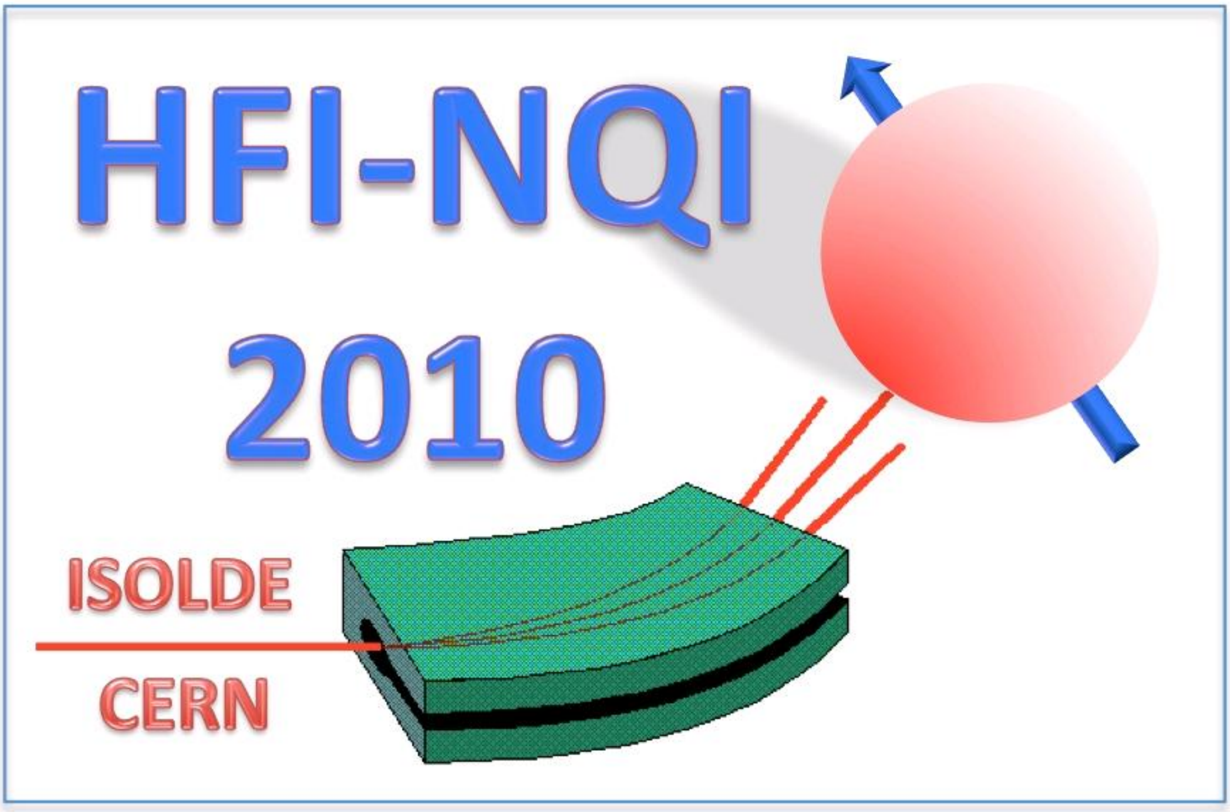
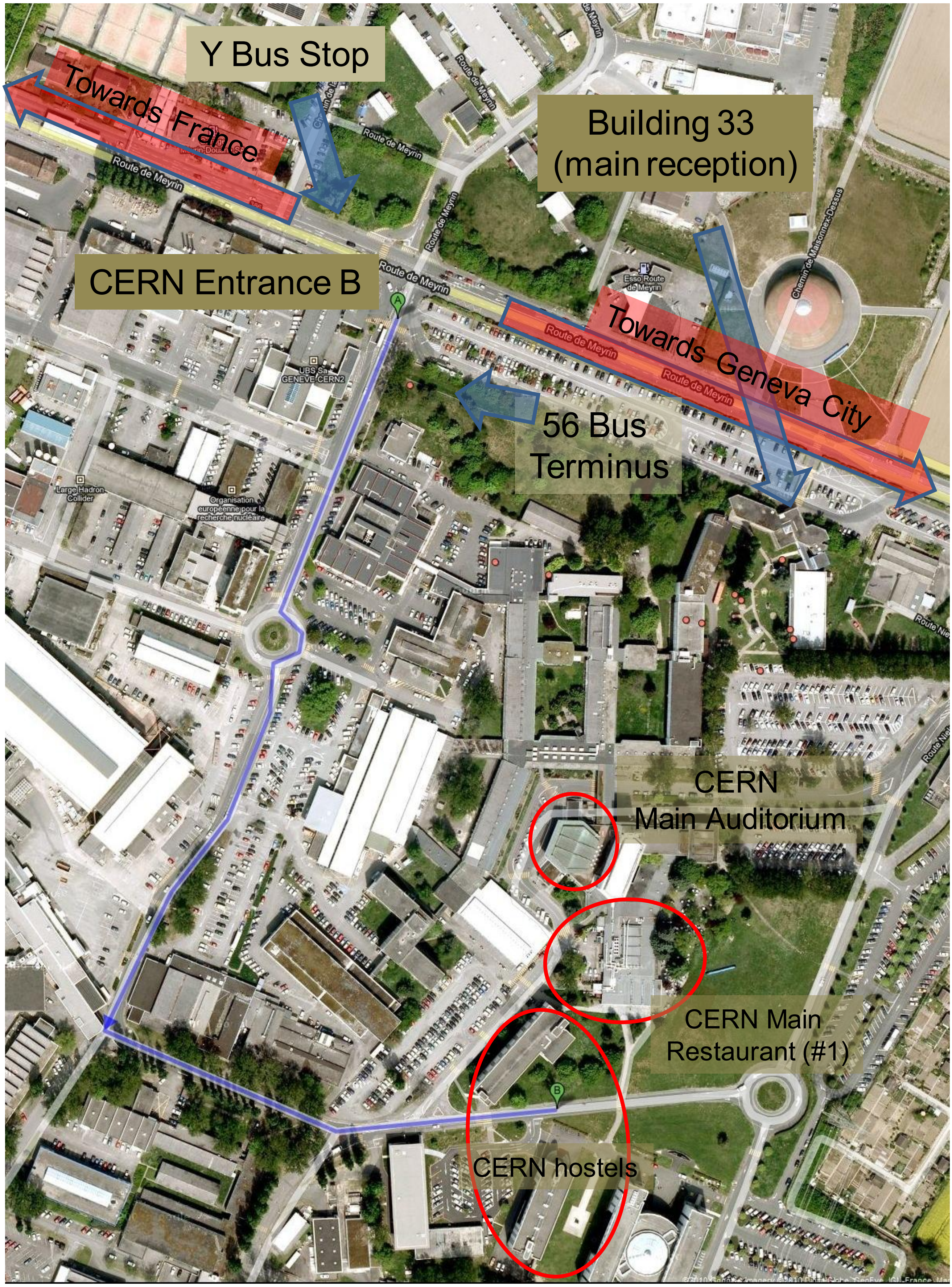


Monday 13 September – 17 September 2010

BOOK OF ABSTRACTS

HFI2010: Guide to CERN



Monday 13th Sept.		Tuesday 14th Sept.		Wednesday 15th Sept.		Thursday 16th Sept.		Friday 17th June	
9:00-9:15	Welcome	9:00-9:20	**Connell**	9:00-9:20	**MacFarlane**	9:00-9:20	**Klauss**	9:00-9:20	**Blaha**
9:15-9:35	**Nörtershäuser**	9:20-9:40		9:20-9:40		9:20-9:40		9:20-9:40	
9:35-9:55		9:40-10:00	**Ko Mibu**	9:40-10:00	**Yoshida**	9:40-10:00	**Hemmingsen**	9:40-10:00	Koch
9:55-10:15	**Severijns**	10:00-10:20		10:00-10:20		10:00-10:20		10:00-10:20	Haas
10:15-10:35		10:20-10:40	Alp	10:20-10:40	Panich	10:20-10:40	Petersen	10:20-10:40	Stone
10:35-10:55	Ohtsubo	10:40-11:10	**coffee break**	10:40-11:10	**coffee break**	10:40-11:10	**coffee break**	10:40-11:10	**coffee break**
10:55-11:25	**coffee break**	11:10-11:30	**Sielemann**	11:10-11:30	**Sergueev**	11:10-11:30	Correia	11:10-11:30	**Kellö**
11:25-11:45	**Mangano/Lhc**	11:30-11:50		11:30-11:50		11:30-11:50	Nagatomo	11:30-11:50	
11:45-12:05		11:50-12:10	Molholt	11:50-12:10	Cadogan	11:50-12:10	Seliger	11:50-12:10	Zacate
12:05-12:25	Yuan	12:10-12:30	Carbonari	12:10-12:30	Wortmann	12:10-12:30	Furman	12:10-12:30	**Haas/conclusion**
12:25-14:00	**lunch**	12:30-14:00	**lunch**	12:30-14:00	**lunch**	12:30-14:00	**lunch**		
14:00-14:20	Deicher	14:00-14:20	Baggio-Saitovich	14:00-14:20	CONFERENCE TOUR	14:00-14:20	Asaji		
14:20-14:40	Valentini	14:20-14:40	D. de Reotier	14:20-14:40		14:20-14:40	Poleshchuk		
14:40-15:00	Munoz	14:40-15:00	Litterst	14:40-15:00		14:40-15:00	Hutchinson		
15:00-15:20	Steffens	15:00-15:20	Salman	15:00-15:20		15:00-15:20	Goncalves		
15:20-15:40	Butz	15:20-15:40	Mishra	15:20-15:40		15:20-15:40	Orlov		
15:40-17:30	POSTER SESSION 1	15:40-17:00	POSTER SESSION 2	15:40-16:00		15:40-17:00	POSTER SESSION 3		
				16:00-17:30					
17:00-19:00	ISOLDE/SM18	17:00-19:00	ISOLDE/SM18			18:00-20:30	Conference		
							Banquet		

Magnetism and Magnetic materials - Bulk and thin layers
Theory: Hyperfine Interactions, Nuclear Moments
Semiconductors, Metals and Insulators
Biology, Chemistry, Medicine
Lattice Dynamics, Ion-Solid Interaction
Surfaces, Interfaces, Thin Films, Nano-structures

Atoms and ions
Resonance Methods
Coherent Phenomena, Synchrotron Radiation, Quantum Optics
Nuclear Moments/Polarization/Models, Fundamental Interactions
New Directions and Developments in Methodology

3rd Joint International Conference on Hyperfine Interactions and International Symposium on Nuclear Quadrupole Interactions

CERN, Geneva, Switzerland

September 13-17 2010

cern.ch/hfi2010

BOOK OF ABSTRACTS

Conference chairs

- Krish Bharuth-Ram (Chair)
- Guido Langouche (Co-Chair)

Local Organizing Committee

- Krish Bharuth-Ram
- Guido Langouche
- Reiner Vianden
- Manfred Deicher
- Wolf-Dietrich Zeitz
- Deena Naidoo
- Guilherme Correia
- Karl Johnston
- Yorick Blumenfeld
- Mats Lindroos
- Jenny Weterings (ISOLDE Secretary)
- Sylvie Padlewski (ISOLDE Secretary)

Program Committee

- Reiner Vianden (Germany)
- Krish Bharuth-Ram (South Africa)
- Ken Ichi Kumagai (Japan)
- Guido Langouche (Belgium)
- Kensaku Matsuta (Japan)
- Alberto F. Pasquevich (Argentina)
- Helena M. Petrilli (Brasil)
- Gary Wulfsberg (USA)
- Pierre Dalmas de Réotier (France)
- Wayne Hutchison (Australia)
- Heinz Haas (Switzerland)

Members of HFI/NQI Executive Committee

- Krish Bharuth-Ram (South Africa)
- Ken Ichi Kumagai (Japan)
- Reiner Vianden (Germany)
- Guido Langouche (Belgium)
- Kensaku Matsuta (Japan)
- Alberto F. Pasquevich (Argentina)
- Helena M. Petrilli (Brasil)
- Gary Wulfsberg (USA)
- Pierre Dalmas de Réotier (France)

International Advisory Committee

- David Ailion (USA)
- Hisazumi Akai (Japan)
- Ercan Alp (USA)
- Tetsuo Asaji (Japan)
- Tatyana Babushkina (Russia)
- Krish Bharuth-Ram (South Africa) EC (Chairman HFI/NQI2010)
- Aidan Byrne (Australia)
- Gary S. Collins (USA)
- Joao Martins Correia (Portugal)
- Stefaan Cottenier (Belgium)
- Manfred Deicher (Germany)
- Wayne Hutchison (Australia)
- Herbert Jaeger (USA)
- Ryosuke Kadono (Japan)
- Ken Ichi Kumagai (Japan)
- Guido Langouche (Belgium)
- Jochen Litterst (Brazil)
- Karl Maier (Germany)
- Kensaku Matsuta (Japan)
- Tadanori Minamisono (Japan)
- Alberto F. Pasquevich (Argentina)
- Helena M. Petrilli (Brazil)
- Mario Renteria (Argentina)
- John A. S. Smith (UK)
- Reiner Vianden (Germany)
- Pawel Wodniecki (Poland)
- Gary Wulfsberg (USA) EC
- Ilan Yaar (Israel)
- Matthew Zacate (USA)
- Sheng-Yun Zhu (China)
- Jonathan Billowes (UK)

PREFACE

This is the third in the series of joint Conferences of the International Conference on Hyperfine Interactions and the International Symposium on Nuclear Quadrupole Interactions, and follows along the lines set at the first and second joint conferences at Bonn and Iguasu Falls in 2004 and 2007 respectively. An international Executive Committee (IEC) on Hyperfine Interactions was established at the meeting in Iguasu Falls, with Professor Reiner Vianden as its first Chair. The IEC was tasked with calling for nominations and managing the election of members of the International Advisory Committee (IAC) and the Program Committee of this conference.

After agreement among the Program Committee members, the topics to be discussed at the conference followed those of the previous conferences, and calls for nominations for Invited talks went out to the IAC, followed by the call for abstracts of proposed presentations from participants. Two Program Committee meetings were held at CERN, the first to agree on the Conference Program and to select the Invited Speakers, and the second to review the submitted abstracts and to select the Oral presentations. Of the 250 abstracts submitted initially a few were found not to fall within the ambit of a HFI/NQI conference.

The Organising Committee (LOC) met several times over the past two years. In this respect the initial contribution of Mats Lindroos on the do's and don't's of organizing an international meeting at CERN was greatly appreciated, as were the continued efforts of Karl Johnston and Jenny Wetterings who together with Sylvie Padlewski formed a very effective and efficient conference secretariat. CERN has proved to be an excellent choice as venue of this conference, not only due to the excitement in the science community that news of LHC has generated, but especially because of the generous support we have received from the CERN management: the Director of CERN agreed to provide free accommodation in the CERN hostels for up to 50 students and participants from developing countries, as well as made available free of charge the CERN auditorium, committee rooms and poster space, while the ISOLDE Coordinator agreed to fund the appointment of the conference secretary. We were able to secure some support from the Abdus Salaam International Centre for Theoretical Physics (ICTP). We are very grateful for all the support, which allowed us to keep the registration fees as low as possible.

On behalf of the Organizing Committee, we wish to express our appreciation to all members of the International Advisory Committee and the Program Committee, and wish you all an intellectually challenging and socially enjoyable conference.

K.Bharuth Ram

Krish Bharuth-Ram
Chair

Guido Langouche
Co-Chair

Monday 13 September 2010

Welcome – Main Auditorium (09:00-9:15)

Atoms And Ions - Main Auditorium (09:15-9:55) *Convener: VIANDEN, Reiner*

09:15 [27]	Recent developments in Collinear Laser Spectroscopy at ISOLDE, CERN. **NOERTERSHAEUSER, Wilfried**

Nuclear Moments, Nuclear Polarization, Nuclear Models, Fundamental Interactions - Main Auditorium (09:55-10:55) *Convener: VIANDEN, Reiner*

09:55 [169]	Recent Progress on Low Temperature Nuclear Orientation Technique and NMRON **SEVERIJNS, Nathal**
10:35 [124]	NMR-ON study of ^{197}PtNi **OHTSUBO, Takashi**

LHC - Main Auditorium (11:25-12:05) *Convener: BLUMENFELD, Yorick*

11:25 [179]	THE LHC **MANGANO, Michelangelo**

NUCLEAR MOMENTS, NUCLEAR POLARIZATION, NUCLEAR MODELS, FUNDAMENTAL INTERACTIONS - Main Auditorium (12:05-12:25) *Convener: BLUMENFELD, Yorick*

12:05 [35]	Study of Dependence of Quasi-Particle Alignment on Proton and Neutron Numbers in A= 80 Region through g-factor measurements. **ZHU, Shengyun, YUAN, Daqing**

SEMICONDUCTORS, METALS AND INSULATORS - Main Auditorium (14:00-15:20) *Convener: HOFSäSS, Hans*

14:00 [51]	Donor-Acceptor Complexes in ZnO **DEICHER, Manfred**
14:20 [25]	Angular correlation studies on ^{172}Lu(^{172}Yb) in GaN and measurement at low Temperature **VALENTINI, Riccardo**
14:40 [59]	PAC study of the dynamic hyperfine interactions at ^{111}In-doped Sc$_2$O$_3$ semiconductor and comparison with ab initio calculations **MUñOZ, Emiliano Luis RICHARD, Diego**
15:00 [32]	Temperature dependence of the hyperfine fields of ^{111}In in sapphire (Al$_2$O$_3$) single crystals **STEFFENS, Michael**

NEW DIRECTIONS, NEW DEVELOPMENTS IN METHODOLOGY - Main Auditorium (15:20-15:40) *Convener: HOFSäSS, Hans*

15:20 [15]	The concept of trajectories in the Data Analysis of Non-axially Symmetric Nuclear Quadrupole Interactions **BUTZ, Tilman**

POSTER SESSION - *mezzanine* (15:40-17:00)

ISOLDE/LHC TOUR - Main Auditorium (17:00-19:00)

Tuesday 14 September 2010

COHERENT PHENOMENA, SYNCHOTRON RADIATION, QUANTUM OPTICS – Main Auditorium (09:00-10:20) - *Convener: DALMAS DE REOTIER, Pierre*

09:00 [171] Quantum Diffusion of Muonium in Diamond **CONNELL, Simon**
09:40 [170] Investigations on thin Fe films and Heusler alloy films using synchrotron-radiation-based Mössbauer spectroscopy **MIBU, Ko**

NEW DIRECTIONS, NEW DEVELOPMENTS IN METHODOLOGY - Main Auditorium (10:20-10:40)

10:20 [86] Recent Methodological Developments in Nuclear Resonant Scattering with Synchrotron Radiation **ALP, Esen Ercan**

MAGNETISM AND MAGNETIC MATERIALS: BULK AND THIN FILMS - Main Auditorium (11:10-12:30) - *Convener: LITTERST, Jochen*

11:10 [151] Magnetism in Iron Implanted Oxides: A Status Report **SIELEMANN, Rainer**
11:50 [47] Mössbauer study of spin-lattice relaxations of dilute Fe^{3+} in MgO **MøLHOLT, Torben**
12:10 [137] Temperature dependence of the magnetic hyperfine field at ^{111}Cd in ZnO doped with Co **CARBONARI, Artur**

MAGNETISM AND MAGNETIC MATERIALS: BULK AND THIN FILMS - Main Auditorium (14:00-15:40) - *Convener: GONçALVES, Joao*

14:00 [130] Fe as Local Probe to follow the Competition between Magnetism and Superconductivity in the New Fe-pnictide Superconductors **BAGGIO SAITOVITCH, Elisa**
14:20 [76] Muon spin relaxation studies of geometrically frustrated magnets **DALMAS DE REOTIER, Pierre**
14:40 [46] Magnetism in Azurite Studied by Muon Spin Rotation **LITTERST, Jochen**
15:00 [97] Measuring the magnetic properties of monolayers of single molecule magnets **SALMAN, Zaher**
15:20 [36] Defect induced magnetic interaction in highly oriented pyrolytic graphite (HOPG): A local investigation using TDPAD method **MISHRA, S.N.**

POSTER SESSION - *Mezzanine* (15:40-17:00)

ISOLDE/LHC TOUR - Main Auditorium (17:00-19:00)

Wednesday 15 September 2010

NEW DIRECTIONS, NEW DEVELOPMENTS IN METHODOLOGY - Main Auditorium (09:00-09:40) - *Convener: GUNNLAUGSSON, Haraldur*

09:00 [172] Beta detected NMR: a New Depth-resolved Probe of Materials at the Nanoscale **MACFARLANE, W. A.**

SURFACES, INTERFACES, THIN FILMS, NANOSTRUCTURES - Main Auditorium (09:40-10:40) - *Convener: GUNNLAUGSSON, Haraldur*

09:40 [173] Development and applications of a Mössbauer camera **YUTAKA, Yoshida**
10:20 [3] Quadrupolar Perturbed NMR in Inorganic Nanomaterials **PANICH, Alexander**

LATTICE DYNAMICS, ION-SOLID INTERACTIONS - Main Auditorium (11:10-12:30) *Convener: MIBU, Ko*

11:10 [174] Synchrotron radiation based TDPAC **SERGUEEV, I.**
11:50 [63] Phonon mode softening at the ferroelectric transition in $Eu_xBa_{1-x}TiO_3$ **CADOGAN, Sean**
12:10 [150] Density of Phonon States at the Fe Sites in Superconducting FeSe as Function of Temperature and Pressure **WORTMANN, Gerhard**

CONFERENCE EXCURSION - (14:00-22:00)

Tour of Annecy (France): 14:00-18:30
Wine tasting, Satigny (Switzerland): 18:30-22:00

Thursday 16 September 2010

SEMICONDUCTORS, METALS AND INSULATORS - Main Auditorium (09:00-09:40)

Convener: MATSUTA, Kensaku

09:00 [175] MuSR studies of High T_c superconductivity in iron pnictides **KLAUSS, H.**

BIOLOGY, CHEMISTRY, MEDICINE, ARCHAEOLOGY, MINERALOGY - Main Auditorium (09:40-10:40) - *Convener: MATSUTA, Kensaku*

09:40 [176] Perturbed Angular Correlation in Bio Systems **HEMMINGSEN, Lars**
10:20 [128] Ab Initio Hyperfine Interactions as a Powerful Tool to Identify the Metal Binding Site in Biological Systems: Cd^{2+} in DNA Bases.**DIVNA PETERSEN, Philippe Alexandre**

RESONANCE METHODS - Main Auditorium (11:10-12:10)- *Convener: EVENSON, Bill*

11.10 Recent advances in emission channeling measurements and relevance to hyperfine interactions **CORREIA, J, Guillerme**
11:30 [98] Precise Nuclear Moments of Extremely Proton-Rich Nuclei ^{23}Al **NAGATOMO, Takashi**

11:50 [67] ^{14}N NQR study of proton position and dynamics in some hydrogen bonded organic ferroelectrics **SELIGER, Janez**

NEW DIRECTIONS, NEW DEVELOPMENTS IN METHODOLOGY - Main Auditorium (12:10-12:30) - *Convener: EVENSON, Bill*

12:10 [7] Entanglement in nuclear quadrupole resonance **FURMAN, Gregory**

BIOLOGY, CHEMISTRY, MEDICINE, ARCHAEOLOGY, MINERALOGY - Main Auditorium (14:00-14:20) - *Convener: COTTENIER, Stefaan*

14:00 [20] Proton Dynamics in One-dimensional Hydrogen-bonding System in Molecular Co-crystals TMP-D2ca and DMP-H2ca **ASAJI, Tetsuo**

THEORY - Main Auditorium (14:20-14:40) - *Convener: COTTENIER, Stefaan*

14:20 [1] DFT Study of Hyperfine Interactions in Some Types of the Complexes **OLESHCHUK, Oleg**

MAGNETISM AND MAGNETIC MATERIALS: BULK AND THIN FILMS - Main Auditorium (14:40-15:40) - *Convener: COTTENIER, Stefaan*

14:40 [90] Low Temperature Nuclear Orientation Studies of the Magnetic Structures of $RNiAl_4$ in Applied Magnetic Fields **HUTCHISON, Wayne**
15:00 [155] Perturbed angular correlation study of the magnetic and structural first-order phase transition in MnAs **GONçALVES, J. N.**

15:20 [18] Anomalous Magnetism and ^{209}Bi Nuclear Spin Relaxation in $Bi_4Ge_3O_{12}$ Crystals **ORLOV, Valery**

POSTER SESSION – *Mezzanine* (15:40-17:00)

CONFERENCE BANQUET – Cruise on Lac Leman (18:00-22:00)

Friday 17 September 2010

THEORY - Main Auditorium (09:00-10:40) - *Convener: PETRILLI, Helena Maria*

09:00 [95] Calculations of Hyperfine parameters in solids based on DFT and using WIEN2k **BLAHA, Peter**
09:40 [30] Electron penetration into the nucleus and its effect on the quadrupole interaction **KOCH, Katrin COTTENIER, Stefaan**
10:00 [108] Quadrupole interaction in the solid halogens - a new (not final) look **HAAS, Heinz**
10:20 [146] *A-priori* calculations of hyperfine interactions in highly ionized atoms: g-factor measurements of pico-second states populated in nuclear reactions. **STONE, Nicholas**

THEORY - Main Auditorium (11:10-11:50) - *Convener: LANGOUCHE, Guido*

11:10 [43] Electric field gradient calculations by quantum chemical methods **KELLOE, Vladimir**

SEMICONDUCTORS, METALS AND INSULATORS - Main Auditorium (11:50-12:10) *Convener: LANGOUCHE, Guido*

11:50 [114] Modelling Complex Diffusion Mechanisms in L12-Structured Compounds **ZACATE, Matthew**

CONCLUSION - Main Auditorium (12:10-12:30)

12:10 [178] CONCLUSION **HAAS, Heinz**

Poster session I: Monday 13 September 15:40 – 17:00

THEORY

PS1-1	157	Density functional calculations of hyperfine parameters in manganites	GONçALVES, J. N.
PS1-2	4	Theoretical calculations on the Electric Field Gradient in HfO_2:Cd and ZrO_2:Cd	TAYLOR, Marcela;
PS1-3		***Moved to Thursday 16 September: Poster session 3***	
PS1-4	71	Electronic and structural properties of ^{181}Ta in anatase and rutile: Experimental study and ab initio calculations	DAS, P
PS1-5	107	The EFG at sp-impurities in Zn and Cd - a new (final?) look	HAAS, Heinz
PS1-6	118	Ab-initio hyperfine fields in Fe-Cr.	SODRE, Ney
PS1-7	119	Ab initio study of the electronic structure and the EFG at Ta sites in HfO_2:Ta & ZrO_2:Ta.	TAYLOR, Marcela Andrea
PS1-8	133	Ab initio calculations and PAC study of ^{111}In-doped $(Hf/Zr)_3Al_2$ and $(Hf/Zr)_4Al_3$ mixed compounds. EFG´s and site preference	ERRICO, Leonardo;
PS1-9	129	Electric Field Gradient and Electronic Properties of Crown Thioether Compounds	NASCIMENTO, Rafael Rodrigues

MAGNETISM AND MAGNETIC MATERIALS: BULK AND THIN FILMS

PS1-10	8	Investigation of hyperfine interactions in $GdCrO_3$ perovskite oxide using PAC spectroscopy	SAXENA, Rajendra
PS1-11	0	Mössbauer studies of the magnetic quasicrystal $Zn_{77}Fe_7Sc_{16}$	NOWIK, Israel
PS1-12	13	Mössbauer and magnetic studies of $(Mn, Zn)_xCo_{1-x}Fe_2O_4$ nanoferrites synthesized by using the citrate precursor preparation technique	MSOMI, Justice
PS1-13	19	Mössbauer spectroscopic study of the kinetics of sigma-phase formation in cold-rolled Fe-V alloys	DUBIEL, Stanislaw
PS1-14	23	Mössbauer and electrical studies of $Mn_xCo_{1-x}Fe_2O_4$ compounds prepared via glycothermal route	ABDALLAH, Hafiz
PS1-15	24	Advances in a Bulk and Surface Properties Studies by using Mossbauer spectroscopy	KAMZIN, Alexander
PS1-16	33	Magnetic hyperfine field in the intermetallic compounds $PrRh_2Si_2$ and $GdRh_2Si_2$ measured with PAC technique using ^{140}Ce as probe nuclei	CABRERA-PASCA, Gabriel

PS1-17	41	Perturbed Angular Correlations Investigations on Magneto-Electric Manganites	MELO MENDONçA, Tânia
PS1-18	44	Magnetic-Electronic Pressure Responase of Ilmenite ($FeTiO_3$)	SIBANDA, Wisdom Nkosilathi
PS1-19	45	Spin and Orbital Order in $FeCr_2S_4$	LITTERST, Jochen
PS1-20	62	Mössbauer Spectroscopy of the New Iron Oxide $Fe_3B_7O_{13}(OH)$	NAKAMURA, Shin
PS1-21	64	Magnetic and electrical transport properties of Ce/Ca substituted perovskite oxides	SHARMA, M. P.
PS1-22	79	Studies of GdZn compound magnetic properties using PAC spectroscopy with ^{140}Ce and ^{111}Cd as probe nuclei	SANTOS, Brianna
PS1-23	93	$DyNi_2Mn$ - Magnetisation and Mössbauer Spectroscopy	CAMPBELL, Stewart
PS1-24	109	Magnetic Hyperfine Interaction of ^{59}Fe in Nickel	MUTO, Suguru
PS1-25	116	Magnetoelectric $AgCrO_2$: A new local insight given by PAC	DE PINHO OLIVEIRA, Goncalo
PS1-26	121	Investigations on $FeSb_2$ by high field ^{57}Fe Mössbauer spectroscopy	REISSNER, Michael
PS1-27	123	Structural, electronic and magnetic properties of Ho substituted $BiFeO_3$ as a function of temperature	NAIDOO, Deena
PS1-28	125	A high temperature NMR study in optimally doped manganites	PANOPOULOS, Nikos
PS1-29	126	Incommensurate modulated spin order and NMR wipeout effect in electron-doped manganites probed by ^{139}La NMR	KOUMOULIS, Dimitrios
PS1-30	144	Magnetism in $CaFe_2As_2$ and Phase Separation in Superconducting $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ Single Crystals: A Mössbauer Study	SANCHEZ, Dalber
PS1-31	153	Magnetic and Electric Properties of Cadmium Films Containing Nanometer Size Clusters of Iron	TRUJILLO, Wiliam
PS1-32	156	Hyperfine local probe study of alkaline-earth manganites $BaMnO_3$ and $SrMnO_3$	GONçALVES, J. N.
PS1-33	161	Mössbauer and XPS studies of $(Mn, Zn)_xCo_{1-x}Fe_2O_4$ ferrites	DOLO, J. J.
PS1-34	166	Tin, Manganese doped chromium iron oxides of composition alpha-$Sn_{0.2}Cr_{1.8-x}Fe_xO_3$ and alpha-$Mn_{0.2}Cr_{1.8-x}Fe_xO_3$	KALENGAY, Mbela
PS1-35	77	Paramagnetism in Mn/Fe implanted ZnO	GUNNLAUGSSON, Haraldur
PS1-36	40	Absence of room temperature ferromagnetism in transition metal doped ZnO nanocrystalline powders from PAC spectroscopy	DOGRA, Rakesh
PS1-37	52	X-ray absorption and magnetic circular dichroism characterizations of $Mo_{1-x}Fe_xO_2$ ($x = 0 - 0.05$) thin films grown by pulsed laser ablation	THAKUR, Pardeep Kumar
PS1-38	29	Features of Structural Transformations in $La_{1-x}Ca_xMn_{0.98}Fe_{0.02}O_{3+\delta}$ ($x = 0.05 - 0.50$)	SEDYKH, Vera
PS1-39	17	Experimental and theoretical study of the σ-phase in Fe-Cr and Fe-V alloys	CIESLAK, Jakub
PS1-40	141	Detection of sub-lattice magnetism in sigma-phase Fe-V compounds by zero-field NMR	DUBIEL, Stanislaw M.

Poster session II Tuesday 14 Sept

SEMICONDUCTORS, METALS AND INSULATORS

PS2-1	26	Search for ferromagnetic ordering in Pd doped wide band gap semiconductors GaN and ZnO	KESSLER, Patrick
PS2-2	28	Evidence of defect pairing for Pd-atoms in Germanium	TIMMERS, Heiko
PS2-3	42	Oxygen ordering in the $HgBa_2CaCu_2O_{6+\delta}$ high-TC superconductor	MELO MENDONçA, Tania
PS2-4	53	Perturbed gamma-gamma angular correlation studies of indium containing 211-MAX phases	JUERGENS, Daniel
PS2-5	55	Perturbed gamma-gamma angular correlation studies of indium free 211-MAX phases	JUERGENS, Daniel
PS2-6	61	Experimental and ab initio study of Ta-doped ZnO semiconductor	MUñOZ, Emiliano Luis; Mr. RICHARD, Diego
PS2-7	66	An In-defect complex as a possible explanation for high luminous efficacy of InGaN and AlInN based devices	KESSLER, Patrick
PS2-8	68	Precise calculation of semiconductor band gaps by means of the LDA-1/2 method	FERREIRA, Luiz
PS2-9	69	Study of annealing behavior of HfO_2 fiber by hyperfine interaction technique.	BANERJEE, D
PS2-10	70	Zr-doped Rutile TiO_2: A Quadrupole Interaction Study	BANERJEE, D
PS2-11	73	Search for "After-Effects" in Cd-doped ZnO semiconductor: PAC experiments supported by ab initio results	MUñOZ, Emiliano Luis
PS2-12	78	APW+lo and TDPAC study of the Electric-Field Gradient at the cation sites of the $^{44}\mathrm{Ti(EC)}\rightarrow{}^{44}\mathrm{Sc}$-doped Sc_2O_3 Semiconductor	RICHARD, Diego; Mr. MUñOZ, Emiliano Luis
PS2-13	81	Electronic and structural properties of the α-Fe_2O_3:Ta semiconductor. Experimental EFG determination and ab initio calculations.	DARRIBA, Germán Nicolás
PS2-14	82	Experimental and ab initio study of the EFG at donor impurities in the Cr_2O_3:Ta semiconductor.	DARRIBA, Germán Nicolás
PS2-15	94	Observation of iron impurities diffusion in silicon under bending stress by Mössbauer spectroscopy	SUZUKI, Kunifumi
PS2-16	100	Observation of long lived Fe^{3+} paramagnetic states in ZnO following the implantation with non-3d elements	NAIDOO, Deena
PS2-17	104	TDPAC study of the phase transitions in $PbTi_{1-x}Hf_xO_3$	ALONSO, Roberto
PS2-18	115	Fitting TDPAC Spectra with Stochastic Models: PolyPacFit	ZACATE, Matthew
PS2-19	117	Fluctuating Hyperfine Interactions: Computational Implementation	EVENSON, William; ZACATE, Matthew
PS2-20	139	Study of hyperfine interactions in CeO_2 nanoparticle by PAC spectroscopy using ^{111}Cd	COSTA, Messias
PS2-21	140	First-principles study of magnetic hyperfine field at Cd probe in Co-doped ZnO semiconductor	PEREIRA, Luciano

PS2-22	142	Electric quadrupole interactions in nano-structured SnO$_2$ as measured with PAC spectroscopy	RAMOS, Juliana
PS2-23	143	Study of the electronic structure and electric field gradient at Cd probe in Co-doped ZnO matrix by first principles calculations	PEREIRA, Luciano
PS2-24	148	TDPAC study of a solid-state reaction doping process of ^{181}Hf (→^{181}Ta) impurities in the Ho$_2$O$_3$ semiconductor	RICHARD, Diego
PS2-25	160	PAC study of the Si-HfO$_2$ system subjected to high energy ball milling	CHAIN, Cecilia Y.
PS2-26	162	Thermal Evolution of Short Range Order in Cu-Hf-Based Amorphous Alloys	DAMONTE, Laura C.
PS2-27	164	Dimensionless Coordinates for Simulations and Theory of Hyperfine Interactions in Materials	EVENSON, William
PS2-28	165	Defects studies in pure and doped In$_2$O$_3$ single crystals by PAC.	QUILLE RAMOS, Ruben
PS2-29	60	Hyperfine parameters of Fe atoms in superconducting FeSe as function of temperature, pressure and magnetic field.	KSENOFONTOV, Vadim
PS2-30	12	Beta-NMR measurement of Cu-58 in Si	MIHARA, Mototsugu
PS2-31	32	Temperature dependence of the hyperfine fields of ^{111}In in sapphire (Al$_2$O$_3$) single crystals	STEFFENS, Michael
PS2-32	84	Nuclear electric quadrupole interactions of ^{111}Cd in the heavy-fermion compound CeCoIn$_5$	FORKER, Manfred

NEW DIRECTIONS, NEW DEVELOPMENTS IN METHODOLOGY

PS2-33	15	The Concept of Trajectories in the Data Analysis of Non-axially Symmetric Nuclear Quadrupole Interactions	BUTZ, Tilman
PS2-34	16	A User-friendly Fully Digital TDPAC-Spectrometer	BUTZ, Tilman
PS2-35	21	Methodology of Quantitative Analysis in Mossbauer Spectroscopy	IRKAEV, Sobir
PS2-36	57	Lattice location of beryllium and boron, measured by thermal-neutron-induced emission channeling measurements	KöSTER, Ulli
PS2-37	112	Advantages of resonant detecting in hyperfine structure investigation by Moessbauer spectroscopy	PANCHUK, Vitaly
PS2-38	152	POLAREX : Study of polarized nuclei - first measurement	GAULARD, Carole
PS2-39	2	Air pollution studied by Mossbauer spectroscopy and synchrotron	ZHANG, Guilin
PS2-40	101	^{57}Mn Implantation Mössbauer Spectroscopy of α-Al2O3 by Anticoincidence Method	KOBAYASHI, Yoshio
PS2-41	92	Kramers-degenerated Spin Systems “NV+n^{13}C” in Diamond for Quantum Magnetometry: Spin-Hamiltonian and Quantum Chemistry Analysis	NIZOVTSEV, Alexander

Poster session III Thursday 16 Sept

BIOLOGY, CHEMISTRY, MEDICINE, ARCHAEOLOGY, MINERALOGY

PS3-1	54	H/D Isotope Effect of 1H MAS NMR Spectra and ^{79}Br NQR Frequencies in Piperidinium and Pyrrolidinium p-Bromobenzoate	HONDA, Hisashi
PS3-2	56	Variations of ^{57}Fe Hyperfine Parameters in Medicaments Containing Ferrous Fumarate and Ferrous Sulfate	OSHTRAKH, Michael
PS3-3	58	Measurements in DNA molecules using Perturbed Angular Correlation Spectroscopy	SILVA, Andréia
PS3-4	80	^{57}Fe Quadrupole Splitting and Isomer Shift in Various Oxyhemoglobins: Study Using Mössbauer Spectroscopy	OSHTRAKH, Michael
PS3-5	91	Quantitative determination of phase transformations of the Tridymite-like FePO$_4$ catalyst pre and post oxidative dehydrogenation reactions to form Alkyl Methacrylates	KHAN, Faiza
PS3-6	113	Chemical states of ^{57}Fe in rock salt type crystals arising from ^{57}Mn	KUBO, Kenya
PS3-7	120	Reduction of Amorphous Fe(III)-hydroxide by the Binary Microbial Culture, Mössbauer Study	CHISTYAKOVA, Nataliya
PS3-8	127	Electric Field Gradient and Electronic Properties of Crown Thioether Compounds	NASCIMENTO, Rafael Rodrigues
PS3-9	131	Beta-NMR as a novel technique using radioactive beams for biophysical studies	STACHURA, Monika
PS3-10	136	Ab-initio study of copper complexes	GONCALVES, Marcos
PS3-11	147	First Principles Electronic Structure Investigation of Order of Singlet and Triplet States of Oxyhemoglobin and ^{57m}Fe Nuclear Quadrupole Interactions	BADU, S. R.
PS3-12	159	Study of hafnium sodium salts of DTPA using PAC Spectroscopy	CHAIN, Cecilia Yamil
PS3-13	34	Negative thermal expansion and pressure induced amorphization in Zirconium tungstate as studied by ^{181}Ta TDPAC	RAMANUJAM, Govindaraj
PS3-14	87	Structural Phase Transitions in a [Chloranilic Acid]-[2-Pyrrolidone] (1:2) Molecular Complex with Hydrogen-Bond Networks	MORIKAWA, Shota
PS3-15	135	Mössbauer characterisation of Copper ferrite as a model system for the Fischer-Tropsch synthesis	CHONCO, Zandile;
PS3-16	74	^{57}Fe Hyperfine Interactions in M1 and M2 Sites of Olivine from Omolon Meteorite: Study Using Mössbauer Spectroscopy	PATRUSHEVA, Daria
PS3-17	85	^{14}N NQR study of selected 1,4-benzoquinonedioximes	SINGH, Nadia
PS3-18	11	Spectroscopic and mineral magnetic studies on some ancient pottery samples	RAMDOSS, Venkatachalapathy
PS3-19	49	Mössbauer Spectroscopic and Mineral Magnetic studies on Archaeological Potteries from Tamilnadu, India	RAMDOSS, Venkatachalapathy
PS3-20	10	Application of Mossbauer spectroscopy in investigation of wall rock alteration at uranium deposit	LIN, Jun

LATTICE DYNAMICS, ION-SOLID INTERACTIONS

PS3-21	14	Debye temperature of sigma-phase Fe-V alloys	DUBIEL, Stanislaw
PS3-22	48	Lattice Location and Diffusion of Interstitial Fe in MgO	MøLHOLT, Torben Esmann
PS3-23	72	Lattice sites of Fe in Al_2O_3 following implantation of ^{57}Mn	GUNNLAUGSSON, Haraldur
PS3-24	96	Mössbauer study of ^{57}Fe in GaAs and GaP following $^{57}Mn^+$ implantation	MASENDA, Hilary

SURFACES, INTERFACES, THIN FILMS, NANOSTRUCTURES

PS3-25	22	Investigation of Nanosized Magnetic Materials by SEDM Technique	SEMENOV, Valentin
PS3-26	37	Size effects on local magnetism of single Fe impurity in nano-crystalline noble metals: A TDPAD investigation	MISHRA, S.N.
PS3-27	38	Zr/Hf/Zr nanostructures studied by perturbed angular correlations	LOPES, Armandina M.
PS3-28	39	Characterization of nanostructured HfO_2 films using Perturbed Angular Correlation (PAC) technique	DE MORAES CAVALCANTE, Fabio Henrique
PS3-29	65	Temperature dependent studies of Zinc nanoferrite synthesized by spray pyrolysis	MATHEW, Jacob; JACOB, Jess
PS3-30	75	Electric field gradients in nanoparticles of $HfAl_2$ and $HfAl_3$ intermetallic compounds	KULINSKA, Agnieszka
PS3-31	89	Laser Deposition of Iron on Graphite Substrates	YAMADA, Yasuhiro
PS3-32	134	Investigation of hyperfine interaction in the nanostructured HfO_2 by PAC spectroscopy	ROSSETTO, Daniel
PS3-33	154	Study of nanoconfigurations in Zircon-Mullite composites using Perturbed Angular Correlations	CHAIN, Cecilia Yamil
PS3-34	158	Synthesis and characterization of nanoparticles of cobalt and nickel ferrites dispersed in mesoporous silicon oxide	BRAGA, Tiago;
PS3-35	163	Mössbauer spectroscopy and neutron diffraction study of the mechanosynthesis of nanocrystalline $MgFe_2O_4$	SEPELAK, V.
PS3-36	110	Room temperature ferromagnetism in MWCNTs synthesized by chemical vapor deposition technique	GAUTAM, Sanjeev

ATOMS AND IONS

PS3-37	145	Test of Variational Methods for Studying Hyperfine Interactions of Molecular and Solid State Systems by Application to Atomic Systems	PINK, R. H.

RESONANCE METHODS

PS3-38	5	Low Frequency Spin Echo in Multiple Pulse NQR Spin Locking	KIBRIK, Gregory
PS3-39	6	Phase transition and proton exchange in 1,3-diazinium hydrogen chloranilate monohydrate	ASAJI, Tetsuo
PS3-40	50	^{127}I NQR and 1H NMR Studies of 4-Aminopyridinium Tetraiodoantimonate(III); Molecular Motion and Phase Transition	TERAO, Hiromitsu
PS3-41	83	Two and three frequency multipulse sequence for NQR of N-14 nuclei.	MOZZHUKHIN, Georgy
PS3-42	102	^{35}Cl NQR in glassy crystal, 2,5-dichlorothiophene	FUJIMORI, Hiroki;
PS3-43	111	^{7}Li quadrupole-perturbed NMR observation of biased Li-ion ordering in the paraelectric phase of weakly substitutionally disordered $K_{1-x}Li_xTaO_3$	ZALAR, Boztjan
PS3-44	149	The cross-correlation effects in relaxation of quadrupolar nuclei in the multipolar spin systems	KUPRIYANOVA, Galina
PS3-45	105	Br NQR relaxation and successive phase transitions of $CH_3NH_3HgBr_3$	NIKI, Haruo

NUCLEAR MOMENTS, NUCLEAR POLARIZATION, NUCLEAR MODELS, FUNDAMENTAL INTERACTIONS

PS3-46	103	Magnetic Moment of Isomeric States in ^{175}Ta	KUMAR, Vivek
PS3-47	106	The quadrupole moments of Zn and Cd isotopes - an update	HAAS, Heinz
PS3-48	122	Magnetic Moment of the 3/2+ State in ^{165}Ho	TANIGAKI, Minoru
PS3-49	99	Electric dipole moment search in ^{129}Xe atom with an optical-coupling nuclear spin oscillator	ASAHI, Koichiro
PS3-50	138	Polarization Creation in Proton-Rich ^{28}P via Charge Exchange Reactions and Measurement of Its Electric Quadrupole Moment	MATSUTA, Kensaku
PS3-51	88	The nuclear quadrupole moment of the 245 keV excited state of ^{111}Cd	ERRICO, Leonardo Antonio
PS3-52	111	^{7}Li quadrupole-perturbed NMR observation of biased Li-ion ordering in the paraelectric phase of weakly substitutionally disordered $K_{1-x}Li_xTaO_3$	ZALAR, Bostjan
PS3-53	31	EFG calculations by the FPLO code	KOCH, Katrin, COTTENIER, Stefaan
		LATE-RECEIVED ABSTRACTS	
PS3-54	181	First Principles Cluster Study of Electronic Structures, Locations and Hyperfine Interactions of Isolated Atoms and Ions in Silicon	PINK, R.H.
PS3-55	180	First Principles Study of Nuclear Quadrupole Interactions in Single and Double Chain DNA and Solid Nucleobases	BADU, S.R.
PS3-56	182	First Principles Study of Muonium Trapping and Associated Magnetic Hyperfine Interactions in Nucleobases in Single and Double Chain DNA and Solid Nucleobases	BADU, S.R.

ORAL SESSIONS
Abstracts

(in chronological order)

Recent developments in Collinear Laser Spectroscopy at ISOLDE, CERN

W Noertershaeuser[1]

[1] *University of Mainz, Germany*

e-mail: wilfried.noertershaeuser@cern.ch

Optical spectroscopy is known to provide very accurate and model-independent data on spins, electromagnetic moments and charge radii of nuclear ground states. Collinear laser spectroscopy is long known to be a general technique, applicable to a large variety of elements, but was also developed continuously towards higher sensitivity and/or accuracy to scope with even more exotic species. At COLLAPS, the collinear laser spectroscopy setup at ISOLDE, we have applied a frequency-comb based technique to measure the charge radii of the beryllium isotopes including the one-neutron halo nucleus Be-11. Here, high accuracy was required and uncertainties in high voltage calibrations had to be eliminated by simultaneous spectroscopy in collinear and anti-collinear geometry. ISCOOL, a radio-frequency cooler and buncher came recently into operation and was for the first time applied at ISOLDE for the spectroscopy of copper and gallium isotopes and increased sensitivity by orders of magnitude. The isotope chains of both isotopes offered surprises concerning the spin values of the neutron-rich isotopes. Moreover, a new technique combining optical pumping and ß-asymmetry detection was applied for isotope shift shift measurements of Mg isotopes. In this way we were able to cover the chain of Mg isotopes across the complete sd shell to study the nuclear shape development during the transition into the island of inversion. In my talk I will present these methodological developments and the outstanding results that were obtained with these techniques at the COLLAPS experiment.

Recent progress with Low Temperature Nuclear Orientation and NMR/ON

Nathal Severijns

Instituut voor Kern- en Stralingsfysica, K.U.Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium, e-mail: nathal.severijns@fys.kuleuven.be

Recent results obtained in low temperature nuclear orientation (LTNO) and nuclear magnetic resonance on oriented nuclei (NMR/ON) experiments obtained with the different existing Nuclear Orientation setups will be reviewed and discussed.

These comprise nuclear moment measurements contributing to the study of nuclear structure in different regions of the nuclear chart, precision beta asymmetry parameter measurements to search for non-standard model components in the weak interaction, as well as solid state studies.

Monday 13th September (10:35-10:55), Nuclear Moments, Nuclear Polarization, Nuclear Models, Fundamental Interactions

NMR-ON study of ^{197}PtNi

T. Ohtsubo,[1] **S. Ohya**[1], **Y. Masamori**[1], **T. Izumikawa**[2], **S. Muto**[3], **K. Nishimura**[4]

[1] *Dept. Phys. Niigata University, 2-8050, Ikarashi, Nishi-ku, Niigata, 950-2181, Japan, e-mail: tohtsubo@np.gs.niigata-u.ac.jp*
[2] *Radioisotope Center, Niigata University, Asahimachi-1, Niigata 951-8510, JAPAN*
[3] *Neutron Science Laboratory, KEK, Tsukuba 305-0801, JAPAN*
[4] *Faculty of Engineering, Toyama University, Toyama 930-8555, JAPAN*

Nuclear magnetic resonance of oriented nuclei (NMR-ON) has been widely applied in the study of the electromagnetic properties of unstable nuclei and hyperfine interactions of dilute impurities in ferromagnetic metals. The hyperfine anomaly arises from the hyperfine interaction of the finite nuclear volume of nuclear magnetization and hyperfine field due to Fermi contact. The difference between the point nuclear magnetic structure and the finite magnetic structure is referred to as the Bohr-Weisskopf effect, which depends on the nuclear structure. In order to study the hyperfine anomalies of Pt isotopes, NMR-ON experiments on ^{197}Pt in Ni was measured.

Samples of ^{197}Pt*Ni* were prepared with thermal neutron irradiation. Thin alloy foils of Pt*Ni* (0.1 at. % of the 96% enriched ^{196}Pt) were irradiated in the reactor at the Japan Atomic Energy Research Institute. After irradiation, the sample was annealed in vacuum for 30 min at 800 °C and was cooled down to about 7 mK using a ^{3}He/^{4}He dilution refrigerator. The β rays from ^{197}Pt were measured by two Si detectors mounted in the refrigerator at 0 and 180° with respect to the external magnetic field of 0.2, 0.4 and 0.6 T. NMR-ON spectra were observed by detecting the β-ray asymmetry change with rf oscillating fields. Fig. 1 shows typical NMR-ON spectra of ^{197}Pt*Ni*. For pure magnetic interaction, the resonance condition is given by $h\nu = | g \{ B_{\mathrm{hf}} + (1+K)B_0 \} | \mu_N$. From least-squares fits of the resonance frequencies vs the external magnetic fields, the resonance frequency at $B_0 = 0$ of $\nu_0(^{197}\mathrm{Pt}Ni) = 230.7(1)$ MHz. Comparing with the magnetic resonance frequency of ^{191}Pt*Ni* [1] and the magnetic moments determined by atomic beam method [2], the hyperfine anomalies of Pt isotopes were deduced; $^{191}\Delta^{197} = 12(5)$ %. It is too large compared with the theoretical value (+0.2%). We also deduce the hyperfine anomaly with ^{195}Pt [3,4] that has a same spin and parity as $^{195}\Delta^{197} = 15(5)$%. From these large values, the experimental value of magnetic moment for ^{197}Pt should be wrong.

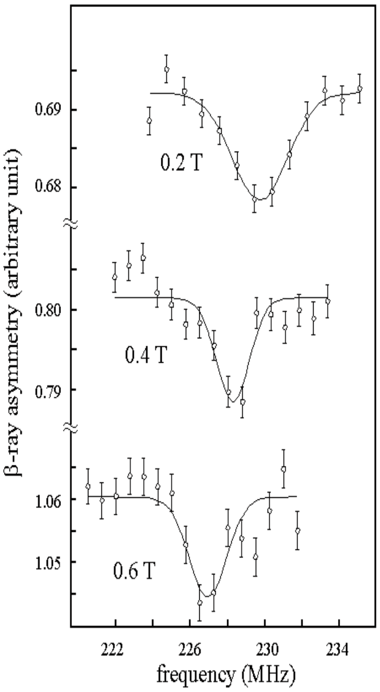


Fig. 1. NMR-ON spectra of ^{197}Pt*Ni*.

References
[1] G. Seewald et al., *Phys. Review B*66, 174401 (2002).
[2] Y.W. Chan et al., *Bull. Am. Phys. Soc.* 13, No.6, 895 CE14 (1968).
[3] M. Kontani and J. Itoh, *J. Phys. Soc. Japan* 22, 345 (1967)
[4] W.G. Proctor and F.C. Yu *Phys. Rev.* 81, 20(1951)

The LHC and its physics programme

Michelangelo Mangano[1]

[1]PH-TH Department, CERN, Route de Meyrin, 1211 Geneva 23, Switzerland

michelangelo.mangano@mac.com

We review the outstanding issues in the understanding of elementary particles and their fundamental interactions, and illustrate the role of the Large Hadron Collider (LHC) in addressing them.

Monday 13th September (12:05-12:25), Nuclear Moments, Nuclear Polarization, Nuclear Models, Fundamental Interactions

Study of Dependence of Quasi-Particle Alignment on Proton and Neutron Numbers in A= 80 Region through g-factor Measurements

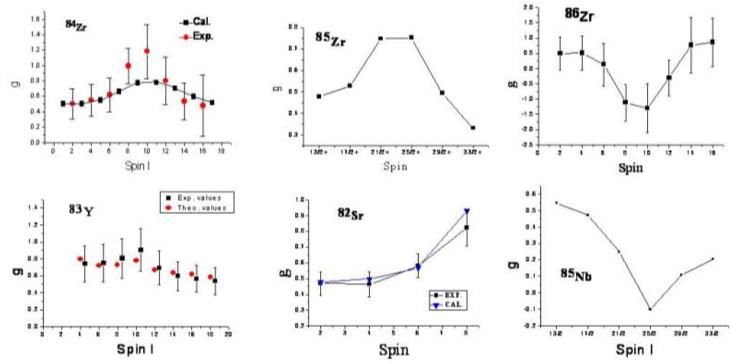
Yuan Daqing, **Fan Ping, Zheng Yongnan, Zuo Yi, Zhou Dongmei, Zhang Qiaoli,**
Wu Xiaoguang, Li Guangsheng, Zhu Lihua, Xu Guoji, Fan Qiwen,
Zhang Xizhen and Zhu Shengyun**

China Institute of Atomic Energy, P.O. Box 275-50, Beijing 102413
Email: zhusy@ciae.ac.cn

The interplay between the collective rotation and the quasi-particle alignment is a significant feature of nuclear structure at high spins. The g-factors of intra-band high spin states of the ground rotational band can provide direct and unique information on quasi-particle alignment since the g-factors of the high-j proton and the high-j neutron are positively large and negatively small, respectively.

The g-factors of high spin states of the ground rotational band in ^{82}Sr, ^{83}Y, ^{84}Zr, ^{85}Nb, ^{85}Zr and ^{86}Zr have been measured in order to study the dependence of quasi-particle alignment on the proton and neutron numbers.

The high spin states of the ground rotational band in ^{82}Sr, ^{83}Y, ^{84}Zr, ^{85}Nb, ^{85}Zr and ^{86}Zr were populated by the fusion-evaporation reactions with the heavy ion beams from the HI-13 tandem accelerator at China Institute of Atomic Energy. The transient -magnetic-field ion implantation perturbed angular distribution (TMF-IMPAD) method was used to determine the g-factors of high spin states along the ground rotational band. The model calculations were also carrried out for some nuclides, which well reproduced the experimentally measured g-factors.



The experimental results are shown in the above figure. It can be seen that for the nuclides ^{84}Zr, ^{85}Zr and ^{86}Zr with Z=40 the proton alignment is followed by the neutron alignment in ^{84}Zr and ^{85}Zr, while the neutron alignment is followed by the proton alignment in ^{86}Zr, and for the nuclides ^{82}Sr, ^{83}Y, ^{84}Zr and ^{85}Nb with N=44 the proton aligns only in ^{82}Sr, the proton aligns first that is followed by the neutron alignment in ^{83}Y and ^{84}Zr and the neutron alignment is followed by the proton alignment in ^{85}Nb. A discussion regard the observed dependence will be presented.

*Supported by National Science Foundation of China under Grant Nos. 10435010 and 10975189

Donor-Acceptor Complexes in ZnO

M. Türker [1], M. Deicher [1], H. Wolf[1], Th. Wichert [1], and the ISOLDE-Collaboration [2]

[1] *Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken, Germany*
manfred.deicher@tech-phys.uni-sb.de
[2] *CERN, CH-1211 Geneva 23, Switzerland*

One of the main obstacles to the technical application of many wide-gap semiconductors represents the difficulty to achieve reliable and sufficient p-type or n-type doping. Possible causes are the electrical compensation of dopants by native defects or other impurities present in the material. For the II-VI semiconductors CdTe, ZnTe, and ZnSe it has been shown [1,2] by perturbed $\gamma\gamma$ angular correlation spectroscopy (PAC) that the concurrent presence of In donors and group-V acceptors leads to the formation of neighboring donor-acceptor pairs. In case of ZnO, the affinity to form donor-acceptor complexes may help to overcome the limitations of p-type doping of this material as outlined in the theoretically proposed concepts of cluster-doping [3] or co-doping [4].

Here, we report on PAC results obtained by co-doping experiments of ZnO using the donor ^{111}In and different group-V acceptors. Fig. 1 shows a PAC spectrum obtained after the implantation of ZnO with ^{111}In and P and after annealing at 850 K. Besides the lattice electric field gradient (EFG) due to the wurtzite structure of ZnO ($\nu_{\mathrm{Q\ Lattice}} = 31$ MHz), two additional EFG caused by the formation of In-defect complexes are observed. They are characterized by two slightly different nearly axially symmetric EFG with $\nu_{Q1} = 175(1)$ MHz ($\eta = 0.1$) and $\nu_{Q2} = 155(2)$ MHz ($\eta = 0$). Due to the wurtzite structure of ZnO having different nearest neighbor distances along the c axis and in the basal plane, respectively, even for identical defect complexes two different EFG are expected to occur. The magnitudes of the EFG observed here are similar to that of the EFG known for In-acceptor complexes in other II-VI semiconductors [1,2]. The nature of the defects in ZnO and the efficiency of different co-doping procedures will be discussed.

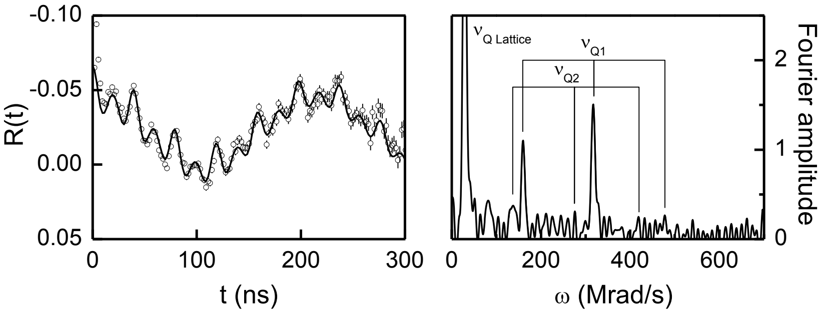


Fig. 1: PAC spectrum (left) and its Fourier transform (right) of ZnO doped with In and P by ion implantation and annealed at 900 K. The measurement was performed with the c-axis perpendicular to the detector plane.

The results of first PAC experiments on the formation of donor-acceptor complexes using group-VII donors in ZnO utilizing the radioactive donor ^{77}Br will be discussed, as well.

This work has been supported by the Bundesministerium für Bildung und Forschung (BMBF) under contract no. 05KK7TS1.

[1] V. Ostheimer, A. Jost, T. Filz, St. Lauer, H. Wolf, and Th. Wichert, *Appl. Phys. Lett.* **69**, 2840 (1996).
[2] S. Lany, P. Blaha, J. Hamann, V. Ostheimer, H. Wolf, and Th. Wichert, *Phys. Rev B* **62** R2259 (2000).
[3] L.G. Wang and A. Zunger, *Phys. Rev. Lett.* **90**, 256401 (2003).
[4] T. Yamamoto and H. Katayama-Yoshida, *Physica B* **302-303**, 155 (2001).

Angular correlation studies on ^{172}Lu(^{172}Yb) in GaN and measurement at low temperature

Riccardo Valentini and Reiner Vianden

Helmholtz – Institut für Strahlen- und Kernphysik der Universität Bonn, Nußallee 14-16, 53115 Bonn, Germany, e-mail: riccardo.valentini@hiskp.uni-bonn.de

For optoelectronic devices semiconductors with large band gap doped with rare earth are used. Doping is generally performed during growth but for more structured doping the ion implantation technique is preferable. The perturbed γγ-angular correlation technique is an ideal tool to study the annealing behavior of semiconductors after implantation. Usually, this method is only able to measure the absolute value but not the sign of the electrical field gradient (EFG) acting onto the quadrupole moment of the implanted probe. An adequate rare earth isotope for such investigations of semiconductors is ^{172}Yb.

The temperature dependence of the hyperfine fields for ^{172}Lu(^{172}Yb) in GaN has been analyzed. The total EFG at the site of this probe is a superposition of the lattice EFG due to the GaN wurtzite structure and the EFG due to the 4f-shell of the rare earth probe itself. The latter is strongly temperature dependent and opposed to the lattice EFG which in contrast is nearly constant since the lattice parameters change only negligibly with temperature.

At elevated temperatures all crystal field split levels of the 4f-shell are equally populated. But at low temperatures the lowest level is occupied preferentially. Sign and magnitude of the EFG produced by the 4f shell can be calculated [1]. Depending on which of the levels is lowest in energy it was possible to determine the sign of the lattice field gradient.

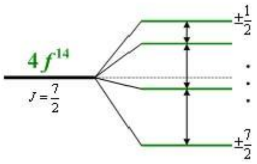


Fig. 1. Splitting of the 4f shell with negative lattice EFG.

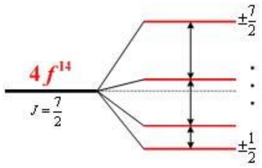
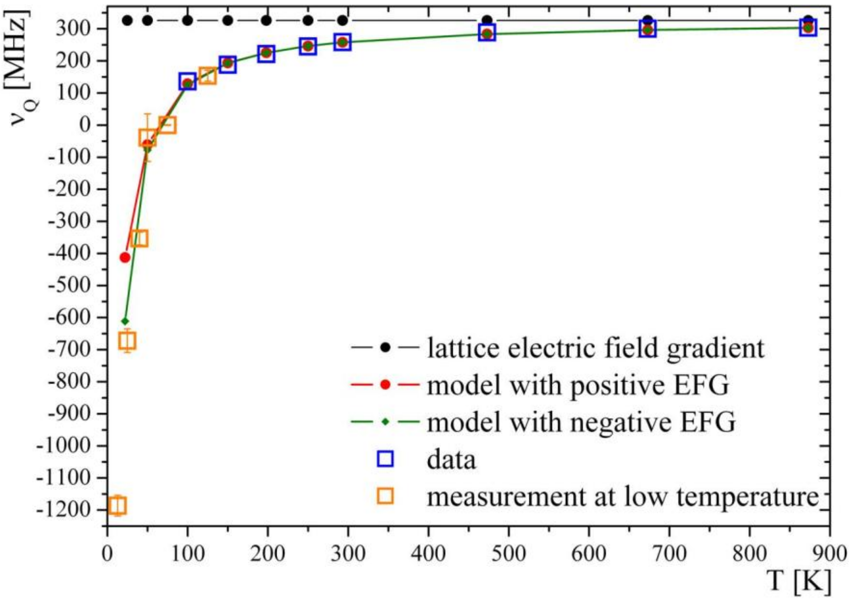


Fig. 2. Splitting of the 4f shell with positive lattice EFG.



References

[1] K.Tomala et al., *Journal of Magnetism and Magnetic Materials* **89**, 143-152 (1990).

PAC study of the dynamic hyperfine interactions at ^{111}In-doped Sc_2O_3 semiconductor and comparison with ab initio calculations

E. L. Muñoz[1], D. Richard[1], A. W. Carbonari[2], L. A. Errico[1] and M. Rentería[1].

[1]*Departamento de Física e Instituto de Física La Plata (IFLP, CCT La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina, e-mail:munoz@fisica.unlp.edu.ar*
[2] *Instituto de Pesquisas Energéticas y Nucleares-IPEN-CNEN/SP, São Paulo, Brazil*

The combined experimental and theoretical approach based on electric-field gradient (EFG) determinations by means of hyperfine interaction measurements and ab initio predictions at impurity atoms has been shown to be a powerful tool to unravel structural and electronic characterizations of impurities in solids, in particular in semiconductor oxides [1-3]

In this work, PAC experiments using ^{111}In-difussed Sc_2O_3 polycrystals have been performed at the IPEN facility in order to measure the Electric-Field Gradient (EFG) at (^{111}In (EC)$\rightarrow$) ^{111}Cd nuclei located at the cation site of the semiconductor lattice. The experimental results are compared with *ab initio* calculations performed with the Full-Potential Augmented Plane Wave plus local orbital (FP-APW+lo) method in the framework of the Density Functional Theory (DFT).

The PAC experiments were carried out in the temperature range 10 K – 900 K. The PAC spectra obtained in these measurements shows two very well-defined quadrupole frequencies along the whole temperature range, pointing to the fact that 100% of the probes are located at both nonequivalent cation sites of the bixbyite structure. Nevertheless, the spectra are dampened at certain intermediate temperatures, indicating the presence of dynamic hyperfine interactions that were analyzed with a perturbation factor based on the Bäverstam and Othaz model [4,5]. The FPAPW+lo calculations were performed using the Wien2K code.

From the *ab initio*-experimental comparison, we can conclude that the Cd impurities localized at the axially symmetric D sites of the crystal structure do not present dynamic interactions while that the Cd probes localized at the asymmetric C sites present appreciable dynamic interactions attributed to the so-called *after-effects* that follow the electron-capture decay of the ^{111}In parent isotope of the ^{111}Cd impurity tracer. This scenario could be supported in terms of the EFG behaviour, predicted by the *ab initio* calculations, at Cd impurities as a function of the charge state of the impurity located at the different cation sites of the structure.

References

[1] Anisotropic Relaxations Introduced by Cd Impurities in Rutile TiO_2: First-Principles Calculations and Experimental Support L.A. Errico, G. Fabricius, M. Rentería, P. de la Presa, and M. Forker.
Physical Review Letters 89, 55503 (2002).
[2] Metal Impurities in an Oxide: Ab Initio Study of Electronic and Structural Properties of Cd in Rutile TiO_2
L.A. Errico, G. Fabricius, and M. Rentería.
Physical Review B 67, 144104 (2003).
[3] Metal Impurities in an Oxide: Ab Initio Study of Electronic and Structural Properties of Cd in Rutile TiO_2
G. N. Darriba, L. A. Errico, P. D. Eversheim, G. Fabricius, and M. Rentería.
Physical Review B 79, 115213 (2009).
[4] U. Bäverstam, R. Othaz, N. De Sousa and B. Ringström, Nucl. Phys. A186, 500 (1972).
[5] A. Abragam and R. V. Pound, Phys. Rev. 92, 943 (1953).

Temperature dependence of the hyperfine fields of ^{111}In in sapphire (Al_2O_3) single crystals

Michael Steffens,[1] **Jakob Penner**[1], **Hassan Kamleh**[2], **Reiner Vianden**[1]

[1] *Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, 53115 Bonn,*
e-mail: steffens@hiskp.uni-bonn.de
[2] *Department of physics, Faculty of Sciences, University of Damascus, Syria*

The decay of ^{111}In to ^{111}Cd via electron capture, accompanied by Auger electrons, leaves the outmost atomic shell of the Cadmium in a highly ionized state.

In PAC measurements, this so called “electron capture after effect” leads to a significant loss of anisotropy and can be associated with a highly fluctuating electric field gradient (EFG).

The recovery of the ^{111}Cd shell by electronic recombination depends on the concentration and the mobility of charge carriers in the material. For insulators, the recombination timescale lies in the nanosecond regime, the generic timescale of hyperfine interaction processes as investigated by the PAC method.

In previous measurements the fraction of undisturbed probe atoms showed a strong and reversible dependence on the sample temperature [1].

Our current approach is to determine and alter the conditions under which electrons are sufficiently available to suppress the “after effect”.

Sapphire single crystals were ion implanted with ^{111}In at the mass separator in Bonn. After rapid thermal annealing the samples were held at temperatures up to 1000 K. To alter the recombination characteristics and to study the influence of acceptor and donator levels, the samples were additionally doped with several concentrations of Si, Cr and P.

References

[1] J. Penner and Reiner Vianden, *Hyperfine Interactions* **158**, 389 (2004)

The Concept of Trajectories in the Data Analysis of Non-axially Symmetric Nuclear Quadrupole Interactions

Tilman Butz[1]

[1] *University of Leipzig, Germany, e-mail: butz@physik.uni-leipzig.de*

The nuclear quadrupole interaction is described as the product of the nuclear quadrupole moment Q with the electric field gradient (EFG) tensor. This is a symmetric, trace-less 3x3 tensor which usually is described by two quantities in the principle coordinate system: the largest component by magnitude is denoted by V_{zz} and the asymmetry parameter is defined as $h = (V_{xx} – V_{yy})/V_{zz}$. Frequently, these two quantities are determined for powder samples as a function of an external variable, e.g. temperature. It is customary to plot both quantities separately versus temperature. This, however, masks any eventual interdependencies of the two quantities. A better way to plot the results is to plot V_{zz} and V_{xx} in a cartesian plot, or better in a Czjzek-plot [1], a variant of the cartesian plot, which is still linear in both variables. Each data pair of V_{zz}/V_{xx} constitutes a point in this plot with temperature being the implicit parameter. Connecting all points by a continuous line yields a trajectory. This trajectory is continuous even when passing over h = 1 where the tensor orientation flips by 90° and the sign of V_{zz} changes.

Interestingly enough, there are many examples where a straight trajectory is observed, i.e. both variables depend linearly on each other. This can be modelled by a linear superposition of two tensors which are simultaneously diagonal and temperature independent:

$V = V1 + a(T)V2$.

The only temperature dependent quantity is a(T), the control parameter. In this situation it is clear that fitting 2n independent parameters for n temperature points is wrong. Instead, a scale factor and a slope should be fitted in addition to n values for a(T), i.e. there are n+2 independent parameters only. The slope is given by the asymmetry parameter of V2, which is the asymptotic asymmetry parameter of V for large a. V2 must have a physical interpretation, contrary to V1 which can be modified by shifting a (unless we know where a must be 0, i.e. if a is an order parameter). The temperature dependence of a contains all solid state information like lattice expansion, lattice vibrations, and changes in the electronic charge density distribution.

The correct strategy for the data analysis would be to analyze the data conventionally, plot the data in the Czjzek-plot, and for a straight trajectory perform a simultaneous fit of all data with n+2 adjustable parameters in a second tier.

Another interesting class of systems can be described by a linear superposition of two tensors which are not simultaneously diagonal in the same principle coordinate system but which share one common coordinate around which the other two rotate. In other words, only a 2x2 matrix has to be diagonalized. The structure of the resulting eigenvalues (Vieta's formula) is such that by using the sum and the product of both the control parameter can be eliminated straightforwardly and second order curves result which must be hyperbolae because we require asymptotes. In this case we require n+3 adjustable parameters, i.e. a scale factor, the asymptotic asymmetry parameter and one off-diagonal element which describes the rotation in addition to n values for a. Again, a simultaneous fit of all data is required in a second tier.

Examples of experiments with linear and hyperbolic trajectories will be given.

References

[1] G. Czjzek, Hyperf, Interact. 14,184, (1984); T. Butz et al., Physica Scripta 54,234, (1996)

MSR in diamond

SH Connell[1], K Bharuth-Ram[2] and SFJ Cox[3]

[1] *Department of Physics, University of Johannesburg, University Road, Johannesburg 2006, South Africa, e-mail: shconnell@uj.ac.za*

[2] *School of Physics, Univ. of KwaZulu-Natal, Durban 4041, South Africa, e-mail: kbr@tlabs.ac.za*

[3] *ISIS Facility, Rutherford Appleton Lab, Chilton, Oxfordshire, OX110QX, UK, e-mail: S.F.J.Cox@rl.ac.u*

Diamond as a material has evolved beyond its roles as a gem or an abrasive to find a niche in modern high technology areas. Examples include radiation detectors, electronic devices, biosensors, X-ray optics and also a promising system for the realization of quantum communication and computation. The reason for the development of these new applications is that the parameters describing the electronic and physical properties of diamond usually represent very extreme values. Indeed, diamond vertex detectors are being considered for the upgrade of some of the LHC experiments. It has recently become possible to take advantage of the interesting properties of diamond, as the synthesis of diamond has reached a point that material with impurities below the part per billion range and residual strain in the order of ten nano-radians has been realized. Hyperfine interactions have played a key role in the study of diamond and the emergence of novel applications. This relates to the characterization of defects and the development of engineered few spin systems. A particular aspect of the defect studies is the elusive hydrogen defect. In MSR studies, muonium is considered a light "isotope" of hydrogen with very similar chemical properties, but with very interestingly different dynamical properties, due to its much lighter mass. It offers a unique opportunity to study the behaviour of hydrogen in diamond at very low concentrations. The studies have revealed details of the elementary muonium atom as well as a molecule involving muonium in the diamond lattice. The dynamics of the muonium, which include quantum diffusion and ionization have also been studied. This contribution reviews MSR in diamond in the context of diamond as a modern material hosting advanced applications.

Investigations on thin Fe films and Heusler alloy films using synchrotron-radiation-based Mössbauer spectroscopy

Ko MIBU[1]

[1]*Nagoya Institute of Technology, Japan*

Recent development in synchrotron-radiation-based nuclear resonant scattering or Mössbauer spectroscopy has opened up new aspects on investigation of materials in the measurements of hyperfine interactions and also of local phonon density-of-states. In Japan a five-year project led by Prof. Seto at Kyoto University is now in progress for further development of these unique techniques. The field of magnetic thin films is also getting a benefit from these new techniques through detection of magnetic hyperfine fields. The method which has mainly been used so far for thin film experiments is "time domain" measurements, where interference patterns of pulsed X-rays resonantly scattered by nuclei are detected as a function of time. However, "energy domain" measurements are more desirable for thin films, which often contain inhomogeneity in the nuclear environments. In our project, a new synchrotron-radiation-based "energy domain" Mössbauer spectroscopic method has been developed, and optimized also for investigations on magnetic thin films. In this presentation, the validity and limitations of this method are demonstrated by showing some experimental results on thin Fe films and Heusler alloy films.

Recent Methodological Developments in Nuclear Resonant Scattering with Synchrotron Radiation

Esen Ercan Alp,[1] Thomas Toellner[1], Wolfgang Sturhahn[1], Jiyong Zhao[1]

[1] *Argonne National Laboratory, USA*

e-mail: alp@anl.gov

The year 2010 marks the 25th anniversary of the first successful demonstration of nuclear resonant scattering using synchrotron radiation. During this period, many different experimental approaches have been developed to observe and conduct meaningful scientific experiments in samples of mineralogical and biological interest. Among these, we can distinguish the development of high-resolution, tunable crystal monochromators, back-scattering crystals, polarization-based optics, interferometric techniques, and creation of of single-line absorbers for direct energy-domain measurements. Some of these are implemented for some subset of the dozen or so different Mossbauer isotopes with transition energies ranging from 6 to 70 keV. Currently, at least 5 different synchrotron beamlines are dedicated fully or partially for this purpose. Some of these facilities, like Sector 3-ID at the APS will be upgraded soon, while some newer facilities are also just coming on-line, like PETRA-III. We will to review the progress made at the APS and the upgrade plans for the 3-ID, the only dedicated beamline in the USA.

Magnetism in Iron Implanted Oxides: A Status Report

R. Sielemann[1] **and the Mössbauer Collaboration at ISOLDE/CERN**[2]

[1]*Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany*

sielemann@helmholtz-berlin.de

[2]*PH Dept. ISOLDE/CERN, 1211 Geneva 23, Switzerland*

Diluted magnetic semiconductors form a special class of magnetic materials which has drawn a lot of attention over the last years both for the interest in the basic physics involved and for possible applications, e.g., in the field of spintronics. However, there is no general agreement on the origin of this type of magnetism. Various coupling mechanisms between the magnetic ions have been proposed, in addition the role of intrinsic defects as well as of unintentional magnetic impurities and precipitations was considered.

Oxides with embedded magnetic ions form a subclass of the magnetic semiconductors. To study magnetism at the atomic level Mössbauer spectroscopy (MS) can be utilized, especially with ^{57}Fe. Since the solubility of 3d magnetic ions in most semiconductors is small, their introduction is difficult. So, implantation is a favorable technique. In addition it creates intrinsic defects and thus may influence (create) magnetic phenomena. With this idea in mind ^{57}Fe MS was performed at the ISOLDE facility at CERN following implantation of radioactive ^{57}Mn ($T_{1/2}$ = 1.5 min) in diverse oxides with a focus on ZnO, one of the most important materials for magnetic semiconductors [1]. The Mössbauer spectra obtained consist to a large part of a magnetic sextet with splitting up to about 50 T and in addition of nonmagnetic components indicating different lattice sites and/or charge states of the Fe atoms. Surprisingly the sextet persists up to measuring temperatures of about 600 K. Experiments performed on other oxides (e.g., MgO, Al_2O_3) show results with partly similar and partly differing features. Detailed MS studies as function of temperature, implanted Mn concentration, pre-doping of the oxides with various magnetic and nonmagnetic ions and in particular experiments with an external magnetic field of 0.6 T show a variety of phenomena with respect to the occurrence of the magnetic fraction and permit attributing it to Fe-ions in a 3^+ paramagnetic state. This observation of a static magnetic pattern is enabled by the unusually long relaxation time > 20 ns even at 600 K though this relaxation time normally strongly decreases with rising temperature. Unlike a first report [2] there is presently no necessity to involve ordered magnetism in the interpretation of the magnetic spectra [3].

The assets of MS in these studies compared to, e.g., the EPR technique (Electron Paramagnetic Resonance) will be discussed.

References

[1] T. Dietl et al., Science **287**, 1019 (2000).

[2] G. Weyer et al., J. Appl. Phys**. 102**, 113915 (2007).

[3] H.P. Gunnlaugsson et al., Appl. Phys. Lett. (manuscript in preparation).

Mössbauer study of spin-lattice relaxations of dilute Fe^{3+} in MgO

T. E. Mølholt[1], **R. Mantovan**[2], **H. P. Gunnlaugsson**[3], **K. Bharuth-Ram**[4], **M. Fanciulli**[2,5], **K. Johnston**[6], **Y. Kobayashi**[7], **G. Langouche**[8], **H. Masenda**[9], **D. Naidoo**[9], **S. Ólafsson**[1], **R. Sielemann**[10], **G. Weyer**[3], **H. P. Gíslason**[1]

[1]Science Institute, University of Iceland, Reykjavík, Iceland, e-mail: tem4@hi.is; [2]Laboratorio MDM-IMM-CNR, Milano, Italy; [3]Department of Physics and Astronomy, Aarhus University, Denmark; [4]School of Physics, University of KwaZulu-Natal, South Africa; [5]Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy; [6]PH Dept, ISOLDE/CERN, 1211 Geneva 23, Switzerland; [7]The Institute of Physical and Chemical Research, Wako, Japan; [8]Instituut voor Kern-en Stralingsfysika, University of Leuven, Belgium; [9]School of Physics, University of the Witwatersrand, South Africa; [10]Helmholtz Zentrum, Berlin, Germany.

We have measured ^{57}Fe emission Mössbauer spectra following 50 – 60 keV implantation of radioactive ^{57}Mn^{+} ($T_{½} = 85.4$ s) at the ISOLDE facility at CERN into MgO single crystals held at 77 – 647 K (Fig. 1). This method allows us to study Fe impurities in concentrations <10^{-4} at.%. The central part of the spectra (Fig. 1) shows lines from Fe^{2+} on distorted lattice sites, substitutional sites, and interstitial Fe sites (see [1] for details). The wings of the spectra show what us in focus here; broad distributions of magnetic hyperfine fields up to ~52 T, evidently slowly relaxing paramagnetic Fe^{3+}.

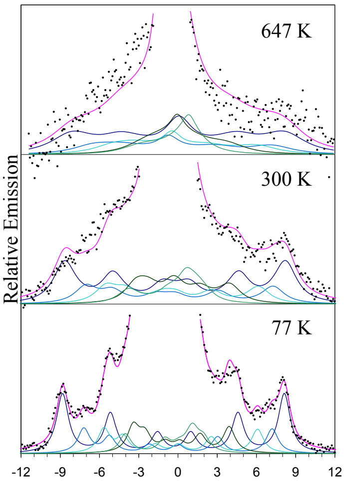


Fig. 1. Show the wings of the ^{57}Fe Mössbauer spectra held at the temperatures indicated.

These have been analysed/simulated with an arbitrary number of Blume-Tjon (BT) sextets [2] (here a minimum of five BT-sextets was needed, constrained by various common para-meters). The relaxation rate parameter W is allowed to vary with temperature. This parameter corresponds to a spin-relaxation rate of $\tau^{-1} = WE_0/(\hbar c)$, where E$_0$=14.4 keV is the energy of the Mössbauer state. The (common) change of the BT-sextets is due to increasing values of W with temperature, which as found to increase to $W \approx 1.5(9)$ mm/s (assuming $W = 0$ mm/s at 77 K). In this range the line shape of the BT-sextets is dominated by broadening of the individual lines by $\Delta\Gamma = 2W$. Figure 2 shows the relaxation rate obtained in this work compared to the results based on EPR measured relaxation rates of dilute Fe^{3+} impurities in MgO [3]. A reasonably good correlation between the two sets of data is obtained, demonstrating the possibility of retrieving spin-lattice relaxation rates using Mössbauer spectroscopy without the application of an external magnetic field. Other applications of this technique will be given at this conference [4].

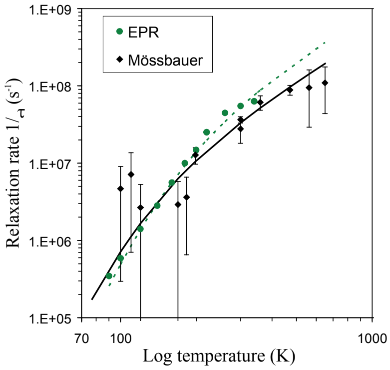


Fig. 2. Spin-lattice relaxation rate of Fe^{3+} from this study compared to relaxation rates from EPR study

References:

[1] T. E. Mølholt et al. (2010) this conference.
[2] M. Blume and J. A. Tjon, *Phys. Rev.* 165, 446 (1968).
[3] R. S. de Biasi and P. D. Portella, *J. Magn. Magn. Mater.*, 15, 737 (1980).
[4] H. P. Gunnlaugsson et al. (2010) this conference.

Temperature dependence of the magnetic hyperfine field at ^{111}Cd in ZnO doped with Co

A. W. Carbonari,[1] **M. E. Mercurio**[1], **M. R. Cordeiro**[1], **R. N. Saxena**[1]

[1]*Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, São Paulo, Brasil, e-mail: carbonar@ipen.br*

The search for room temperature ferromagnetism in wide band gap semiconductor oxides has been quite intensive in the last years. In particular, ZnO has attracted attention since theoretical calculations[1,2] have indicated that ZnO when doped with a transition metal like Co or Mn should present ferromagnetism at room temperature. The results instead of clarifying this issue have however brought more doubts. While many experimental studies confirm the occurrence of ferromagnetism, several others do not observe magnetic order in such compounds. Hyperfine interactions, by their nature seem to be very suited to investigate these materials and tell something about the existence and origin of the magnetism in such compounds. In the present work powder and bulk samples of ZnO doped with 10 % of Co were prepared by sol-gel method from highly pure metallic Zn(99.9999%) and Co(99.9999%). The samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS) and perturbed gamma-gamma angular correlation (PAC) spectroscopy. In order to carry out PAC measurements carrier-free ^{111}In nuclei were introduced during preparation of the samples and used as probe nuclei in Zn sites. The XRD patterns showed that no second phase appeared and SEM images indicated that the samples are highly homogeneous. PAC measurements were carried out in the temperature range from 50 K to 295 K and the results at 295 K before cooling down showed that samples of ZnO doped with Co have the same electric quadrupole frequency reported in literature for pure ZnO. This observation indicates that Co ions are substituted for Zn ions and have a similar electronic structure of Zn ions. Below room temperature one of the samples showed a combined magnetic and electric hyperfine interaction from which a magnetic hyperfine field around 1.9 T has been extracted. The temperature dependence of this field showed unusual behavior indicating a first order transition around 300 K which suggests a different type of magnetism.

References

[1] T. Dietl, H. Ohno, F. Matsukura, J. Cibert, D. Ferrand, Science **287**, 1019 (2000).

[2] K. Sato and H. Katayama-Yoshida, Hyperfine Interact. **136/137**, 737 (2001)

Fe as Local Probe to follow the Competition between Magnetism and Superconductivity in the New Fe-pnictide Superconductors

E. Baggio Saitovitch[1] ,D. R. Sánchez[2], M. Alzamora[1] and J. Munevar[1], S. L. Budko[3], P. C. Canfield[3], G. F. Cheng[4], N. L. Wang[4], H. H. Wen[5]

[1]*Centro Brasileiro de Pesquisas Físicas. Rua Xavier Sigaud 150, Urca 22290-180. Rio de Janeiro, Brasil.*
[2]*Universidade Federal Fluminense, Av. Milton Tavares de Souza, 24210-346 Niterói. Rio de Janeiro, Brasil.*
[3]*Ames Laboratory, U.S. DOE and Iowa State University, Ames, Iowa 50011, USA*
[4]*Beijing National Lab. for Condensed Matter Physics, C. A. of Sciences, Beijing 100080, China*
[5]*National Laboratory for Superconductivity, Institute of Physics, and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China*

The ^{57}Fe Mössbauer spectroscopy has been used to follow the appearance of magnetic order and structural transition induced by composition or temperature changes in some Fe-pnictide compounds. Superconductivity was established in undoped compounds by F, K and Na in $CeFeAsO_{1-x}F_x$, $Ba_{1-x}K_xFe_2As_2$ and $Sr_{1-x}Na_xFe_2As_2$. The studies have been performed on some $RFeAsO_{1-x}F_x$ (R = Ce, Nd) polycrystalline samples of as well as in $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ single crystal samples. Other Mössbauer studies have shown evidence for magnetism and superconductivity on $Sr_4V_2O_6Fe_2As_2$, and $Sr_4Sc_2O_6Fe_2As_2$ would show a magnetic ordering without a homogeneous structure. The magnetic transition temperature and the type of transition will be discussed, as well as the coexistence of magnetism and superconductivity.

Muon spin relaxation studies of geometrically frustrated magnets

Pierre Dalmas de Reotier,[1] **Alain Yaouanc**[1]

[1] *CEA Grenoble, France e-mail: pierre.dalmas-de-reotier@cea.fr*

Highly frustrated magnetic systems (HFMS) are characterised by exotic ground states which include unconventional magnetic orders, spin liquids, spin glasses, spin ices,... The muon spin rotation and relaxation (µSR) techniques are well known for their ability to detect magnetic phase transitions and for their sensitivity to spin dynamics over a broad time window. They are therefore ideally suited for the study of HFMS.

We shall show that µSR reveal features which are specific to HFMS such as the ubiquitous spin dynamics which are observed for temperatures approaching the absolute zero. While these dynamics are not unexpected in systems with large ground state degeneracy, they are much more surprising in HFMS with a long-range magnetic order.

The interplay between static and dynamic properties results in completely unexpected responses in µSR experiments. In some case, an interpretation of these experiments following conventional practice even leads to flawed conclusions. This has been the motivation for a deeper insight into the fate of µSR measurements, which has led in turn to unravel some characteristics of the HFMS.

The paper will be illustrated by examples taken from µSR investigations on geometrically frustrated magnets with a structure based on triangles or tetrahedra. When relevant, they will be discussed in the light of results obtained by other microscopic techniques.

Magnetism in Azurite Studied by Muon Spin Rotation

M. Kraken[1], F.J. Litterst[1], S. Süllow[1], A. Wolter[2], B. Wolf[3], M. Lang[3], Ch. Baines[4], H. Luetkens[4]

[1] *IPKM, TU Braunschweig, 38106 Braunschweig, Germany, e-mail: j.litterst@tu-bs.de*

[2] *IFW Dresden, 01069 Dresden, Germany, e-mail: a.wolter@ifw-dresden.de*

[3] *Physikaisches Institut University Frankfurt, 60438 Frankfurt a.M., Germany,*

e-mail:michael.lang@physik.uni-frankfurt.de

[4] *NUM, PSI, 5232 Villigen, Switzerland, e-mail: hubertus.luetkens@psi.ch*

The natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ represents a new type of low-dimensional frustrated quantum spin system with a diamond spin chain as basis. From specific heat [1] there is evidence for a phase transition at ca. 1.8 K which however is magnetically still ill-defined. Earlier muon spin rotation experiments [2] have indicated a magnetic transition yet no systematic study has been reported. We have performed zero field and transverse field muon spin rotation experiments at Paul Scherrer Institut Villigen (Switzerland) in the temperature range from 0.02 K to 6 K on polycrystalline powder and a single crystal. We could corroborate the appearance of magnetic order below 1.9 K from spontaneous muon spin rotations with frequencies following a magnetization curve indicating 2-dimensional correlations. There is evidence for a further change in magnetic structure below about 500 mK. The ordered magnetic Cu moments can be estimated to be only on the order of some tenths of a Bohr magneton in agreement with recent neutron scattering data [3].

References

[1] H. Kikuchi, et al., *Phys. Rev. Lett.* **94**, 227201(2005).

[2] H. Kikuchi, et al., *Progress of Theoretical Physics Supplement*. **159**, 1 (2005)

[3] K. Rule, et al., *Phys. Rev.* **B 81** in print (2010)

Measuring the magnetic properties of monolayers of single molecule magnets

Z. Salman,[1] S. J. Blundell,[2] K. H. Chow,[3] S. R. Giblin,[4] R. F. Kiefl,[5,6]
W. A. MacFarlane,[7] M. Mannini,[8] E. Morenzoni,[1] G. D. Morris,[6] T. Prokscha,[1]
R. Sessoli,[8] A. Suter [1]

[1] Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, e-mail: zaher.salman@psi.ch
[2] Clarendon Laboratory, Department of Physics, Oxford University,Parks Road, Oxford OX1 3PU, UK
[3] Department of Physics, University of Alberta, Edmonton, AB, Canada, T6G 2G7
[4] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Oxfordshire, OX11 0QX, UK
[5] Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1
[6] TRIUMF, 4004 Wesbrook Mall, Vancouver, BC, Canada, V6T 2A3
[7] Department of Chemistry, University of British Columbia, Vancouver, BC, Canada V6T 1Z1
[8] Dipartimento di Scienze Chimiche, Universita di Catania & INSTM UdR di Catania, viale A. Doria 6, 95125 Catania, Italy

A promising strategy to encode information in molecular units is provided by single molecule magnets (SMMs), chemically identical nanoscale clusters of exchange-coupled transition metal and associated ligands. SMMs have been used to study a variety of quantum phenomena and may find applications in quantum information processing. The assembly of these systems on surfaces is currently investigated as this represents a necessary prerequisite for magnetic memory applications. However, the effect of the surface on an SMM is still not well understood. This is due to the small quantity of magnetic material contained in a (sub)monolayer which prevents the use of conventional techniques. Here we overcome this obstacle by using a novel proximal magnetometry techniques utilizing polarized muons and nuclei as an implanted local probe to investigate magnetic properties of such monolayers of SMMs. We anticipate that this method will provide a powerful tool to improve our understanding of the influence of the surface on a grafted SMM.

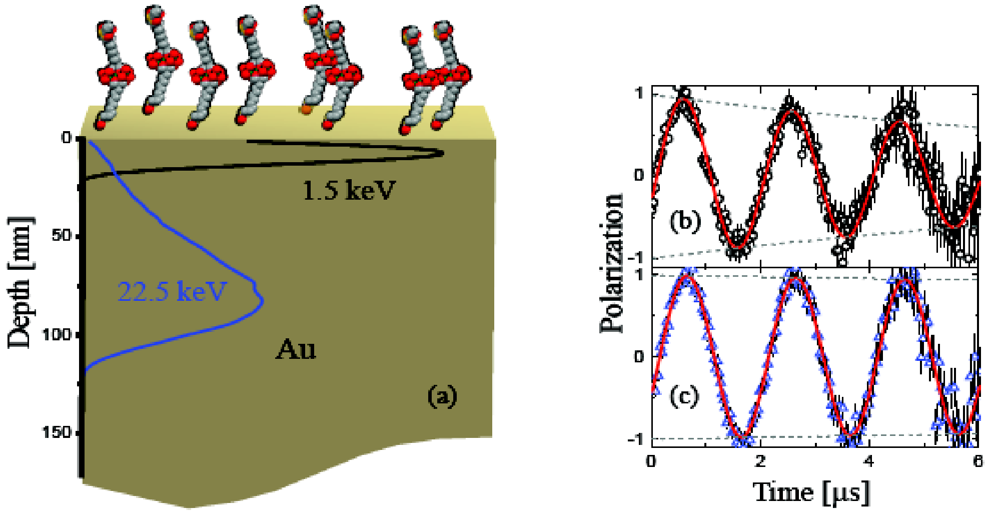


Fig. 1. (a) A schematic view of a monolayer of SMMs grafted on Au film. The stopping distribution of muons in Au at E = 1.5 and 22.5 keV are also shown. Typical muon spin precession spectra in the rotating reference frame measured at T = 6 K, B0 = 110 mT and implantation energy (b) 1.5 keV and (c) 22.5 keV. The damping of the precession signal in (b) is due to the dipolar magnetic field from the SMM monolayer.

Defect induced magnetic interaction in highly oriented pyrolytic graphite (HOPG): A local investigation using TDPAD method.

S.N. Mishra,[1] **S.K. Mohanta,**[1,2] **S.K. Srivastava**[2]

[1]*Dept. of Nuclear and Atomic Physics, Tata Institute of Fundamental Research, Mumbai-400005, India,*
e-mail: mishra@tifr.res.in
[2]*Dept. of Physics and Meteorology, Indian Institute of Technology, Kharagpur-721302, India*

Defect induced magnetism in carbon based systems have long been the subject under extensive investigation, not only for the nature of magnetism in s, p electron systems but also for its potential to practical applications. The discovery of ferromagnetism at room temperature in pure carbon materials has given a new impetus for magnetic studies in graphite and other carbon materials [1,2]. It has been suggested that defects play a key role for the ferromagnetic ordering observed in graphite.

Here, we present magnetic hyperfine field of ^{19}F measured by time differential perturbed angular distribution technique. The ^{19}F probes were produced via the heavy-ion reaction ^{12}C(^{12}C,αp)^{19}F using pulsed ^{12}C beam at an energy of 40 MeV. The energetic ^{12}C beam impinging on a 1 mm thick HOPG sample, used as the stopper, also creates high concentration of defects. The approach adopted here, thus serves the dual purpose of creating defects and studying the magnetic interactions arising thereof. For the detection of hyperfine fields we have used the $5/2^+$ isomeric state in ^{19}F with half-life $T_{1/2}$=88.5 ns, g-factor g_N = 1.44 and, quadrupole moment Q = -0.12 b which offers high sensitivity towards magnetic interactions. Typical spin rotation spectra R(t) measured for ^{19}F in HOPG are shown in Fig 1. The R(t) spectra show superposition of two frequencies having ω_L = 64 and 93 MHz and intensity ratio of 45:55 at 15 K. Fig 2 shows the temperature dependence of the magnetic hyperfine field B_{hf} derived from the expression $B_{hf} = (\hbar\omega_L/g_N\mu_N B_{ext})-B_{ext}$. The ω_L for the two components show distinctly different temperature dependence yielding B_{hf} ~5 kG and 0.8 kG at T = 0. The observed results indicate the presence of strong magnetic interaction in HOPG. Supported by *ab-initio* calculations performed for a number of defect configurations around a F impurity in graphite, we assign the high field component to substitutional site with single vacancy/interstitial C, and the low field component to F at substitutional/interstitial sites without any vacancy

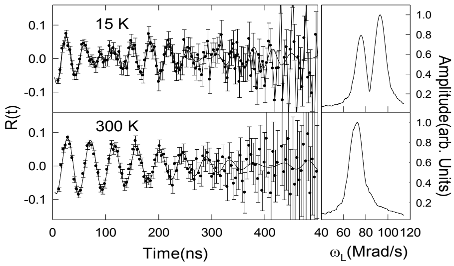


Fig 1. Spin rotation spectra at 15 and 35K .

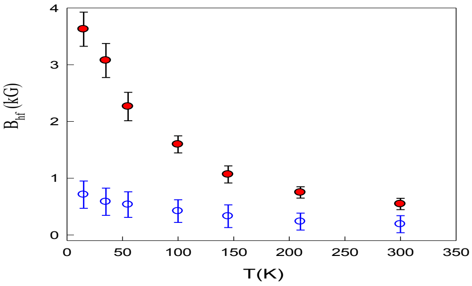


Fig 2. Hyperfine field as a function of temperature.

References
[1] T. Makarova et al., *Carbon based magnetism*, Amsterdam: Elsevier; p. 371-96 (2006).
[2] P. Esquinazi et al., *Phys. Rev. B* **66**, 024429 (2002).

Beta detected NMR: a New Depth-resolved Probe of Materials at the Nanoscale

W.A. MacFarlane[1]

[1]*Chemistry Department, University of British Columbia, Vancouver, Canada*

I will describe the beta detected NMR and NQR facility at TRIUMF which has been developed over the last decade, motivated by the need for depth resolved probes of the electromagnetic properties of solids, particularly in thin film heterostructures, where many new phenomena of both fundamental and practical interest arise.

The principal probe used is a 28 keV beam of $^{8}Li^{+}$ optically polarized in-flight at TRIUMF's ISAC facility. I will then present some recent results from diverse areas including spintronic materials and heterostructures and superconductors.

Wednesday 15th September (9:40-10:20), Surface Interfaces, Thin Films, Nano-Structures

Development and Applications of Mössbauer Spectroscopic Microscope

Yutaka Yoshida[1], **Kazuo Hayakawa**[1], **Kenichi Yukihira**[1], **Masahiro Ichino**[1],
Yuki Akiyama[1], **Hiroto Kumabe**[1], **Hiroyoshi Soejima**[2]

[1] *Shizuoka Institute of Science and Technology, Toyosawa 2200-2, Fukuroi-city, Shizuoka 437-8555, Japan, e-mail: yoshida@ms.sist.ac.jp*
[2] *Shimadzu Corporation, Nishinokyo-Kuwabaracho 1, Nakagyo-ku, Kyoto 604-8511, Japan*

We developed a mapping technique for ^{57}Fe Mössbauer spectroscopy using a Multi-Capillary X-ray lens (MCX or Soejima-Kumakhov lens), which provided a space resolution down to 50 μm [1, 2]. There are, however, strong demands to study sub-micrometer-scale structures in materials science. Presently, we are challenging to improve the space resolution using a Fresnel-Zone Plate (FZP), which is known to provide a possibility to focus X-ray beam down to several 10 nm in diameter, if one would use it at a beam line of synchrotron facilities where a strong and sharp X-ray beam is available. In our laboratory, therefore, we combine a FZP with the MCX in order to focus 14.4 keV γ-rays down to hundreds nanometers. The focal distance is 48 mm from the outlet of FZP lens. The experimental or and 3.7 GBq-^{57}Co source mounted on a Mössbauer transducer. In order to evaluate the spot size of the combined γ-ray lens, the transmission counts of 14.4 keV γ-rays are measured as functions of the X or Y positions of the Ta-knife-edge collimators by a Si-PIN detector. The measuring time is 55000 sec at each position. After subtracting the background from the original data (red points in Fig.2), we obtained the blue data points which shows two sharp peaks of the 1st order diffraction at around 155 μm close to the beam center. In addition, two broad peaks appear at around 125 and 75 μm, which correspond to the 2nd order diffractions. The position of the Ta knife-edge appears to be about 10μm deviated to the direction of the FZP from the exact focal position. Considering the focusing geometry and the half-width of the sharp peaks, the spot size expected at the focal position can be estimated about 3 μm in diameter. The mapping images will be shown in the lecture.

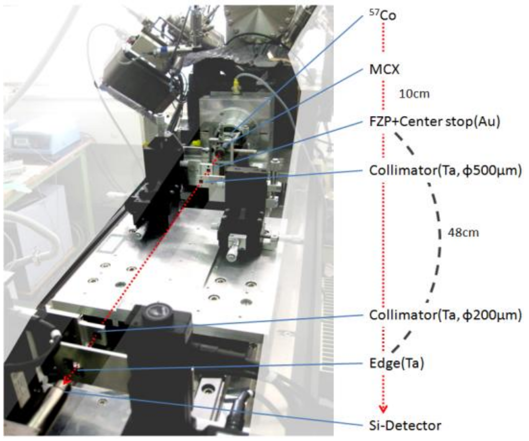


Fig. 1 Experimental set-up using a MCX and FZP combined lens.

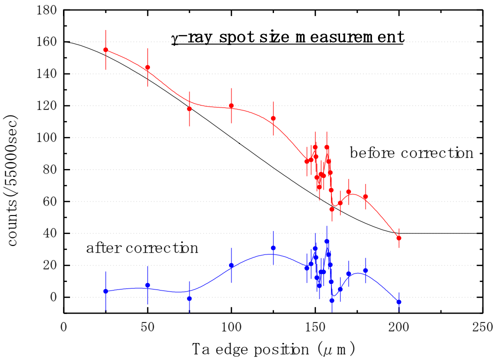


Fig. 2 14.4 keV-γ-ray counts as function of Ta-edge collimator, suggesting that the spot size is about 3 μm at the focus point.

References

[1] Y. Yoshida, K. Suzuki, K. Hayakawa, K. Yukihira, H. Soejima, "Mössbauer spectroscopic microscope", Hyperfine Interact., **188**, 121 (2009).
[2] Y. Yoshida, et.al, in Proceedings of ICAME2009, Vienna, *J. Phys.: Conf. Ser.*217, 012003, (2010).

Quadrupolar Perturbed NMR in Inorganic Nanomaterials

A. M. Panich[1]

[1]Department of Physics, Ben-Gurion University of the Negev, P.O.Box 653,
84105 Be'er Sheva, Israel
e-mail: pan@bgu.ac.il

Inorganic nanostructures reveal a number of applications in electronics, magnetic recording, as low-friction and nano-bio materials. However, our knowledge about properties of inorganic nanomaterials is still limited. Quadrupolar perturbed NMR is an excellent tool in studying the local site symmetry, chemical bonding and electronic structure of inorganic nano-particles comprising quadrupole nuclei. I will review my own and literature data on NMR spectra and relaxation measurements of quadrupole nuclei in several inorganic nano-compounds such as boron nitride nanotubes, vanadium oxide nanotubes and molybdenum sulfide fullerenes. Detailed analysis of the spectra and their comparison with those in bulk samples will be done. The obtained findings allow us making conclusions about the local crystal structure, electronic structure and bonding in the inorganic nanosized compounds.

Synchrotron radiation based TDPAC

I. Sergueev

European Synchrotron Radiation Facility, BP220, F-38043 Grenoble, France,

e-mail:sergueev@esrf.fr

Mössbauer spectroscopy and time differential perturbed angular correlations (TDPAC) are classical nuclear spectroscopy techniques used to study hyperfine interactions. They both measure hyperfine splitting of the excited nuclear state with ns-μs lifetime. On the other hand, the collective over nuclear ensemble nature of the Mössbauer effect expressed in the recoil-free emission and absorption, leads to the difference in the applicability of the methods and, sometimes, to the different sensitivity to the hyperfine interactions. From this point of view, it would be important to combine two techniques in the study of the hyperfine interactions at the same nucleus. However, due to different requirements to the properties of mother isotopes, the application of MS and TDPAC to study the same element is very difficult.

The nuclear resonant scattering of synchrotron radiation is a technique which allows one to overcome this problem. The spatially coherent nuclear forward scattering (NFS) is the time analogue of the Mössbauer spectroscopy. On the other hand, the spatially incoherent, single-nucleus resonant scattering [1], SRPAC, is closely related to TDPAC and can be measured in parallel to NFS.

In SRPAC the intermediate nuclear level is not excited "from above" via a cascade originating from the decay of a radioactive parent like in TDPAC, but “from below", i.e. from the ground state, during incoherent nuclear resonant scattering of SR. Directional selection and timing by the first detector in TDPAC are replaced in SRPAC by the direction and the timing of the incident flash of synchrotron radiation. The absence of the cascade in SRPAC allows one to investigate the excited states which can hardly or even cannot be studied by TDPAC, e.g. the Mössbauer isotopes ^{57}Fe [2], ^{119}Sn [3], ^{61}Ni [4], ^{160}Gd, ^{174}Yb. In addition, SRPAC does not depend on recoil energy. This gives possibility to continue Mössbauer investigations of hyperfine interactions into regions where the Lamb-Mössbauer factor vanishes, i.e. in soft matter or for the high-energy Mössbauer transitions even at ambient temperatures.

In this presentation the basic features of SRPAC will be described underlining the similarity and the difference with conventional TDPAC and with Mössbauer spectroscopy. Several examples of application of the method will be presented: study of the glass transition using the iron contained glass former [2], study of quadrupole interaction in the β-tin, study of magnetic hyperfine interactions in the nickel metal [4].

References

[1] A.Q.R.Baron, A.I.Chumakov, R.Rüffer et al., *Europhys. Lett*. 34, 331 (1996).
[2] I.Sergueev, U.van Bürck, A.I.Chumakov et al., *Phys.Rev. B* 73, 024203 (2006).
[3] C.Strohm, I.Sergueev, and U. van Bürck, *Europhys. Lett*. 81, 52001 (2008).
[4] I. Sergueev, O.Leupold, H.-C.Wille et al., *Phys. Rev. B* 78, 214436 (2008).

Phonon mode softening at the ferroelectric transition in $Eu_xBa_{1-x}TiO_3$

W.N. Rowan-Weetaluktuk[1], D. H. Ryan[1], A.O. Sushkov[2], S. Eckel[2], S. K. Lamoreaux[2], O.P. Sushkov[3], J. M. Cadogan[4a], M. Yethiraj[5] and A.J. Studer[5]

[1] Department of Physics, McGill University, Montreal, QC, H3A2T8, Canada
[2]Department of Physics, Yale University, New Haven, CT, 06520-8120, USA.
[3] School of Physics, University of New South Wales, Sydney, NSW, 2070, Australia.
[4]Department of Physics and Astronomy, University of Manitoba, Winnipeg, MB, R3T2N2, Canada.
[5]Bragg Institute, ANSTO, PMB 1, Menai, NSW 2234, Australia.
[a] e-mail: cadogan@physics.umanitoba.ca

The ferroelectric $Eu_xBa_{1-x}TiO_3$ system is being studied as part of a project to search for the permanent electric dipole moment of the electron [1]. Part of this work involves understanding the materials properties of the system. Doping $BaTiO_3$ with europium drives the ferroelectric transition down from 278 K [2] at x=0, to 0 K by x<0.75. The Eu-doped materials are weakly conducting, so detecting the ferroelectric transition by either capacitive methods or bulk susceptibility is difficult, however the phonon mode softening that accompanies the formation of the orthorhombic ferroelectric phase leads to a characteristic reduction in the Mössbauer-Lamb (or "*f* ")–factor [3]. ^{151}Eu Mössbauer measurements on two samples of $Eu_{0.5}Ba_{0.5}TiO_3$ have confirmed the presence of the phonon mode softening centred at 180 K, but also revealed an unexpected result. The signal from divalent europium (Eu^{2+}) dominates the spectra of both samples; however, we found that 9-12% of the europium was present as Eu^{3+}. While initially ascribed to unreacted Eu_2O_3, neither xrd nor neutron diffraction showed any evidence for this, or any other trivalent europium impurity. More surprisingly, the temperature dependence of the *f*-factor shows a much stronger response in the Eu^{3+} component than in the Eu^{2+} one, clearly indicating that the trivalent europium is present within the $Eu_{0.5}Ba_{0.5}TiO_3$ phase and ruling out any possibility of phase separation or impurity effects. Preliminary analysis of neutron powder diffraction data rules out the possibility that some of the europium might be located on titanium sites and the origins of the enhanced phonon softening at the Eu^{3+} site remain unclear.

References

[1] A.O. Sushkov, S. Eckel and S.K. Lamoreaux, Phys. Rev. A 81 (2010) 022104.

[2] G. Shirane et al.. Phys. Rev. **105** (1957) 856

[3] V.G. Bhide and M.S. Hedge, Phys. Rev. **B5** (1972) 3488

Density of Phonon States at the Fe Sites in Superconducting FeSe as Function of Temperature and Pressure

V. Ksenofontov[1], G. Wortmann[2*], A.I. Chumakov[3], T. Gasi[1], S. Medvedev[1,4], T.M. McQueen[5], R.J. Cava[5], and C. Felser[1]

[1] *Institut Anorg. Analyt. Chemie, Universität Mainz, D-55099 Mainz, Germany*
[2] *Department Physik, Universität Paderborn, D-33095 Paderborn, Germany*
[3] *European Synchrotron Radiation Facility, BP220, F-38043 Grenoble Cedex, France*
[4] *Max-Planck-Institute for Chemistry, D-55128 Mainz, Germany*
[5] *Department of Chemistry, Princeton University, Princeton NJ 08544, USA*

The temperature and pressure dependence of the partial density-of-phonon states (phonon-DOS) at the iron sites in superconducting (sc) $Fe_{1.01}Se$ was studied by ^{57}Fe nuclear inelastic scattering (NIS) of synchrotron radiation, a method well adapted for these studies as function of temperature and pressure [1,2]. As proved by a recent study of the isotope effect at the Fe sites on the sc temperature T_c in FeSe, superconductivity is intrinsically connected with the Fe phonon modes [3]. The sc properties of the present $Fe_{1.01}Se$ sample and their pressure dependencies were well characterized in previous studies using various methods, including ^{57}Fe-Mössbauer spectroscopy [4-7]. The high energy resolution in the present ^{57}Fe-NIS study allows for a detailed observation of spectral properties in the phonon-DOS not observed before, e.g. shifts of all spectral features to higher energies by ~4% with decreasing temperature from 296 K to 10 K. No detectable changes in the partial Fe phonon-DOS were observed at the tetragonal–orthorhombic transition around 100 K [7,8]. An applied pressure of 6.7 GPa, combined with an increase of the sc temperature T_c from 8 K to 34 K [8], resulted in an increase of the optical phonon-mode energies by ~12%, and an even more pronounced increase in energies of the lowest-lying transversal acoustic modes. Despite of these strong pressure-induced changes in the partial Fe phonon-DOS we conclude that the pronounced increase of T_c in $Fe_{1.01}Se$ with pressure cannot be described in the framework of classical electron-phonon coupling [8]. This suggests the importance of spin fluctuations for the observed superconductivity [9]. The present results are discussed in conjunction with the phonon-DOS of $FeSe_{0.5}Te_{0.5}$ X-tals, studied including its polarization dependence by ^{57}Fe-NIS [10], where T_c = 15 K was observed at ambient pressure. Finally we present a synopsis of the complementary information on the sc $Fe_{1.01}Se$ and $FeSe_{0.5}Te_{0.5}$ systems, obtained from the elastic channel, ^{57}Fe-ME [4-7], as well as from the inelastic channel, ^{57}Fe-NIS [8, 10], of the ^{57}Fe(14.4 keV)-Mössbauer resonance.

References:

[*] *wortmann@physik.upb.de*

[1] A.I. Chumakov et al., Phys. Rev. B 54, R9596 (1996).
[2] R. Lübbers, H.F. Grünsteudel, A.I. Chumakov, G. Wortmann, Science 287, 1250 (2000).
[3] R. Khasanov et al., arXiv:1002.2510.v1.
[4] T.M. McQueen et al., Phys. Rev. B 79, 014522 (2009).
[5] S. Medvedev et al., *Nature Mater.* ***8****, 630 (2009).*
[6] V. Ksenofontov et al., contribution to this conference.
[7] T.M. McQueen et al., Phys. Rev. Lett. 103, 057002 (2009).
[8] V. Ksenofontov et al., Phys. Rev. B (in print); see arXiv:1004.2007.
[9] T. Imai et al., Phys. Rev. Lett. 102, 177005 (2009).
[10] V. Ksenofontov, G. Wortmann, T. Gasi, J. Deisenhofer, V. Tsurkan, C. Felser (unpublished)

μSR studies of High-Tc superconductivity in iron pnictides

H.-H. Klauss
Technische Universität Dresden, Germany
h.klauss@physik.tu-dresden.de

We have determined the electronic phase diagrams of several iron pnictide high-T_c superconductors based on the ROFeAs (1111 family) with electron Flour and isovalent Phosphorus doping and (Sr,Eu)Fe_2As_2 (122 family) with Cobalt doping. The nature of the change from the magnetically ordered to the superconducting state in $LaO_{1-x}F_xFeAs$ was determined by means of x-ray scattering, μSR and Moessbauer spectroscopy [1-3]. The results prove an important role of the structural orthorhombic distortion disappearing exactly at the SDW magnetism and superconductivity phase boundary accompanied by a delicate nanoscale order revealed recently from NMR.

Superconductivity and the interplay of iron and rare earth magnetic order in the iron-pnictide systems $RO_{1-x}F_xFeAs$ and $ROFeAs_{1-x}P_x$ with R=Ce, Gd, Pr, Sm has been studied by μSR, Moessbauer spectroscopy and high resolution XRD. We find that the undoped compounds show very different magnetic coupling strength of the rare earth ion to the antiferromagnetic iron layers ranging from independent order to strong polarization of the rare earth moments by the ordered iron [4]. Similar to $LaO_{1-x}F_xFeAs$ the orthorhombic phase transition in $REO_{1-x}F_xFeAs$ is also intimately connected to the suppression of magnetic order and the appearance of superconductivity.

Finally, we present recent studies on (Ba,Sr,Eu)Fe_2As_2 based pnictide superconductors. We present a quantitative description of coexistence of magnetism and superconductivity from combined ARPES and μSR measurements and the anisotropy of the electronic properties determined in these single crystal studies [5].

References:

[1] H.Luetkens, H.-H. Klauss et al., Phys. Rev. Lett.,101 (097009), 2008
[2] H.-H. Klauss, H. Luetkens et al., Phys. Rev. Lett., 101 (077005), 2008
[3] H. Luetkens, H.-H. Klauss et al., Nature Materials, 8 (305), 2009
[4] H. Maeter et al., Phys. Rev. B 80 (094524), 2009
[5] R. Khasanov et al., Phys. Rev. Lett., 102 (187005), 2009

Applications of perturbed angular correlation (PAC) of γ-rays spectroscopy in biological systems

Lars Hemmingsen

Department of Basic Sciences and Environment, Faculty of Life Sciences, University of Copenhagen,
Thorvaldsensvej 40, 1871 Frederiksberg C, Denmark, lhe@life.ku.dk

PAC spectroscopy was first applied in biochemistry in 1968, in a study of serum albumin [1]. Over the following 4 decades a number of publications have appeared, demonstrating that PAC spectroscopy is a useful tool for the study of biomolecules [2]. Selected applications of PAC spectroscopy in will be presented, with a particular focus on the biological role of metal ions in catalysis, protein structure and folding, design of heavy metal ion binding proteins, protein-protein interaction in photosynthesis.

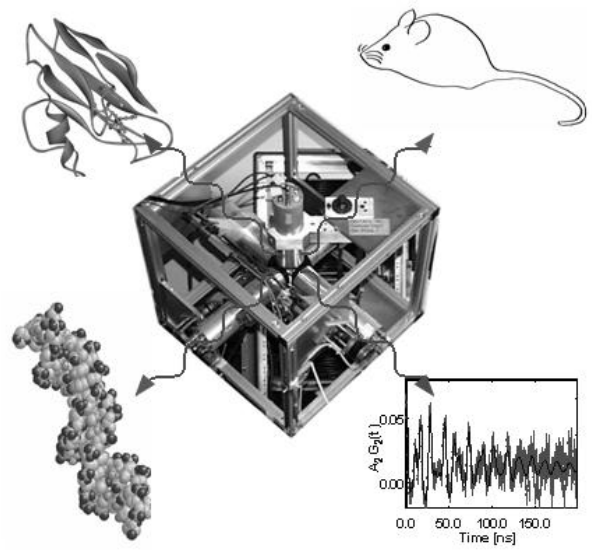


Figure 1. *PAC instrument at the centre and illustration of γ-rays emitted in various directions. The γ-rays point to experimental data (lover right), and three applications in biochemistry: DNA (lower left), a protein (upper left), and in vivo experiment (upper right).*

References

[1] T.K. Leipert, J.D. Baldeschwieler, D.A. Shirley, Nature 1968, 220, 907-909.
[2] Hemmingsen L., Sas K.N., Danielsen E., Chem. Rev. 2004, 104, 4027-4062.

Ab Initio Hyperfine Interactions as a Powerful Tool to Identify the Metal Binding Site in Biological Systems: Cd^{2+} in DNA Bases.

Philippe Alexandre Divina Petersen (1), M.B.Gonçalves (1), H.M.Petrilli (1),
A. dos Santos Silva(2), A.L. Lapolli (2), A.W. Carbonari (2)

(1) Universidade de São Paulo, Instituto de Física, Departamento de Física de Materiais e Mecânica DFMT.
e-mail:petersen@if.usp.br
(2) Instituto de Pesquisas Energéticas e Nucleares, IPEN, São Paulo

Hyperfine interactions can be a powerful tool to identify local environments in many different systems. Recently it has been drawn attention to the possible application of the Time Differential Perturbed Angular Correlation (TDPAC) technique to study differences in the Nuclear Quadrupole Coupling constants (υ_Q) at Cd probes in mouse DNA infected with the *Trypanosoma Cruzi*. The electric contribution to the hyperfine interaction is usually expressed as the nuclear quadrupole coupling frequency υ_Q which is given by the product of the nuclear quadrupole moment Q and the Electric Field Gradient (EFG) at the nucleus. The EFG can be theoretically obtained from an *ab initio* electronic structure calculation. The $^{111}In \rightarrow {}^{111}Cd$ β decay can be used in a TDPAC measurement to investigate the Cd metal binding to DNA. The interaction of the metal with the DNA bases can change many aspects of the base pairing [1]. Here we study electric hyperfine properties of Cd bound to some DNA bases. The methodology used for the electronic structure calculations is based on the Kohn Sham [2] scheme of the Density Functional Theory (DFT) and the Car-Parrinello [3] method. We use the Projector Augmented Wave [4] method as embodied in the (CP-PAW) computational code. The results of EFG and energies are discussed as function of water molecules present in the Cd^{2+} environment and compared with TDPAC measurements at Cd probes in mouse DNA infected with the *Trypanosoma Cruzi*.

References

[1] J. V. Burda, J. Sponer, J. Leszczynski, P. Hobza, *J. Phys. Chem. B.*, 101, 9670 (1997).
[2] W. Kohn, L. J. Sham, *Phys. Rev. B.*, 140, 1133 (1965).
[3] P. E. Blöchl, *Phys. Rev. B.*, 50, 17953 (1994).
[4] R. Car e M. Parrinello, *Phys. Rev. Lett.* 55, 2493 (1985).

Recent advances in Emission Channeling measurements and relevance to Hyperfine Interactions

J. G. Correia and U. Wahl

ITN, Instituto Tecnológico e Nuclear, Sacavém, Portugal

Hyperfine interactions are due to the coupling of the nuclear quadrupole and magnetic moments with the electric field gradient and magnetic fields present inside a material, respectively. “Hyperfine Techniques” can then deliver unique information to enlighten atomic and electronic phenomenology on a nanoscopic scale, provided their signal will be fitted with the right model and then properly interpreted. During the last two decades big advances have been made for the interpretation of hyperfine data. Powerful first principle calculation methods of charge densities in materials provide today reliable tools for the interpretation of hyperfine parameters. Still, these methods rely on establishing an atomic model with the only input of the initial atomic coordinates, which are then allowed to relax to more energetically favorable positions. This brings us to the point that, since the hyperfine parameters are extremely sensitive to both relaxations and the atomic position of the probing atom, a technique that can provide precise local scale information about impurity element position can be of great use for the modeling of the atomic configurations used to interpret the hyperfine parameters.

This talk introduces the emission channeling (EC) technique, which uses the fact that charged particles (in this case electrons), emitted from implanted radioactive isotopes, are guided by the potential of atomic rows and planes while traveling through a single crystal. The resulting anisotropic electron emission patterns around low-index crystal directions are characteristic for the lattice site occupied by the emitting atom and are measured with a 2-dimensional energy- and position-sensitive Si detector of 22 × 22 pixels. This technique allows one to measure the lattice location of a very low concentration of impurities with accuracy down to 0.1 Å. The combination of position sensitive detectors developed at CERN in the frame of high-energy particle detection with the ISOLDE radioactive beam facility provides a huge number of radioactive element probes to be measured with high precision. Selected case study examples will be shown as well as the perspectives for improving this technique with new highly pixilated electron detectors recently developed at CERN.

Precise Nuclear Moments of Extremely Proton-Rich Nuclei ^{23}Al

T. Nagatomo,[1, 3] **K. Matsuta,**[2] **H. Ueno,**[3] **M. Mihara,**[2] **A. Yoshimi,**[3] **Y. Ichikawa,**[3]
K. Yamada,[3] **H. Kawamura,**[3] **A. Ozawa,**[4] **T. Moriguchi,**[4] **Y. Ishibashi,**[4] **K. Asahi,**[5]
M. Uchida,[5] **K. Suzuki,**[5] **T. Inoue,**[5] **Y. Hasama,**[5] **H. Iijima,**[5] **T. Sumikama**[6]
and T. Minamisono[7]

[1] *International Christian University, Osawa 3-10-2, Mitaka, Tokyo 181-8585, Japan, e-mail: nagatomo@nt.icu.ac.jp*
[2] *Osaka University, Machikaneyama 1-1, Toyonaka, Osaka 560-0043, Japan*
[3] *RIKEN Nishina Center, Hirosawa 2-1, Wako, Saitama 351-0198, Japan*
[4] *University of Tsukuba, Tennodai 1-1-1, Tsukuba, Ibaraki 305-8577, Japan*
[5] *Tokyo Institute of Technology, Ookayama 2-12-1, Meguro-ku, Tokyo 152-8550, Japan*
[6] *Tokyo University of Science, Yamazaki 2641, Noda, Chiba 278-8510, Japan*
[7] *Fukui University of Technology, Gakuen 3-6-1, Fukui, Fukui 910-8505, Japan*

Nuclear magnetic moment μ and the electric quadrupole moment Q of the ground state of ^{23}Al have been precisely measured by the β-NMR/NQR technique. The one-proton-separation energy of ^{23}Al is very small (125 keV) and so ^{23}Al is expected to have an exotic structure. Recently, a large reaction cross section of ^{23}Al at the intermediate energy (~36*A* MeV) was reported [1,2] and that indicated the possibility of the proton-halo structure of ^{23}Al. In previous work, we successfully obtained NMR signal of ^{23}Al in a Si single crystal which had enough precision to determine the spin and parity of the ground state as $I^{\pi} = 5/2^{+}$ [3]. In present work, we have remarkably improved the precision of $\mu(^{23}\mathrm{Al})$ and have obtained the quadrupole coupling constant *eqQ* of ^{23}Al in Al_2O_3 for the first time to discuss details of the nuclear structure.

Experiment was performed at RIKEN Nishina Center. Unstable ^{23}Al beam were produced through high-energy nuclear collisions of 100*A* MeV $^{24}Mg^{12+}$ ions and ^{9}Be. The nuclear spin polarization of ^{23}Al were produced by restriction of the outgoing momentum and the emission angle relative to the primary beam by utilizing the projectile-fragment separator RIPS at RIKEN. After the separation, the polarized ^{23}Al ions (~ 90% purity) were implanted into single crystals of Si and α-Al_2O_3 for the μ and Q measurements, respectively. By use of the β-NMR/NQR method at the room temperature, we have precisely determined the μ moment as $|\mu| = 3.8881(14)$ μ_N, and Q moment as $|Q| = 168(10)$ mb as shown in Fig. 1 together with the best-fit-shape function. From the results, we will discuss the possible nuclear structure of ^{23}Al by comparison with the mirror nuclei ^{23}Ne and the other nuclei which locates around ^{23}Al such as ^{22}Mg that is known to have well-deformed structure.

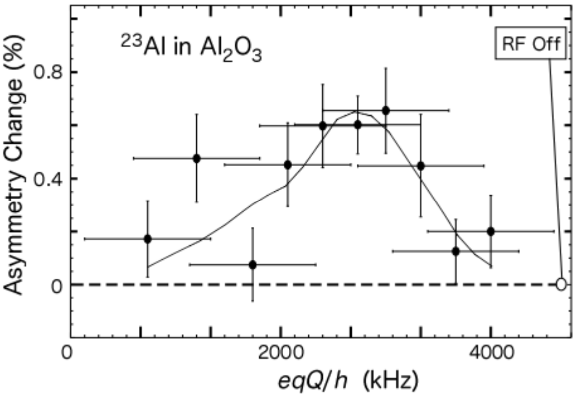


Fig.1 Obtained β-NQR spectrum of ^{23}Al in Al_2O_3
at room temperature.

References
[1] X.Z. Cai et al., *Phys. Rev. C* **65**, 024610 (2002).
[2] H.Y. Zhang et al., *Nucl. Phys. A* **707**, 303 (2002).
[3] A. Ozawa et al., *Phys. Rev. C* **74**, 021301(R) (2006).

^{14}N NQR study of proton position and dynamics in some hydrogen bonded organic ferroelectrics

Janez Seliger[1,2], Veselko Ţagar[1], Tetsuo Asaji[3]

[1] *"Jozef Stefan" Institute, Jamova 39, 1000 Ljubljana, Slovenia, e-mail: janez.seliger@fmf.uni-lj.si*
[2] *Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia*
[3] *Department of Chemistry, College of Humanities and Sciences, NihonUniversity, Sakurajosui 3-25-40, Setagaya-ku, Tokyo 156-8550, Japan*

Three hydrogen bonded organic systems: phenazine–chloranilic acid (1:1), 1,2-diazine–chloranilic acid (2 : 1) and 2,3,5,6-tetra(2'-pyridyl)pyrazine-chloranilic acid (1:2) have been recently studied by ^{14}N nuclear quadrupole resonance (NQR). Several ^{1}H-^{14}N nuclear quadrupole double resonance techniques have been used to obtain the ^{14}N NQR spectra.

In phenazine-chloranilic acid (1:1) the ^{14}N NQR parameters suggest that donor orbital populations of the two nitrogen atoms in a phenazine molecule become nonequivalent in the ferroelectric phase below $T_c = 253$ K, while they are both equal in the paraelectric phase. In the deuterated compound besides the ferroelectric transition at $T_c = 286$ K, a neutral to ionic transition was found at T = 188 K associated with the proton transfer from chloranilic acid to phenazine.

Protons involved in the H-bond system in 1,2-diazine–chloranilic acid (2 : 1) are assumed to be in jumping motion in the double-minimum potential corresponding to the two extreme electronic states of O-H…N and O^{-}…H-N^{+}. The ^{14}N nuclear quadrupole coupling tensor is used to determine the population of the states. The NQR data suggest that not only the population but also the electron distribution of the extreme electronic states itself changes with temperature.

The complete ^{14}N nuclear quadrupole resonance spectrum has been measured in ferroelectric and paraelectric 2,3,5,6-tetra(2'-pyridyl)pyrazine-chloranilic acid (1:2) The quadrupole coupling tensors are assigned to various nitrogen positions in the crystal structure. Two types of asymmetric N-H…N hydrogen bonds are observed in the ferroelectric phase. A slow dynamics influencing the ^{14}N NQR spectrum and relaxation has been observed in the paraelectric phase. The analysis of the ^{14}N NQR spectra in the paraelectric phase shows that above T^{c} each hydrogen bond exchanges between the two types observed in the ferroelectric phase. The change of the type of hydrogen bond is associated with the transfer of protons within the bond.

References

[1] T. Asaji et al., *J. Phys.: Condens. Matter* **19,** 226203 (2007)
[2] J. Seliger et al., *Phys. Chem. Chem. Phys.* **11**, 2281 (2009)
[3] J. Seliger et al., *Phys. Chem. Chem. Phys.*, 12, 3254 (2010)

Entanglement in nuclear quadrupole resonance

Gregory Furman[1] Victor Meerovich[1], Vladimir Sokolovsky[1]

[1] Physics Department, Ben Gurion University, P.O.B. 653, Beer Sheva, 84105,

e-mail: gregoryf@bgu.ac.il

Quantum systems in an entangled state [1] can be used as a primary quantum information channel to perform computational [2], communicational [3], metrological [4, 5] and cryptographic tasks that are impossible for classical systems. These possible applications of entangled quantum states stimulate intensive research in the fields of generation and manipulation of them. Entangled states may appear in various systems of interacting quantum particles, such as phonons, ions, electron, nuclear spins, and of a single particle interacting with environment.

We study entanglement between quantum states of multi level spin system of a single particle considering a nucleus with spin 3/2 in both the internal electric field gradient and the external magnetic field. It was shown that entanglement is achieved by applying a magnetic field to a single particle at low temperature (5 mK). In this temperature range, the numerical calculation revealed the coincidence between magnetization and concurrence. As a result, the magnetization can be used as an entanglement witness for such systems.

References

[1] C. H.Bennett , G.Brassard , C.Crepeau , R.Jozsa , A.Peres , and W. K.Wootters , Phys. Rev. Lett. 70, 1895 (1993).
[2] C.H. Bennett and G.Brassard , Proceedings of IEEE International Conference on Computers, Systems and Signal Processing, Bangalore, India, pp. 175-179, December 1984.
[3] P.Shor, in Proceedings of 35th Annual Symposium on the Foundations of Computer Science (IEEE Computer Society, Los Alamitos, CA, 1994), p. 124-134.
[4] P. Cappellaro , J. Emerson , N. Boulant , C. Ramanathan , S. Lloyd , and D. G. Cory , Phys. Rev. Lett., 94, 020502 (2005).
[5] C.F.Roos, K.Kim, M.Riebe, R. Blatt, Nature 443, 316 (2006).

Proton Dynamics in One-dimensional Hydrogen-bonding System in Molecular Co-crystals TMP-D_2ca and DMP-H_2ca

T. Asaji[1], **D. Amino**[1], **N. Tago**[1], **M. Mizuno**[2]

[1] *Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo 156-8550, Japan, e-mail: asaji@chs.nihon-u.ac.jp*

[2] *Department of Chemistry, Graduate School of Natural Science & Technology, Kanazawa University, Kanazawa 920-1192, Japan*

Recently, hydrogen-bonded supramolecular co-crystals have attracted much interest in aim for functional materials such as ferroelectrics [1]. By use of ^{35}Cl nuclear quadrupole resonance (NQR) we have studied an organic ferroelectric, phenazine(Phz)-chloranilic acid (H_2ca) co-crystal, Phz-H_2ca, and found an electric field gradient fluctuation probably due to a proton dynamics in hydrogen bond [2]. For the detection of rather slow motion of proton in the hydrogen-bonding system, NQR spin-lattice relaxation of the nearby atom will be quite sensitive. In the co-crystal of tetramethylpyrazine (TMP) with H_2ca, TMP-H_2ca, the spin-lattice relaxation time (T_1) of ^{35}Cl NQR showed a steep decrease with increasing temperature above *ca.* 250 K. The decrease could be explained by the Arrhenius law with the activation energy of 35 kJ mol^{-1} [3]. In the present paper we studied a possible proton motion in another compound with a similar one-dimensional hydrogen bond, DMP-H_2ca, the co-crystal between 2,6-dimethylpyrazine (DMP) and H_2ca. The isotope effect on the hydrogen motion by deuteration of the acid hydrogen in TMP-H_2ca was also studied. Fig. 1 shows temperature dependence of ^{35}Cl T_1 of TMP-D_2ca compared with that of TMP-H_2ca. By the deuteration the activation energy increased to 50 kJ mol^{-1}. The deuteron motion was confirmed by ^{2}H NMR spin-lattice relaxation measurements which resulted in the activation energy of 49 kJ mol^{-1}. Fig. 2 shows temperature dependence of ^{35}Cl T_1 of DMP-H_2ca. In this compound the relaxation is dominated by lattice vibration suggesting no transfer motion of proton between the acid and base molecules.

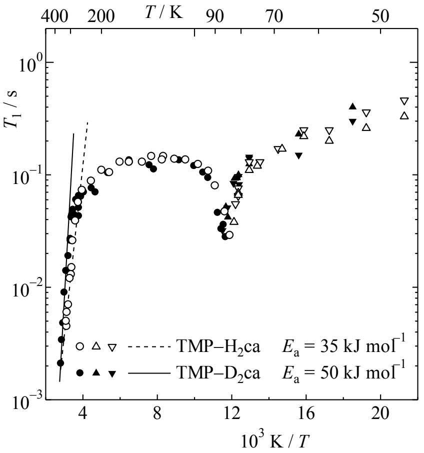


Fig. 1 ^{35}Cl NQR T_1 of TMP-H_2ca.

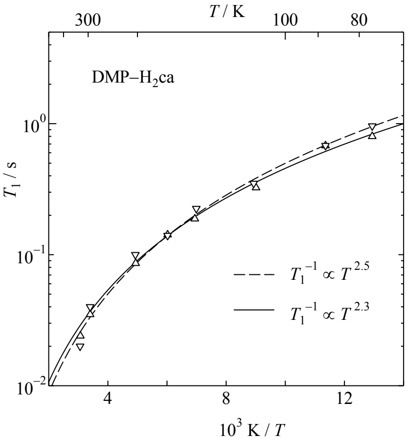


Fig. 2 ^{35}Cl NQR T_1 of DMP-H_2ca.

References

[1] S. Horiuchi and Y. Tokura, *Nature Materials* **7**, 357-366 (2008).

[2] T. Asaji, J. Seliger, V. Ţagar, M. Sekiguchi, J. Watanabe, K. Gotoh, H. Ishida, S. Vrtnik, and J. Dolinšek, *J. Phys.: Condens. Matter* **19**, 226203 (2007).

[3] T. Asaji, Y. Yoshimura, and D. Amino, *Hyperfine Interact.* **179**, 1-7 (2007).

DFT Study of Hyperfine Interactions in Some Types of the Complexes

O. Kh. Poleshchuk, **N. O. Khramova, A. V. Fateev**

Tomsk State Pedagogical University, 634041, Komsomolskii 75, Tomsk, Russia,
e-mail: poleshch@tspu.edu.ru

Structure and bonding in Lewis acid-base complexes has long been a subject of much chemical interest. Clearly, notions of intrinsic strength and compatibility of the acid and base should be important, and basic chemical ideas relating to acidity and basicity are expected to apply. Central to most simple theories of Lewis acidity is the idea that both ionic and covalent interactions play important roles in stabilizing the donor-acceptor bond [1].

In this report, we present a DFT calculations based on a microwave spectroscopic, nuclear quadrupole resonance and Mössbauer investigation of the donor-acceptor complexes formed from metal halides such as $PtCl_2$, $PtCl_4$, XeF_2, AuCl, AgCl, $SbCl_5$, $SnCl_4$, $TiCl_4$, $SnBr_4$, $NbCl_5$, $TaCl_5$, ICl, I_2, IBr with organic ligands. All ligands have a different basicity and softness. Therefore, it is of interest to investigate these complexes with a different acids and to compare their structural and electronic properties.

The full optimisation of geometry was carried out using some DFT functionals achieved within the GAUSSIAN'03 program. The calculations of the complexes were carried out with different basis sets: SDD, DGDZVP and 3-21G*. The quadrupole coupling constants of the central atoms and the formation energy of some of the complexes has been broken down using the extended transition state (ETS) scheme implemented in the ADF package. There are bases to consider, that the relativistic effects basic for such heavy atoms should be considered by the zero order regular approximation (ZORA) that is more reliable than the widely used Pauli formalism.

An analysis of the quality of the calculations that employ pseudo-potentials and all-electron basis sets for the halogen compounds was carried out. The ZORA method is shown to be a viable alternative for the calculation of halogen coupling constants in molecules [2]. In addition, the ZORA model, in contrast to the pseudo-potential model, leads to realistic values of all metal nuclear quadrupole coupling constants [3].

The calculated energy terms can be identified with three main components of the chemical bond, i.e. Pauli repulsion, electrostatic attraction and covalent interaction. As a result, we receive the answer to a question about the relative contributions of covalent and electrostatic interactions to the donor-acceptor bond. If for the transition element complexes the electrostatic bonding is larger than covalent bonding while for the non-transition element complexes the tendency opposite.

In the language of the theory of hard and soft acids and bases, the calculated energy gaps involve direct mixing of the donor and acceptor orbitals. Energy of the bonds, calculated from the general energy of molecules with ZPE corresponded as formation energy of the ETS scheme, and to experimental enthalpy of the complex formation. The electron density on the nucleus obtained by our calculations substantially corresponded to the known Mössbauer data.

References

[1] G. Frenking., K. Wichmann et al., Coord. Chem. Rev. 238-239, 55 (2003).
[2] O. Kh. Poleshchuk, V. Branchadell, B. Brycki, A. V. Fateev, A. Legon, J. Mol. Struct. Theochem 760, 173 (2006).
[3] O. Kh. Poleshchuk, V. Branchadell, R. A. Ritter, A. V. Fateev, Hyperfine Interactions, 181, 27 (2008).

Low Temperature Nuclear Orientation Studies of the Magnetic Structures of $RNiAl_4$ in Applied Magnetic Fields

W.D. Hutchison,[1] K. Nishimura[2]

[1] *School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Australian Defence Force Academy, Canberra 2600, Australia, e-mail: w.hutchison@adfa.edu.au*
[2] *Graduate School of Science and Engineering, The University of Toyama, Toyama 930-8555, Japan, e-mail: nishi@eng.u-toyama.ac.jp*

The family of metamagnetic compounds $RNiAl_4$ (R = rare earth) exhibits a range of interesting magnetic behaviours. There are multiple magnetic phases, and crystal field driven differences in anisotropy and behaviour when different rare earth ions (R) are present in the compound. $TbNiAl_4$ is one illustrative example. It has two phase transitions (three phases) as a function of temperature in low applied magnetic field, and also at least three phases as a function of applied magnetic field at low temperature [1]. Aligned with the first of these field driven transitions is a large inverse magneto-caloric effect (MCE) [2]. Recent neutron diffraction studies carried out on single crystal $TbNiAl_4$, in applied magnetic fields, show the onset of an incommensurate antiferromagnetic ordered phase above the first field induced phase transition [3]. This observation vindicates the existence of the higher entropy state at higher applied field that is required for an inverse MCE but contradicts the predictions of other authors who suggest a spin flop transition [4].

Low Temperature Nuclear Orientation (LTNO) can also be usefully applied to $TbNiAl_4$ and other $RNiAl_4$ compounds to investigate magnetic structure. In the case of the Tb compound, neutron activation is used to create *in situ* ^{160}Tb LTNO probes. However, as we found recently, $TbNiAl_4$ crystals must be annealed after thermal neutron irradiation in order to remove damage and restore full gamma-ray anisotropy [5]. In this paper, we present new LTNO results for annealed $TbNiAl_4$, in applied fields extending to 9 tesla. These results support the model of magnetic struture revealed by the earlier neutron diffraction studies. LTNO is also applied to crystals of compounds with R = Nd and Pr. These additional studies magnetic fields sufficient to traverse the respective first metamagnetic transitions were also used and behaviours similar to the $TbNiAl_4$ case were observed.

References

[1] W.D. Hutchison, D.J. Goossens, K. Nishimura, K. Mori, Y. Isikawa, A.J. Studer, J. Magn. Magn. Mater. **301,** 352 (2006) and references therein.
[2] L. Li, K. Nishimura and W.D. Hutchison, Solid State Comm., **149**, 932-936 (2009).
[3] W.D. Hutchison *et. al.*, *in preparation*.
[4] T. Mizushima, Y. Isikawa, A. Mitsuda, K. Kobayasi, F. Ishikawa, T. Goto, S. Kawano, J. Magn. Magn. Mater. **272–276**, e475 (2004)
[5] W.D. Hutchison, D.H. Chaplin and K. Nishimura, Hyperfine Interactions, **177**, 38-43 (2007).

Perturbed angular correlation study of the magnetic and structural first-order phase transition in MnAs

J. N. Gonçalves[1], V. S. Amaral[1], A. M. L. Lopes[2], J. G. Correia[3], H. Haas[3]

[1] Departmento de Física and CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal
[2] CFNUL, Av. Prof. Gama Pinto 2, P-1699 Lisboa, Portugal
[3] Instituto Tecnológico e Nuclear, E.N. 10, 2686-953 Sacavém, Portugal

The MnAs compound[1] shows a first-order transition at ~42 °C, with structural (hexagonal-orthorhombic), magnetic (FM-PM) and electrical conductivity changes, and associated magnetocaloric, magnetoelastic and magnetoresistance effects. At ~120 °C it undergoes a second-order transition, becoming paramagnetic hexagonal. We report a study in the temperature range of -190-140 °C, using the γ- γ Perturbed Angular Correlation method, complemented by first principles calculations.
The radioactive ion probe ^{77}Se, with the double gamma decay cascade, implanted as ^{77}Br, at ISOLDE-CERN laboratory is used to determine the Electric Field Gradient (EFG) and Magnetic Hyperfine Field (MHF) across the first-order phase transition encompassing the pure and mixed phase regimes in cooling and heating cycles. In the hexagonal phase the spectra is determined by the MHF whereas in the orthorhombic phase MHF is zero. The fractions of each phase are determined as a function of temperature. The temperature irreversibility of the first-order phase transition is seen locally, at the local atomic scale sensitivity of the hyperfine field, by the hysteresis of the fractions of each phase, in agreement with macroscopic magnetization and X-ray powder diffraction measurements. The MHF of the hexagonal phase is the same at a given temperature, irrespective of measuring on cooling or heating the sample, even in the phase coexistence region. The values of hyperfine parameters obtained using first-principles density functional theory with the LAPW method (Wien2k code[2]) are compared with the experimental results, considering the Se probe at both Mn and As sites, with the clear assignment of the probe location to the As sites.

References

[1] We thank Prof. S. Gama for supplying the sample.
[2] Blaha P, Schwarz K, Madsen G, Kvasnicka D and Luitz J, 2001.
WIEN2k, an Augmented-Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Technische Universitat Wien (ISBN 3-9501031-1-2)

Anomalous Magnetism and ^{209}Bi Nuclear Spin Relaxation in $Bi_4Ge_3O_{12}$ Crystals

V.G. Orlov[1], E.A. Kravchenko[2], Tetsuo Asaji[3], G.S. Sergeev[1], Yu.F. Kargin[4], A.N. Vasil'ev[5], O.S. Volkova[5]

[1]*Russian Research Center "Kurchatov Institute", Moscow 123182, Russia*
E-mail: orlov@mbslab.kiae.ru
[2]*Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow 119991, Russia*
[3]*Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo 156-8550, Japan*
[4]*State Institute of Metallurgy and Material Science, Russian Academy of Sciences, Moscow 119991, Russia*
[5]*Moscow State University, Faculty of Physics, Moscow 119991, Russia*

Unique magnetic properties were earlier found by measuring the NQI parameters in a number of bismuth (III) oxy compounds with s- and p-electrons hitherto classified as diamagnetic [1]. In α-Bi_2O_3 single crystal the magnetoelectric effect and paramagnetism depending on magnetic prehistory of the sample were observed [1].

In $Bi_4Ge_3O_{12}$ (BGO), local magnetic fields (H_{loc}) of the order of 20-30 G were found by modeling the Zeeman split ^{209}Bi NQR spectra and spin-echo envelope [2-3]. A dramatic increase in the ^{209}Bi line intensity was observed for this compound in the Zeeman fields (H_e) hence revealing a remarkable elongation of the nuclear spin-spin relaxation time T_2 under the influence of H_e [4]. This stimulated relaxation studies of the BGO crystals doped with the "magnetic" atoms Cr, Nd, Pr, Gd.

Here, we present the results of a study of the ^{209}Bi nuclear quadrupole spin-spin and spin-lattice relaxation in pure and doped BGO single crystals in the temperature range 4.2−300 K.

Various mechanisms (quadrupole, crystal electric field, electron spin fluctuations) governing the temperature dependence of the spin-lattice relaxation time T_1 in pure and doped samples at different temperature ranges are considered.

Unlike T_1, the spin-spin relaxation time T_2 for pure and Nd-doped samples only weakly depended on temperature over the whole temperature range studied. Doping BGO with paramagnetic atoms strongly elongated T_2, the elongation being also observed under the influence of weak external magnetic fields.

The magnetization of doped BGO crystals vs. magnetic field and temperature was measured using a SQUID magnetometer. The temperature behavior of magnetic susceptibility for the Nd-doped BGO crystal evidenced for the presence of the crystal electric field effects. The curves of magnetization vs. magnetic field measured for the Gd-doped BGO crystal under field cooling and zero-field cooling conditions were markedly different, although this difference was less pronounced than that for the α-Bi_2O_3 crystal [1].

References

[1] E.A. Kravchenko, V.G. Orlov, and M.P. Shlykov, *Russian Chem. Rev.* 75, 77 (2006).
[2] E.A. Kravchenko, Yu.F. Kargin, V.G. Orlov, T. Okuda, K. Yamada, *JMMM*, 224, 249 (2001).
[3] E.A. Kravchenko, V.G. Orlov, V.G. Morgunov, M.P. Shlykov, *Hyperfine Interact.* 180, 437 (2007).
[4] E.A. Kravchenko, V.G. Morgunov, V.G. Orlov, Yu.F. Kargin, *JETP Letters*. 86, 390 (2007).

Summary:

The ^{209}Bi nuclear quadrupole spin-lattice and spin-spin relaxation were studied in the BGO single crystals which exhibit, as was previously found, anomalous magnetic properties. The results revealed unexpectedly strong influence on the relaxation processes of tiny amounts of paramagnetic atoms (0.1-0.5 mol%) inserted into the BGO crystals.

Friday 17th September (9:00-9:40), Theory: Hyperfine Interactions, Nuclear Moments

Calculations of Hyperfine parameters in solids based on DFT and using WIEN2k

Peter Blaha

Inst. Materials Chemistry, TU Vienna, A-1060 Vienna, Austria,
e-mail: pblaha@theochem.tuwien.ac.at

I will review briefly the underlying concepts of electronic structure calculations in solids and more specifically describe density functional theory and the APW+lo method as implemented in the WIEN2k code [1]. Special emphasis will be given to explain the calculations of isomer shifts, magnetic hyperfine fields and electric field gradients (EFG) and in particular I'll discuss how we can interpret the results and what we can learn from a particular hyperfine parameter. For the case of several fluoro-aluminates I'll demonstrate the strong dependency of the EFG (and even more of the asymmetry parameter η) on the exact atomic positions, which makes it mandatory to optimize the internal coordinates since often the experimentally determined positions are not accurate enough [2]. Mössbauer spectroscopy is also a very valuable tool to study matter under extreme conditions and recently [3] we could explain the large change of the EFG with pressure in (Mg,Fe)SiO_3, a very important material in the lower mantle of the earth. Finally I'll discuss EFGs, isomer shifts and hyperfine fields in $YBaFe_2O_5$ (Fig.1), a material which exhibits a Verwey transition between a charge-ordered and valence-mixed state [4] with temperature. During this transition the crystal structure, the magnetic order, the charge state and the hyperfine parameters change dramatically.

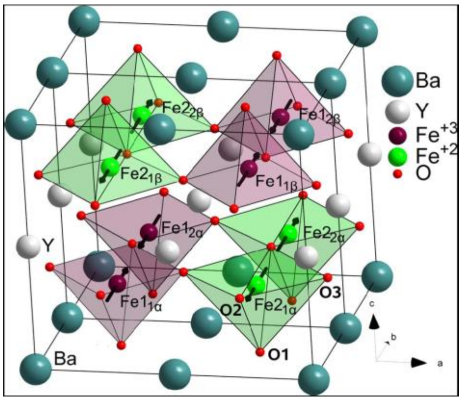


Fig. 1. Geometric and magnetic structure of the CO phase of $YBaFe_2O_5$

References

[1] P.Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J.Luitz, WIEN2K, an augmented plane wave+local orbitals program for calculating crystal properties, TU Vienna, Austria (2001). http://www.wien2k.at.
[2] M. Body, C. Legein, J. Buzare, G. Silly, P. Blaha, C. Martineau, F. Calvayrac: J. Phys.Chem. A, 111, 11873 (2007).
[3] H.Hsu, K.Umemoto, P.Blaha and R.Wentzcovitch, Earth Planet. Sci. Lett. 294, 19 (2010)
[4] C.Spiel, P.Blaha, K.Schwarz, Phys.Rev.B 79, 115123 (2009).

Electron penetration into the nucleus and its effect on the quadrupole interaction

Katrin Koch,[1] **Klaus Koepernik,**[2] **Dimitri Van Neck,**[3] **Helge Rosner,**[1] **Stefaan Cottenier**[3]

[1] Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, DE-01187 Dresden, Germany, e-mail: katrinkoch79@googlemail.com
[2] IFW Dresden, Institute for Solid State Research, P.O. Box 270116, DE-01171 Dresden, Germany
[3] Center for Molecular Modeling, Ghent University, Technologiepark 903, BE-9052 Zwijnaarde, Belgium, e-mail: Stefaan.Cottenier@ugent.be

A series expansion of the interaction between a nucleus and its surrounding electron distribution provides terms that are well-known in the study of hyperfine interactions: the familiar quadrupole interaction and the less familiar hexadecapole interaction. If the penetration of electrons into the nucleus is taken into account, various corrections to these multipole interactions appear. The best known correction is a scalar term related to the isotope shift and the isomer shift. This contribution discusses a related tensor correction, which modifies the quadrupole interaction if electrons penetrate the nucleus: the quadrupole shift. We describe the mathematical formalism and provide first-principles calculations of the quadrupole shift for a large set of solids. Fully relativistic calculations that explicitly take a finite nucleus into account turn out to be mandatory. Our analysis shows that the quadrupole shift becomes appreciably large for heavy elements. Implications for experimental high-precision studies of quadrupole interactions and quadrupole moment ratios are discussed.

This contribution brings alive the analysis that is reported in Ref. [1], updated with very recent experimental follow-up work [2].

References
[1] K. Koch, K. Koepernik, D. Van Neck, H. Rosner, S. Cottenier, Physical Review A 81 (2010) 032507
[2] D. Dewald, J. Grabow, in preparation.

Quadrupole interaction in the solid halogens – a new (not final) look

H. Haas[1]

[1] Instituto Tecnológico e Nuclear, Estrada Nacional 10, P-2685 Sacavém, Portugal, and
CERN/EP-SC, CH-1211 Geneve-23, Switzerland, e-mail: heinz haas@cern.ch

The nuclear quadrupole interaction in the molecular crystals of chlorine, bromine and iodine has been studied very early after the introduction of the NQR method. One should thus believe that precise experimental results are available. It will be argued here that for Cl_2 and Br_2 this is not the case at all.

Obviously several attempts on interpreting the existing data have been made. Actually already in the first theoretical analysis [1] doubts on the results for solid Br have been raised, but afterwards ignored. In a pioneering work really free from parameters the EFG for solid Cl_2, Br_2 and I_2 was calculated with the density functional method FLAPW [2]. The comparison of the calculated asymmetry parameters η with experiment was inconclusive, however.

The intermolecular interaction that creates η also will have an influence on the interaction frequency when compared to the free molecule value ν_0. Since precise experimental data for this shift $\delta\nu/\nu_0$ are available, here an attempt is described to treat both effects on the same footing. The same method previously used to determine the halogen nuclear quadrupole moments [3] was therefore applied to the free halogen molecules and the solids. The results are summarized in Table 1:

Table1: Calculated EFG (10^{21} V/m^2) and derived frequency shift compared to experimental shift; calculated η compared to published and estimated "corrected" value

	Cl_2	Br_2	I_2
EFG(mol)	57.3	113.0	152.9
EFG(sol)	54.1	97.9	120.0
$\delta\nu/\nu_0$(cal)	0.055	0.134	0.215
$\delta\nu/\nu_0$(exp)	0.025	0.055	0.119
η(cal)	0.071	0.183	0.318
η(pub)	0.0-0.2	0.200	0.175
η(cor)	0.033	0.076	0.176

It is obvious that the FLAPW calculations overestimate the frequency shift by a factor of about 2 in all three cases. It is thus extremely likely that the same holds also for η. Under the assumption that the degree of overestimation for $\delta\nu/\nu_0$ and η is the same, "corrected" values for η may be obtained. This results in a perfect agreement with the precisely known value for I_2. It could be demonstrated with FLAPW calculations of expanded unit cells that the effects of the intermolecular interaction on $\delta\nu/\nu_0$ and η are correlated. From these calculations also for the first time a realistic theoretical result for the sublimation enthalpies is obtained. It may be hoped that the interpretation presented here will act as a stimulus for new experiments and theoretical treatments that can describe the intermolecular interaction better than FLAPW.

References

[1] R. Bersohn, *J. Chem. Phys.* 36, 3445 (1962)
[2] P. Blaha and K. Schwarz, *J. Mol. Struct. (Theochem)* 261, 355 (1992)
[3] H. Haas and H.M. Petrilli, *Phys. Rev. B* 61, 13588 (2000)

A-priori calculations of hyperfine interactions in highly ionized atoms: g-factor measurements of pico-second states populated in nuclear reactions.

N. J. Stone,[1,2] J. R. Stone[1,2], P. Jonsson[3] and C. Froese Fischer[4]

[1] University of Oxford, OX1 3PU Oxford, UK e-mail: n.stone@physics.ox.ac.uk
[2] University of Tennessee, Knoxville TN 37996, USA
[3]Malmo University, S-20506 Malmo, Sweden
[4]NIST, Gaithersburg, MD 20899, USA

The recoil-in-vacuum [RIV] method, which uses attenuation of angular distributions to measure nuclear excited state g-factors, has been shown, in a recent experiment on a ^{132}Te beam, to offer attractive possibilities for application with radioactive ion beams [RIBs] when combined with modern detector arrays [1]. The more usual Transient Field method struggles with limited beam intensity [2]. The magnetic hyperfine interaction acting on the nuclei of the recoiling ions was calibrated using states of known lifetime and g-factor. It is of clear importance to establish how these interactions vary with element and ionization state in order to discover how the RIV approach may be best utilized. The ability to calculate lifetimes and hyperfine interaction strengths in complex electronic levels of multiply ionized atoms has advanced markedly with modern computation techniques. Dirac-Hartree-Fock multi-configuration model [3] calculations, applied to systems ranging from 5-electron Fe ions to 23-electron Te ions will be presented. The results, compared with recent RIV experiments, show great promise that such calculations can provide parameter free, a-priori, calibrations for RIV experiments. The calculations are readily adapted to any nuclear level spin, allowing extension of measurement beyond the usual 2^+, 4^+ states of even-even isotopes to levels in odd-A and odd-odd isotopes.

Projected experiments based not only on Coulomb excitation, but also on fusion reactions and fission fragments will be described.

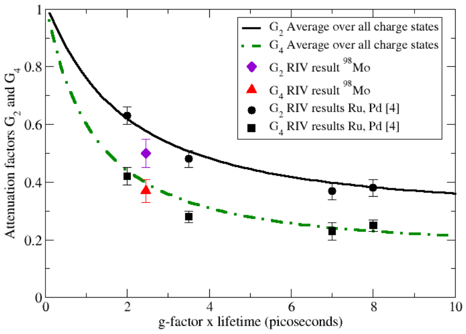


Fig. 1. Calculated and measured [4] attenuation coefficients for Pd, Ru and Mo ions.

References

[1] N.J.Stone et al., *Phys.Rev.Lett.* 94, 192501 (2005) .
[2] N.Benczer-Koller et al., *Phys.Lett.* 664, 241 (2008).
[3] P.Jonsson et al., Comp.Phys.Com. 177, 597 (2007).
[4] A.E.Stuchbery, private communication, 2010

Electric field gradient calculations by quantum chemical methods

Vladimir Kellö

Department of Physical Chemistry, Comenius University, SK-842 15 Bratislava, Slovakia

The electric field gradient, which from the point of view of the given nucleus is a measure of the inhomogeneity of the external electric field of all other charges, is a molecular property of the first order and can be determined from the knowledge of the electronic wave function and positions of nuclei. Since for accurate calculations we have to use highly sophisticated electron correlation approximations like the Coupled Cluster Singles and Doubles with non-iterative Triples CCSD(T) method, which does not fulfill the Hellmann-Fyenman theorem, and therefore we are forced to use so-called derivatives methods instead of calculating the expectation value of the given operator. Inclusion of relativistic effects in calculation of electric field gradients is inevitable [1]. If one– or two–component relativistic methods (*e.g.* DKH, IOTC) are exploited, the usual method of computing, which is just a counterpart of the nonrelativistic scheme leads to the change of picture effect [2] manifested by significant inaccuracies of the calculated property values. Different techniques how to avoid the change of picture effect will be discussed [3-5].

The combination of experimental nuclear quadrupole coupling constant obtained from microwave spectra and theoretical electric field gradient provides currently the best source of nuclear quadrupole moment values, at least for light elements. A series of such determinations of nuclear quadrupole moments will be presented [6-11].

References:

[1] M. Iliaš, V. Kellö, M. Urban; Acta Phys. Slovaca, in press.
[2] V. Kellö, A. J. Sadlej; Int. J. Quantum Chem., **68**, 159 (1998).
[3] M. Pernpointner, M. Seth, P. Schwerdtfeger; J. Chem. Phys., **108**, 6722 (1998).
[4] V. Kellö, A. J. Sadlej; J. Chem. Phys., **112**, 522 (2000).
[5] V. Kellö, A. J. Sadlej; J. Chem. Phys., **120**, 9424 (2004).
[6] V. Kellö, A. J. Sadlej, P. Pyykkö, D. Sundholm, M. Tokman; Chem. Phys. Letters, **304**, 414 (1999).
[7] V. Kellö, A. J. Sadlej; Mol. Phys., **96**, 275 (1999).
[8] V. Kellö, P. Pyykkö, A. J. Sadlej, P. Schwerdtfeger, J. Thyssen; Chem. Phys. Letters, **318**, 222 (2000).
[9] J. Bierroń, P. Pyykkö, D. Sundholm, V. Kellö, A. J. Sadlej; Phys. Rev A, **64**, 052507 (2001).
[10] L. Demovič, V. Kellö, A. J. Sadlej, S. A. Cooke; J. Chem. Phys., **124**, 184308 (2006).
[11] V. Kellö, A. J. Sadlej; Collect. Czech. Chem. Commun. **72**, 64 (2007).

Modeling Complex Diffusion Mechanisms in $L1_2$-Structured Compounds

M. O. Zacate[1], M. Lape[1], M. Stufflebeam[2] and W. E. Evenson[2]

[1] *Dept. of Physics and Geology, Northern Kentucky University, Highland Heights, KY 41099, USA, e-mail: zacatem1@nku.edu*

[2] *Dept. of Physics, Utah Valley University, Orem, UT 84058, USA, e-mail: bill@evenson.ch*

We report a computational procedure developed to explore and, hopefully, to distinguish various complex diffusion mechanisms in materials through analysis of hyperfine spectra. We have given initial attention to intermetallic compounds, which are of special interest because complex diffusion mechanisms, whereby diffusing species change sublattices or multiple defect species cooperate in diffusion, can be important diffusion processes.

When a hyperfine probe serves as a tracer in the diffusion process, it is subjected to hyperfine interactions induced by evolving arrangements of defects as they move in the diffusion process. It is not practicable to enumerate all possible arrangements of defects near probes, but it is sufficient to construct a model by considering only those arrangements that are most probable and that create the largest perturbations of the hyperfine field. Such a model contains each Hamiltonian of the defect configurations under consideration and all rates of transition among the configurations. Even when limiting consideration of contributions to electric field gradients (EFGs) caused by defects in the first-neighbor shell of a probe, the number of distinct Hamiltonians can be cumbersomely large.

In this work, we describe a method developed to determine all Hamiltonians of a model and the jump rates among them. In the first step, all possible configurations of defects within a specified range of the hyperfine probe are determined, subject to constraints on which types of defects are allowed, on numbers of defects, and on possible defect jump paths. In the second step, a list is made of unique EFGs arising from the allowed defect configurations within a cutoff distance from the probe, and the connectivity from one EFG to another is determined. In the third step, the rates of transition among EFG states are expressed in terms of defect concentrations and defect jump rates. Finally, a stochastic model is used to calculate PAC spectra for fluctuations among the possible configurations.

Using this method, stochastic models for complex diffusion mechanisms in $L1_2$-structured compounds were developed. Under the approximation that only defects in the near neighbor shell of the PAC probe will have a significant influence on the EFG, the model for the divacancy mechanism has 45 unique EFGs and the model for the 6-jump mechanism has 588 unique EFGs.

This work is funded in part by NSF grant DMR 06-06006 (Metals Program) and computational resources were provided in part by KY EPSCoR grant RSF 012-03.

POSTER ABSTRACTS

Poster session I

Monday 13th September 2010

15:40 – 17:00

Mezzanine

PS1-1-157

Density functional calculations of hyperfine parameters in manganites

J. N. Gonçalves[1], **V. S. Amaral**[1], **J. G. Correia**[2], **H. Haas**[2]

[1] *Departmento de Física and CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal*
[2] *Instituto Tecnológico e Nuclear, E.N. 10, 2686-953 Sacavém, Portugal*

The manganites $RMnO_3$ are a current topic of research due to the interesting interplay of various orders resulting in effects such as colossal magnetoresistance and multiferroism. The hyperfine quantities, electric field gradient and magnetic hyperfine field, highly sensitive to the neighboring charge density, can be used in the experiments to probe local atomic environments. First-principles density functional theory calculations can be compared with experiments to help in its interpretation and to assess the quality of different theoretical methods.

We present the results of calculations with the density functional theory (DFT) linear augmented plane wave (LAPW) method, with the Wien2k code[1] implementation, in the pure manganite compounds. The calculated hyperfine parameters are studied in a systematic way, for series of rare-earth (La, Pr, Y, Eu, Gd, Ho, Er, Yb) and alkaline-earth (Ca, Sr, Ba) compounds with respect to the ionic radius, structure (hexagonal/orthorhombic), different magnetic orders (F/A-AF, etc.) and calculated electronic structure. The sensitivity of the EFG to different exchange-correlation approximations (GGA, GGA+U and LDA+U) is also discussed. The presence of a diluted radioactive probe, as ^{111m}Cd for PAC measurements, is also taken into account by proper expansion of cells.

References

[1] Blaha P, Schwarz K, Madsen G, Kvasnicka D and Luitz J, 2001. WIEN2k, an Augmented-Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Technische Universitat Wien (ISBN 3-9501031-1-2)

PS1-2-4

Theoretical calculations on the Electric Field Gradient in HfO_2:Cd and ZrO_2:Cd

M. Taylor[1], L. Errico[1,2] and R.E. Alonso[1]

[1] Departamento de Física, Fac. de Ciencias Exactas, Instituto de Física La Plata. CC 67, CP 1900 La Plata, Argentina
e-mail: errico@fisica.unlp.edu.ar
[2] Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, Pergamino, CP 2700, Buenos Aires, Argentina

Zirconia-based materials and HfO_2 are in the focus of interest for many years due to their outstanding electrical and mechanical properties. HfO_2 and ZrO_2 are very similar in their crystallographic and electronic structure. They have three polymorphs at atmospheric pressure: their low-temperature phase is monoclinic, increasing the temperature they transform to a tetragonal phase, and finally to a cubic phase as temperature increases.

HfO_2 and ZrO_2 were largely studied with the Perturbed Angular Correlations (PAC) technique with the $^{181}Hf \rightarrow ^{181}Ta$ probe. But a reliable model for the electric field gradient were present recently for Ta-doped HfO_2 [1]. PAC experiments with the $^{111}In \rightarrow ^{111}Cd$ were less common, and as far as we know, only two works were reported in the literature [2, 3]. In this work, we analyze the EFG at the Cd site for the doped monoclinic structure of ZrO_2 and HfO_2. The theoretical results are compared with those determined experimentally by means of PAC spectroscopy. Our calculations are based on the Density Functional Theory (DFT), with the Local Density approximation (LDA) and the Generalized Gradient Approximation (GGA) for the exchange correlation potential, as implemented in the WIEN2k version of the Full Potential APW+LO. Different charge states for the Cd impurity are analyzed, and their influence on the hyperfine parameters is discussed.

References

[1] R. E. Alonso et al., Phys. Rev. B 78, 165206 (2008).
[2] J. Luthin et al., Phys. Rev. B 57, 15272 (1998)).
[3]M. Forker et al., Phys. Rev. B 77, 054108 (2008).

PS1-3-31

Electric-Field Gradient calculations with the full-potential code FPLO

Katrin Koch,[1] **Helge Rosner,**[1] **Klaus Koepernik**[2]

[1]*MPI for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany,*
e-mail: katrinkoch79@gmail.com, rosner@cpfs.mpg.de
[2] *IFW Dresden, Institute for Solid State Research, P.O. Box 270116 01171 Dresden, Germany,*
e-mail: k.koepernik@ifw-dresden.de

The ultimate goal of solid state physics is to explain the properties of solids, based on nothing more than the quantum interactions between their elementary building blocks: electrons and nuclei. The daily work of solid state experimentalists and theoreticians can be considered as making steps towards this goal. In this process, cross-links between theory and experiment are particularly useful. An example of a quantity that can both be calculated and measured with high accuracy, is the electric-field gradient (EFG). It contains valuable information about many aspects of solids, as for instance the electron density, the crystal structure, magnetism or chemical bonding.

An EFG module was recently implemented into the FPLO code [1]. The FPLO package (www.fplo.de) is a full-potential local-orbital minimum-basis code [2, 3] to solve the Kohn-Sham equations on a regular lattice using the local spin density approximation (LSDA). The situation of a chemically disordered structure is covered by a CPA solver [4], relativistic effects can be treated in a related 4-component code [5], and the LSDA+U formalism is implemented [6].

In this poster, we show several examples where the calculation and evaluation of the EFG helped to gain deeper insight into some fundamental properties of solids.

References

[1] K.Koch Koch *Dissertation TU Dresden* (2009).
[2] K. Koepernik and H. Eschrig, *Phys. Rev. B* **59**, 1743 (1999).
[3] I. Opahle, K. Koepernik, and H. Eschrig, *Phys. Rev. B* **60**, 14035 (1999).
[4] K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig, *Phys. Rev. B* **55**, 5717 (1997).
[5] H. Eschrig, M. Richter, I. Opahle, *Relativistic Solid State Calculations, in: Relativistic Electronic Structure Theory,* Part 2. Applications Theoretical and Computational Chemistry, vol.13, pp.723 - 776, Elsevier, (2004)
[6] H. Eschrig, K. Koepernik, and I. Chaplygin, *J. Solid State Chemistry* 176, 482 (2003).

PS1-4-71

Electronic and structural properties of ^{181}Ta in anatase and rutile: Experimental study and *ab initio* calculations

P. Das[1], **D Banerjee**[2], **S K Das**[2], **T. Butz**[3]

[1] *Variable Energy Cyclotron Centre, Kolkata 700064,India,e-mail:*
parnika@vecc.gov.in
[2] *Radiochemistry Laboratory, Variable Energy Cyclotron Centre,*
Bhabha Atomic Research Centre, 1/AF Bidhan nagar, Kolkata 700064, India
[3] *Universität Leipzig, Fakultät für Physik und Geowissenschaften,*
Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

The study of the properties of Titanium Dioxide (TiO_2) has been a subject of interest for its wide ranging applications in different fields. However, the current renewal of interest in this material is due to the synthesis of TiO_2 nanoparticles and its numerous potential applications [1]. As it is well known that the hyperfine-interaction measurements provide local information as a result of the interaction at the probe nucleus and the surrounding electronic charge distribution, in this study we report the result of hyperfine interaction measurement at ^{181}Hf ($\rightarrow^{181}$Ta) probes present as an impurity in the anatase phase of TiO_2. In addition, we have performed first principle calculations in both phases of TiO_2, anatase and rutile, and analyzed the electronic environment around the Tantalum probe atom.

We have performed our calculations based on the density functional theory (DFT) with local orbitals in addition to the augmented plane wave (APW+LO) method as embodied in the WIEN2K code [2]. In order to introduce the Ta impurity a 2×2×3 super cell with 72 atoms in case of rutile and a 2×2×1 super cell with 48 atoms in case of anatase were constructed. Thereafter one of the Ti atoms was replaced by a Ta atom in each case. We optimized the internal position parameter of all atoms and kept the lattice parameters constant. It is observed that for relaxation beyond optimum oxygen nearest neighbor (ONN) distance the change in the electric field gradient (EFG) at Ta sites is insignificant. Calculations were performed with the optimized structure in each case and a reasonable agreement is observed with the experimental results as shown in the table below. However, the nonzero value of η for anatase has been attributed to a large distribution width of ω_Q and the poor crystallinity of the anatase sample [3]. We find no significant change in EFG calculated with a charged Ta state in either case. Calculations are in progress to elucidate the variation in experimentally measured TDPAC parameters in Zr-doped rutile TiO_2 carried out recently by us.

System	Theor. / Exp. V_{ZZ} x 10^{17} (VCm^{-2})	Theor. / Exp. η	References
Anatase	5.87 / 4.62(1)	0.0 / 0.22(1)	[3]
Rutile	14.16 / 13.65(10)	0.48 / 0.56(1)	[3]

References

[1] Seung baek Ryu et al., *Physical Review B* **77**, 094124 (2008).
[2] P. Blaha*, An Augmented Plane Wave+Local Orbitals Programe for Calculating Crystal Properties* (Technische Universität, Wien, 2001).
[3] S. K. Das et al., *Journal of Physics and Chemistry of Solids* **70**, 778-781 (2009).

PS1-5-107

The EFG at sp-impurities in Zn and Cd – a new (final?) look

H. Haas,[1] **J.G. Correia**[1]

[1] *Instituto Tecnológico e Nuclear, Estrada Nacional 10, P-2685 Sacavém, Portugal, and*

CERN/PH-IS, CH-1211 Geneve-23, Switzerland, e-mail: heinz haas@cern.ch

The measurement of the nuclear quadrupole interaction at impurities in simple metals with nuclear methods, the PAC and PAD techniques in particular, has produced a great number of precise experimental data. For the 4sp and 5sp impurities in the strongly deformed hexagonal metals Zn and Cd the data set is almost complete. It has allowed to develop a qualitative understanding of the trends observed. Within a rigid band model [1] the sign change at group V impurities could be explained. Several early theoretical calculations with different methods have confirmed the conclusions but failed to reach quantitative agreement with the experimental data. The local lattice relaxation around the impurities has generally been blamed for this problem. The present work has been started to include this effect by the use of very large (150 atoms) supercells and the precise FLAPW method.

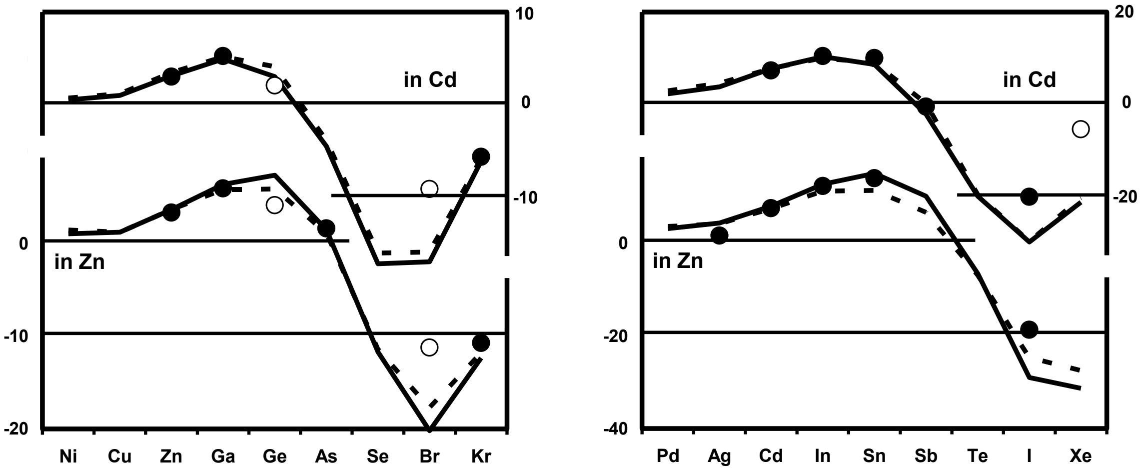


Fig. 1: EFG (in 10^{21} V/m^{2}) for 4sp and 5sp impurities in Zn and Cd. Lines: calculated, Broken lines: 64 atoms supercell, Dots: experimental (open dots: Q only estimated)

For the cases where the nuclear quadrupole moments (Q) are reliably known the calculations reproduce quantitatively the data, with two exceptions: Ag in Zn and I in Zn and Cd. In the first case a generally not very reliable nuclear orientation measurement has been the data source [2]. For the second case the pioneering β-γ PAC experiment [3], however, appears quite reliable. A remeasurement with a different technique would be worthwhile. Whenever Q has only been estimated, strong disagreement is found. In these three cases (^{67}Ge, ^{77}Br, ^{123}Xe) it is felt that the present work results in the first reliable value for Q. The qualitative features found can be understood in the rigid band model. An extensive estimation of the theoretical errors has been made using calculations with a 64 atoms supercell.

References
[1] H. Haas, *Z. Naturforsch. A* 41, 78 (1986)
[2] E. van Walle et al., *Phys. Rev. B* 26, 1109 (1983)
[3] H. Ooms et al., *Hyperfine Interactions* 11, 1 (1981)

PS1-6-118

AB-INITIO HYPERFINE FIELDS IN Fe-Cr

Ney Sodré[a], Helena M. Petrilli[a], Cláudio G. Schön[b]

(a) Departamento de Física dos Materiais e Mecânica,
Instituto de Física da Universidade de São Paulo, São Paulo – SP, Brazil, email:neysodre@if.usp.br
(b) Departamento de Engenharia Metalúrgica e de Materiais.
Escola Politécnica da Universidade de São Paulo, CEP 05508-900 São Paulo -SP, Brazil,email:schoen@usp.br

Fe-Cr alloys form the basis of many industrially important steels, in particular, of the stainless steels. In recent years interest on Fe-Cr alloys grew due to the excellent resistance to irradiation induced swelling of ferritic stainless steels, which are expected to be key materials for developing critical structural components in advanced nuclear reactors. Iron-chromium alloys are characterized by extensive mutual solubility in the bcc phase at high temperatures, with small positive enthalpy of mixing and by complex magnetic interactions [1]. All this justifies the investigation of the constitution, thermodynamics and complex magnetic interactions of the bcc Fe-Cr alloys.

In this work we focus on the the hyperfine fields at the Fe sites in bcc-based Fe-Cr alloys, determined from first principles calculations. We use the Full-Potential Linear Augmented Plane Wave method (FP-LAPW) as embodied in the WIEN2k code [02]. This method allows the computational of very precise total energies and charge densities in metallic compounds due to its full potential feature and is, one of the most accurate methods for electronic structure calculations in solids, specially metals.

Our hyperfine fields are discussed in the light of the theoretical and experimental results in the literature.

References

[1] Inden, G., C. G. Schön . Thermodynamic self-consistency issues related to the Cluster Variation Method: the case of the BCC Cr-Fe (Chromium - Iron) system. CALPHAD 32 (2008) 661- 668.
[02] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka and J. Luitz, *WIEN2k*, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2

Key-words: Fe-Cr alloys, magnetic ordering, WIEN2k, FP-LAPW, intermetallic compounds.

PS1-7-119

Ab initio study of the electronic structure and the EFG at Ta sites in HfO_2:Ta y ZrO_2:Ta.

R. E. Alonso[1], **M. Taylor**[1], **L. A. Errico**[1,2] **and A. López-García**[3]

[1] Departamento de Física e Instituto de Física La Plata (IFLP, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Casilla de Coreo 67, 1900 La Plata, Argentina.
[2]Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, Pergamino, CP 2700 Buenos Aires, Argentina.
3Instituto de Física La Plata IFLP, CONICET
e-mail: taylor@fisica.unlp.edu.ar

Hafnia (HfO_2) and zirconia (ZrO_2) are wide band gap semiconductors with high dielectric constants and very similar properties. Both oxides have monoclinic structure at room temperature that transforms into tetragonal and cubic at respectively higher temperatures. Besides both oxides display technological interest because their high temperature melting point as well as its chemical stability.

By adding small amounts of impurities present different structures that have important technological applications such as electrolytes for combustion cells, catalytic substrates and protecting coatings.

Both, HfO_2 and ZrO_2 have been widely studied using Time Differential Perturbed Angular Correlations spectroscopy (TDPAC) using ^{181}Hf→^{181}Ta probes. Up to now the analysis of TDPAC results was based in the simple assumption that probes are inert in the sense that they do not introduce any crystalline or electronic distortion.

In this contribution we present a first principles study (using the full-potential linear augmented plane wave plus local orbital, APW+lo) of structural, electronic and hyperfine properties of Ta impurities localized at cationic sites in monoclinic HfO_2 and ZrO_2. Due to the agreement between the experimental results obtained by TDPAC and our calculations of the electric field gradient tensor (EFG) it was possible to deduce the Ta charge state at 300 K. It was also possible to calculate the structural distortions induced by the impurities in both oxides. From these results the role played by the Ta impurity to create the EFG can be determined.

PS1-8-133

Ab initio calculations and PAC study of ^{111}In-doped $(Hf/Zr)_3Al_2$ and $(Hf/Zr)_4Al_3$ mixed compounds. EFGs and site preference

L. A. Errico[1], H. M. Petrilli[2], L. A. Terrazos[3], A. Kulińska[4,5], P. Wodniecki[4],
K. P. Lieb[5], M. Uhrmacher[5], J. Belosevic-Cavor[6], and V. Koteski[6].

[1] *Dto. de Física and Instituto de Física La Plata (CONICET-UNLP), Fac. de Cs. Exactas, UNLP, Argentina and*
Universidad Nacional del Noroeste Bonaerense (UNNOBA),Pergamino, Argentina
[2] *Instituto de Fisica, Universidade de Sao Paulo, CP 66318, Sao Paulo, SP, Brazil*
[3] *Universidade Federal de Campina Grande, Centro de Educaçăo e Saude, Brazil*
[4] *Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland*
[5] *II. Physikalisches Institut, Georg-August-Universität, 37077 Göttingen, Germany*
[6] *VINCA Institute of Nuclear Sciences, 11001 Belgrade, Serbia*
e-mail: errico@fisica.unlp.edu.ar

Hyperfine interactions and, in particular, electric field gradients (EFG), constitute a very sensitive tool to investigate the local environment of probe nuclei. Their measurement using Perturbed Angular Correlation (PAC) spectroscopy can provide detailed information on structural and electronic properties. In a well defined single-phase crystal with known lattice structure the interpretation of such measurements is usually not too difficult. But, in more complicated cases, such as multi-phase samples or systems with several crystallographic sites, the interpretation of the various EFG fractions is by no means straightforward. Arguments based on point charge summations or symmetry considerations may fail, since the chemical nature of the impurity causing structural distortions of its neighborhood is not taken into account. To unravel these complex cases, a realistic theory which models different structural and electronic scenarios is mandatory.

In the last decade, a systematic study of the EFGs of $^{181}Hf \rightarrow {}^{181}Ta$ and $^{111}In \rightarrow {}^{111}Cd$ probe nuclei in the full series of hafnium and zirconium aluminides has been carried out [1]. Recently, successful attempts have been made in the compounds Zr_4Al_3 and Hf_4Al_3 to assign the EFGs of $^{181}Hf \rightarrow {}^{181}Ta$ probes to the possible lattice sites and even to distinguish among the lattice structures deduced from X-ray diffraction. Indeed, these EFGs have given evidence of substitutional Zr/Hf sites [2], as confirmed by calculations using the full-potential augmented plane wave + local orbitals formalism (APW+lo).

The present work addresses the more complicated problem of which lattice sites $^{111}In \rightarrow {}^{111}Cd$ probes prefer in these aluminides. Evidently these probe atoms are different from the constituents of the aluminides. We report here on a theoretical and experimental study of the quadrupolar hyperfine interactions of ion-diffused $^{111}In \rightarrow {}^{111}Cd$ probes in polycrystalline isostructural $(Zr/Hf)_4Al_3$ samples containing small admixtures of the phases $(Zr/Hf)_3Al_2$. Strong preference of ^{111}In solutes for the $(Zr/Hf)_3Al_2$ minority phases was observed. Detailed calculations of the EFGs and energetic considerations using the APW+lo theory allowed us to assign unambiguously the observed four EFG fractions to the various lattice sites of $^{111}In \rightarrow {}^{111}Cd$ in $(Zr/Hf)_3Al_2$ and to explain the preferential site occupation of ^{111}In in the minority phases.

References

[1] P. Wodniecki, A. Kulińska, B. Wodniecka, M. Uhrmacher, and K. P. Lieb, Hyperfine Interact. 158, 339 and 429 (2005), and references given there.
[2] P. Wodniecki, A. Kulińska, B. Wodniecka, S. Cottenier, H. M. Petrilli, M. Uhrmacher, and K. P. Lieb, Europhys. Lett. 77, 43001 (2007).

PS1-9-129

Electric Field Gradient and Electronic Properties of Crown Thioether Compounds

Rafael Rodrigues do Nascimento,[1] **F. C. D. A. Lima,**[1] **M. B. Gonçalves,** [1] **H. M. Petrilli** [1]

[1]*Universidade de São Paulo, Instituto de Física, Departamento de Física*
dos Materiais e Mecânica, Grupo Nanomol,P-66318, São Paulo, Brazil, email:
rafaelr@if.usp.br

Crown thioethers are organic molecules that can act as molecular, metal and radioisotope carriers, ion-sensitive electrodes, phase transfer reagents and etc [1]. When these lock and key compounds are functionalized with radioisotopes, they present promising possibilities to be applied in drug design to treat and diagnose diseases. The Time Differential Perturbed Angular Correlation (TDPAC) technique has been suggested in the literature, in connection with different radioactive probes, to aid in this study [2,3]. An important issue to be addressed in the case of biomedical applications is the structural stability of the Crown thioethers, under different conditions, what can be done through state of the art ab initio electronic structure calculations. Here we study the electronic, structural and electrical hyperfine properties of some Crown thioethers complexed with Ag or Cd. We try to reproduce the different situations faced when there is a β decay of ^{111}Ag to ^{111}Cd as seen in a TDPAC experiment. We use the CP-PAW code, which is an all electron ab initio method in the Kohn-Sham scheme of the DFT [4] combining the Car-Parrinello quantum molecular dynamics [5] and the Projector Augmented Wave basis (PAW) set [6]. Our Electric Field Gradient (EFG) results are in a very good agreement with measurements [7] when the Cd$^+$ atom is used to mimic the experimental situation. We also discuss the similarity in the electronic structures before and after the decay. We demonstrate in this issue the importance to evaluate the correct charge state in the ab initio analysis.

References

[1] Schubiger P. A., Alberto R. and Smith A., *Bioconjug. Chem*., 7, 165 (1996).
[2] Ctortecka B., PhD Thesis, Faculty of Physics and Earth Science, Universität Leipzig, 1999.
[3] Tröger W., *Hyperfine Interactions*, 120/121, 117-128 (1999).
[4] Kohn W. and Sham L. J., *Phys. Rev. B*., 140, 1133 (1965).
[5] Car R. and Parrinello M., *Phys. Rev. Lett*., 55, 2493 (1985).
[6] Blöch P., *Phys. Rev. B*, 50, 17953 (1994).
[7] Heinrich F., Ctortecka B. and Troger W., *Hyperfine Interactions*, 158, 79-88 (2004).

PS1-10-8

Investigation of hyperfine interactions in $GdCrO_3$ perovskite oxide using PAC spectroscopy

Renilson A. da Silva, [1] **R.N. Saxena,** [1] **A.W. Carbonari,** [1] **G.A. Cabrera-Pasca**[1]

[1]*Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, São Paulo, Brazil, e-mail:* *rnsaxena@ipen.br*

Perturbed angular correlation (PAC) measurements have been carried out in the anti-ferromagnetic $GdCrO_3$ perovskite oxide using ^{111}In (^{111}Cd) and ^{181}Hf(^{181}Ta) nuclear probes. The radioactive parent nuclei ^{111}In and ^{181}Hf were introduced in the compound through a chemical process during sample preparation. The PAC measurements were carried out in the temperature range 20-300 K. Measurements with the ^{181}Ta indicated a unique quadrupole interaction above 170 K and a combined electric quadrupole and magnetic dipole interactions below this temperature. The observed interactions were assigned to the probe nuclei substituting Cr sites in $GdCrO_3$. Measurements with ^{111}Cd showed two quadrupole interactions. Only one of the fractions however, showed a combined electric and magnetic interaction in the temperature rage 20-170 K which was assigned to ^{111}Cd probe substituting Cr site. The other fraction was attributed to the Gd site. The present results are compared with those of $LaCrO_3$ and $NdCrO_3$.

PS1-11-0

Mössbauer studies of the magnetic quasicrystal $Zn_{77}Fe_7Sc_{16}$

I . Nowik,[1] **R. H. Herber**[1], **T. J. Sato**[2]

[1]*Racah Institute of physics, The Hebrew University, Jerusalem 91904, Israel, nowik@vms.huji.ac.il*

[2]*Neutron Science Laboratory, Institute for Solid State Physics, University of Tokyo, 106-1 Shirakata, Tokay, Ibaraki 319-1106, Japan*

Recent publications [1,2] reported detailed studies, by a variety of methods including Mössbauer spectroscopy [2], of the icosahedral quasicrystal $Zn_{77}Fe_7Sc_{16}$. However the Mössbauer absorber used was extremely thick (1mg/cm^2 of ^{57}Fe) which is more than 20 mean free paths for the 14.4 γ radiation. Thus the interpretation of the many spectra in terms of a distribution of hyperfine parameters, without considering the thick absorber problem, is in serious doubt. We have repeated some of the measurements, with the material studied in [1], however with a very thin absorber (3 mg/cm^2 of natural iron), to be able to analyze the spectra in terms of various physical models. The experimental spectra, Figure 1, (5.1 K to 296 K) were least square fitted with a pure Gaussian distribution of quadrupole interactions at temperatures 8.1 K to 296 K, and an additional Gaussian distribution of magnetic hyperfine fields in the spectra at 5.1 K to 7.1 K. However the low temperature spectra (below 7.1 K) can also be fitted, to the same χ^2, with a dynamical model, using the formulas given in [3], in which superparamagnetic clusters fluctuate, close to and below the spin glass freezing temperature (T_f ~7.5 K). Our conclusions are: (a) Indeed the iron ions are distributed in this quasicrystal in an almost random manner, simulated by a Gaussian distribution of quadrupole interactions extending even to negative values, which artificially resembles a two peak distribution [2]. (b) The spectra below T_f exhibit a broad symmetric shape, indicating random angles between the magnetic hyperfine field and the main axis of the electric field gradient. (c) The experimental spectra do not have the resolution required to distinguish between the static or dynamic model, with which the spectra were fitted.

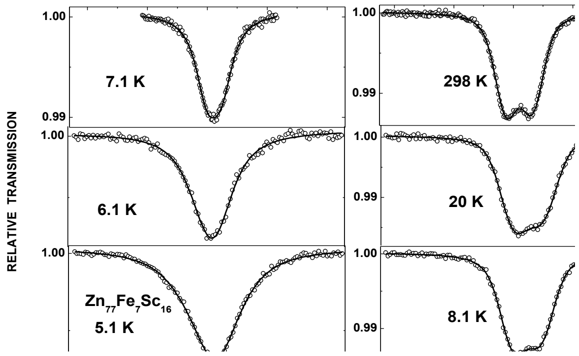


Fig. 1 Mössbauer spectra of $Zn_{77}Fe_7Sc_{16}$.Note the different velocity scales for left and right spectra.

References

[1]T. J. Sato, S. Kashimoto, C. Masuda, T. Onimaru, I. Nakanowatari, K. Iida, R. Morinaga and T. Ishimasa, *Phys. Rev.* **B77**, 014437 (2008).

[2] K. Al-Qadi, P. Wang, Z. M. Stadnik, and J. Przewoznik, *Phys. Rev.* **B79**, 224202 (2009).

[3] I. Nowik and H.H. Wickman, *Phys. Rev. Letters* **17**, 949-51 (1966).

PS1-12-13

Mössbauer and magnetic studies of (Mn, Zn)$_x$Co$_{1-x}$Fe$_2$O$_4$ nanoferrites synthesized by using the citrate precursor preparation technique

J. Z. Msomi,[1] **T. Moyo**[2] **, H. M. I. Abdallah**[2]

[1]*Department of Physics, University of Free State, P/Bag X13, Phuthaditjhaba 9866, South Africa, E-mail: msomijz@qwa.uovs.ac.za*
[2]*School of Physics, University of KwaZulu-Natal, Durban 4000, South Africa, E-mail: moyo@ukzn.ac.za*

(Mn, Zn)$_x$Co$_{1-x}$Fe$_2$O$_4$ ($0 \leq x \leq 1.0$) fine powders with particle sizes of about 4 nm have been produced by citrate precursor method. The evolution of the properties as a function of grain sizes and compositions has been investigated by x-ray diffraction, Mössbauer and magnetization measurements (4 – 350 K). Transformation from ferrimagnetic behavior to paramagnetic state is observed with increasing Zn concentration. The ZnFe$_2$O$_4$ and MnFe$_2$O$_4$ fine powders show enhancement of magnetic transition temperatures which decreases with increasing grain size. The Curie or Neel temperature enhancement is explained on the basis of redistribution of Zn and Mn ions at both tetrahedral (A) and octahedral (B) sites in nanosize samples. The FC and ZFC magnetization curves show spin-glass like behavior in (Mn, Zn)$_x$Co$_{1-x}$Fe$_2$O$_4$ nano ferrites. The variations of coercive field, saturation magnetization and remanance as a function of x and particle diameters are also presented in this work.

PS1-13-19

Mössbauer spectroscopic study of the kinetics of σ-phase formation in cold-rolled Fe-V alloys

B. F. O. Costa[1], J. Cieslak[2] and S. M. Dubiel[2]

[1] *CEMDRX Department of Physics, University of Coimbra, P-3004-516 Coimbra, Portugal*
[2] *Faculty of Physics and Computer Science, AGH University of Science and Technology, PL-30-059 Kraków, Poland,*
e-mail: dubiel@novell.ftj.agh.edu.pl

The bcc-Fe-V alloy system is not stable, for a wide range of compositions around 50%, and upon annealing, the α-phase transforms, either into the σ-phase, or into the ordered metastable B2-phase, depending on the annealing temperature. The B2 is claimed to be a precursor of the σ-phase. In this study we were interested in the effect of temperature on the α-to-σ phase transformation in plastically deformed Fe-V samples. Ingots of an equiatomic Fe-V alloy were cold-rolled down to form platelets of ~200 μm thickness, which were next isothermally annealed at temperatures between 600°C and 800°C for different periods. Samples prepared in that way were investigated at room temperature by X-ray diffraction and Mössbauer Spectroscopy. The former gave direct evidence on the existence of the σ-phase, and indirect on the formation of the B2 superstructure via a decrease of the lattice parameter. Mössbauer spectra, that dramatically changed their shape on annealing, gave thereby evidence that the hyperfine field has significantlylly decreased, which is an indication of the formation of the B2 superstructure. Assuming that the shape of the sub-spectrum corresponding to the B2 superstructure does not depend on the annealing time, the kinetics of the σ-phase formation was followed by studying a temperature dependence of the average hyperfine field.

The results obtained with this procedure are discussed in terms of the Avrami-Johnson-Mehl equation, which yielded kinetics parameters such as the Avrami exponent, n, and the time constant, k. The values of the former are related with the mechanism responsible for the transformation, while the activation energy of the σ-phase formation was determined from the time constant, assuming the Arrhenius law.

PS1-14-23

Mössbauer and electrical studies of $Mn_xCo_{1-x}Fe_2O_4$ compounds prepared via glycothermal route

Hafiz Abdallah,[1] **Thomas Moyo**[1], **Justice Msomi**[2]

[1] *School of Physics, University of KwaZulu-Natal, Durban 4000, South Africa, e-mail: abdallah@ukzn.ac.za*
[2] *Department of Physics, University of Free State, P/Bag X13, Phuthaditjhaba 9866, South Africa*

Manganese-cobalt ferrite powders ($Mn_xCo_{1-x}Fe_2O_4$ with x varying from 0.0 to 0.6), have been produced by glycothermal process from pure metal chlorides. Single phase cubic spinel structure and nanophase structure of the as-synthesized samples were confirmed by X-ray diffraction (XRD) and by transmission electron microscope (TEM). The results show that the produced powders have grain sizes in the range 7 to 13 nm. Fe-57 Mössbauer spectra for as-synthesized and for annealed samples at 700ºC (in Ar atmosphere for 1 hour) are found to be similar. No significant changes in the spectra are observed across the composition range studied. The variations of grain sizes, lattice parameters and Mössbauer parameters as a function of composition have also been investigated. Bulk samples in the form of pellets were also produced from the as-synthesized compounds for resistivity measurements. The temperature dependence of the electrical resistivity for the samples sintered at 1050°C were studied using the four-probe method, from room temperature to about 110°C in a PID controlled oven. The resistivity is observed to vary linearly with $T^{-1/2}$ [1]. This result is discussed in the context of the granular nature of the compounds where electrons can be assumed to tunnel between charged and neutral grains.

References

[1] P. Sheng, B. Abeles and Y. Arie, Phys. Rev. Lett. 31, No. 1, 44 (1973).

PS1-15-24

Advances in a Bulk and Surface properties Studies by using Mossbauer spectroscopy

Alexander Kamzin[1]

[1] *Ioffe PhysicalTechnical Institute TAS, St-Petersburg, 194021 Russia,*
e-mail: Kamzin@ioffe.mail.ru

At present time is very important to study the surface magnetic properties, as well as to understand those relations with bulk properties of crystals. The best way for this was to use experimental methods which provide a possibility to compare surface and bulk properties directly. In 1988 [1,2] we have combined different type of Mossbauer Spectroscopy (MS): Transmission gamma-rays MS (TMS), Conversion Electrons MS (CEMS) and Conversion X-rays MS (XMS) in one method. So, we find possibilities to extract information simultaneously from the bulk and from the surface layers of crystal by combining Mossbauer Effect measurements on radiation with a different track-length in material. Later this method was named by U. Gonser "Simultaneous Triple Radiation Mossbauer Spectroscopy" (STRMS) [3].

With the help of this method and equipment we have investigated a processes on the surface at the phase transition (spin reorientation phase transition? At Neel or Curie points) in the bulk of crystal.

In the given report is observed the results of the studding the surface properties of bulk crystals. as well as the processes on the surface at the phase transiotion (at Curie or Neel point, at spin-reorientation) in the bulk. There has been shown by theoretical analysis that the experimental results obtained by STRMS are of crucial importance for understanding of fundamental magnetic properties.

Author expresses gratitude to the Russian Fund for Fundamental Research (grant 09-02-90447) for supporting this work

References

[1] A.S.Kamzin et al., International Conference "Physics of Transition Metals". USSR-1988. Proceed. pt.II, p.271
[2] A.S.Kamzin et al., Sov.Tech.Phys.Lett. 16, 616 (1990)
[3] U.Gonser et al., Hyperfine Interactions 66, 95 (1991)

PS1-16-33

Magnetic hyperfine field in the intermetallic compounds $PrRh_2Si_2$ and $GdRh_2Si_2$ measured with PAC technique using ^{140}Ce as probe nuclei

G.A Cabrera-Pasca,[1-2] **B. Bosch-Santos**[1], **A.W. Carbonari**[1], **R.N. Saxena**[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, São Paulo, Brazil*
, e-mail: gpasca@usp.br
[2] *Instituto de Física da Universidade de São Paulo, IFUSP/SP, São Paulo, Brazil*

Perturbed angular correlation (PAC) technique has been used to measure the magnetic hyperfine field (B_{hf}) in the antiferromagnetic isostructural compounds $PrRh_2Si_2$ and $GdRh_2Si_2$ using $^{140}La \rightarrow ^{140}Ce$ as probe nuclei. Since the intermediate level in ^{140}Ce at 2083 KeV with $J^{\pi} = 4^{+}$ used in the PAC measurement has a very small quadrupole moment, one observes only the magnetic interaction with this probe. The samples were prepared by arc melting the constituent metals Ce(99.9%), Rh(99.98%) and Si(99.9999%) in estoiquiometric proportions followed by annealing in vacuum at 900°C during 5 days. The samples were analyzed by X-ray diffraction, which confirmed single phase in both cases corresponding to the $ThCr_2Si_2$ structure. The radioactive parent nuclei ^{140}La, obtained by the neutron irradiation of La, were introduced as a highly dilute impurity (<0.1%) into the compounds during arc melting process. The PAC measures were performed in the temperature range of 10 K to 70 K in the case of $PrRh_2Si_2$ and 10 K to 105 K in the case of $GdRh_2Si_2$. While the temperature dependence of B_{hf} for $PrRh_2Si_2$ follows a typical behavior expected for a second order magnetic transition, the behavior in the case of $GdRh_2Si_2$ is anomalous. The values of hyperfine field (B_{hf}) at 10 K, determined from the present measurements are 129.5(5) T and 25.6(4) T respectively for $PrRh_2Si_2$ and $GdRh_2Si_2$. This difference is explained by the difference in the mechanism for the formation of magnetic moments in the two compounds. The Neél temperatures (TN) were determined to be 70.6(3) K and 106 (1) K respectively for $PrRh_2Si_2$ and $GdRh_2Si_2$ in good agreement with values found in the literature.

PS1-17--41

Perturbed Angular Correlations Investigations on Rare-Earth Manganites

Tania M. Mendonça,[1] **Armandina M.L. Lopes**[2], **João N. Gonçalves**[3], **João G. Correia**[4], **Pedro B. Tavares**[5], **Vítor S. Amaral**[3], **João Pedro Araujo**[1], **Céline Darie**[6]

[1] *IFIMUP and IN – Institute of Nanosciences and Nanotechnology, Dep. De Física da Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal, e-mail: tania.de.melo.mendonca@cern.ch*
[2] *Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-002 Lisboa, Portugal*
[3] *Departamento de Física and CICECO, Universidade de Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*
[4] *Instituto Tecnológico e Nuclear, E.N.10, 2686-953 Sacavém, Portugal*
[5] *Centro de Química – Vila Real, Departamento de Química, Universidade de Trás-os-Montes e Alto Douro, 5001-911 Vila Real, Portugal*
[6] *Institut Néel, CNRS, Av. des Martyrs 25, F-38042 Grenoble CEDEX 9, France*

The perturbed angular correlation (PAC) technique was applied to study the rare-earth (R) local environment in a series of rare-earth manganites ($RMnO_3$, R=Nd, Sm, Eu, Gd, Ho, Y, Er, Yb, and Lu). By measuring the electric field gradients (EFG) at the rare-earth site, the charge distribution of the R neighborhood was fully characterized. The EFG were studied as a function of the rare earth ionic radius (R_I) and the results were interpreted with the help of ab-initio calculations using the density functional full potential augmented plane wave (FLAPW) method.

The experimental and simulated results show two different EFG distributions for all compounds. Different local environments were observed depending in the crystalline structure (orthorhombic or hexagonal) being only one directly attributed to the rare-earth crystalline site. The existence of intrinsic nanoscale electronic inhomogeneities scenario associated to subtle distortions around the R-O polyhedra is discussed.

PS1-18-44

Magnetic-Electronic Pressure Response of Ilmenite ($FeTiO_3$)

W. N. Sibanda[1], G. R. Hearne[2] and D. Naidoo[1]

[1]*School of Physics, University of the Witwatersrand, P Bag 3, Wits 2050, Johannesburg, South Africa, email:wisdom.sibanda@students.wits.ac.za*

[2]*Department of Physics, University of Johannesburg, P O Box 524, Auckland Park, 2006, Johannesburg, South Africa.*

Polycrystalline powders of synthetic and natural ilmenite ($FeTiO_3$) assemblages pressurized in a diamond anvil cell have been studied at room temperature using ^{57}Fe Mössbauer spectroscopy to elucidate the magnetic-electronic pressure response of different ilmenite samples. Natural ilmenite samples used included an untreated sample derived from the Hillindale mining area in KwaZulu-Natal, South Africa and a heat treated sample (to increase oxidation) from the same source. Asymmetry in the Mössbauer lineshape (doublet) profile is initiated at low pressure and persists to the highest pressure in all samples. This is especially evident in the synthetic sample which has a symmetric doublet (and only Fe^{2+}) at ambient pressure. The asymmetry is perhaps attributed to Fe^{3+} emerging (i.e., pressure-induced oxidation). Metal-metal charge transfer along the *c*-axis of the unit cell between face sharing octahedra of Fe^{2+} and Ti^{4+} cations may be one , albeit, contentious explanation for this [1,2]. If we consider the asymmetry in the relative intensities of the doublet to be a result of an increase in the ferric-ferrous ratio from charge transfer (and not from texture effects or the GKE), then the following quantitative behavior is obtained. The Fe^{3+}/Fe^{2+} ratio in the heat treated sample as deduced from the theoretical fits to the data shows a gradual increase of 0.28 to 0.38 in the pressure range 0 GPa to 14 GPa, the highest pressure reached for that sample. The phase abundance of the ferric component in the synthetic sample increases from 0 to 15% at 18.5 GPa, then seems to decrease at higher pressure as a structural transition ensues. A perovskite high pressure phase initiates at ~18 GPa corresponding to Fe^{2+} in dodecahedral coordination. It coexists in ever increasing abundance, and over a wide pressure range with the corundum-type low-pressure phase (i.e., sluggish transition at room temperature). The relative content of Fe^{2+} in the perovskite phase increases at the expense of Fe^{2+} in the low-pressure ilmenite phase. The trend observed in the abundances of the ferric and ferrous components of the ilmenite-corundum structure of the untreated natural sample is similar to what is seen in both the heat treated and synthetic samples. In the low pressure region (up to 4 GPa), the Fe^{3+}/Fe^{2+} ratio in the untreated natural sample increases significantly and thereafter continues to increase into a “plateau” region. The ratio is ~0.10 at ambient conditions and ~0.30 at 15 GPa, the highest pressure attained in the study of this sample.

References

[1] X. Wu et al., *Physical Review B* **79**, 094106 (2009)
[2] S. Takele et al., *Journal of Physics: Condensed Matter,* **16**, 2707-2718 (2004)

PS1-19-45

Spin and Orbital Order in $FeCr_2S_4$

J. Engelke[1], F.J. Litterst[1], A. Krimmel[2], A. Loidl[2], F.E. Wagner[3], and G.M. Kalvius[3]

[1] *IPKM TU Braunschweig, 38106 Braunschweig, Germany, e-mail: j.litterst@tu-bs.de*
[2] *Experimentalphysik V, Universität Augsburg, 86135 Augsburg, Germany, e-mail: alois.loidl@physik.uni-augsburg.de*
[3] *Physics-Department TU München, 85747 Garching, Germany, e-mail:kalvius@ph.tum.de*

The spinel $FeCr_2S_4$ has been studied intensely during the past for its magnetic and orbital ordering properties. Ferromagnetic coupling occurs between the B-site Cr. The A-site Fe^{2+} couples antiferromagnetically to the Cr sublattice. The ferrimagnetic order is driven by the Cr coupling. Recent muon spin rotation data [1] give strong evidence that the earlier claimed magnetic structures are in fact more complex. The collinear ferrimagnetism found between the Curie temperature T_C=165 K and 50 K changes to an incommensurate, probably helical structure. Close to the ordering/reorientation temperatures considerable spin disorder is detected. Below 10 K orbital order is found.

Several attempts have been reported for an interpretation of the iron hyperfine spectra based on the assumption of collinear magnetic structures. We present new experimental Mössbauer spectroscopic data and a new strategy of analysis taking into account the magnetic correlation results obtained from muon spin rotation. The influence on spectral shape by changing Jahn-Teller dynamics will be discussed. Special emphasis is given to the interpretation of the spectra close to the spin reorientation near 50 K and near the orbital ordering transition indicating the splitting of the orbital ground state of Fe^{2+} and a possible formation of an orbital glass state.

References

[1] G. M. Kalvius et al., *J. Phys.: Condens. Matter* **22,** 052205 (2010)

PS1-20-62

Mössbauer Spectroscopy of the New Iron Oxide $Fe_3B_7O_{13}(OH)$

Shin Nakamura[1] ,**Yorihiko Tsunoda**[2], **Ippei Nomoto** [3], **Hirohiko Sato** [3]

[1] *Department of Physics, Teikyo University, Utsunomiya 320-8551, Japan, e-mail: shin@koala.mse.teikyo-u.ac.jp*
[2] *School of Science and Engineering, Waseda University, Shinjuku-ku, Tokyo 169-8555, Japan*
[3] *Department of Physics, Chuo University, Bunkyo-ku, Tokyo 112-8551, Japan*

Boracite $Fe_3B_7O_{13}(OH)$ is a new ion oxide synthesized by hydrothermal method [1]. The crystal structure is trigonal ($R3cH$) with the lattice constants of a=8.590Å and c=21.107Å (hexagonal notation) at room temperature. Iron ion, Fe^{2+}, occupies a pentahedral site. Three pentahedrons share the upper corner, which is probably occupied by OH^- ion [2,3], and thus three Fe^{2+} ions form a triangular cluster in the c-plane. The material is an antiferromagnet with T_N=4.9 K. Ising-like behavior is observed [1]. In order to investigate the local structure and the magnetic structure, we have applied ^{57}Fe Mössbauer spectroscopy. The spectra were measured in conventional transmission geometry by using ^{57}Co-in-Rh as the γ-ray source. The powdered specimen was used as an absorber.

The paramagnetic spectrum at 293 K is shown in Fig.1. The spectrum is composed of a paramagnetic doublet with sharp line widths (0.24mm/s), indicating that there is only one crystallographic Fe site. The room-temperature value of isomer shift (IS) is 1.16mm/s, which indicates that the Fe ions are in high spin Fe^{2+} state. The quadrupole splitting (QS) is very large (3.21mm/s) due to the valence electron contribution. The spectrum at 4.2 K, just below T_N, is shown in Fig.2. The spectrum is a well-resolved hyperfine sextet with sharp line widths (0.30mm/s), indicating that the hyperfine field (H_{hf}) glows rather rapidly below T_N. We can obtain the best fit curve with the parameters; IS=1.29mm/s, QS=3.52 mm/s H_{hf}=3.6T, asymmetry parameter η=0.5, and Euler angles θ=20° and ϕ=0°. By evaluating the principal axis of electric field gradient (EFG) from the lattice contribution, we can deduce that each three Fe^{2+} magnetic moment is directed from Fe^{2+} ion to OH^- ion. Taking into account that the system is antiferromagnetic as a whole, a probable magnetic structure is 6-sublattice model, which is consistent with that derived from the static magnetic properties [1].

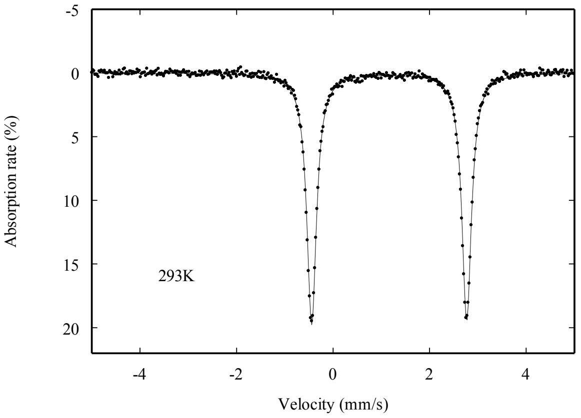


Fig. 1.Paramagnetic spectrum at 293 K.

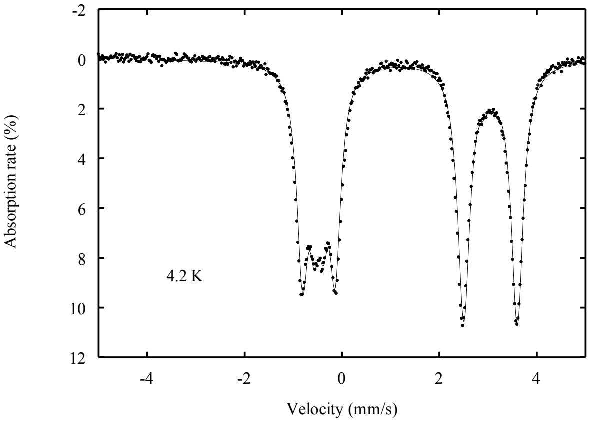


Fig. 2.Magnetically ordered spectrum at 4.2 K.

References

[1] H. Sato, et al., in preparation.
[2] D. Andreica, et al., *Ferroelectrics*, 204 (1997) 73.
[3] U. Werthmann, et al., *Z.Kristallogr.*215 (2000) 393.

PS1-21-64

Magnetic and electrical transport properties of Ce/Ca substituted perovskite oxides

M.P. Sharma[1], Anjali Krishnamurthy[1], Bipin K. Srivastava[1] and V. Ganesan[2]

[1]Department of Physics, University of Rajasthan, Jaipur – 302 004(India)
E-mail: mps.phy@gmail.com
[2]UGC-DAE Consortium for Scientific Research, Indore – 452 017(India)

Magnetic and electric transport studies have been made on cerium - calcium substituted perovskites $La_{1-2x}Ce_xCa_xMnO_3$ for x = 0.05, 0.10 and 0.15, prepared by solgel method. Magnetization and electrical measurements are reported in the temperature range 20 K – 300 K and in fields upto 8 kOe and 2K – 300K and in fields upto 14 T respectively. All the samples undergo paramagnetic to ferromagnetic transition. Among the Ce/Ca substituted samples LCeCaM15 is highly disordered. Addition of 10 atomic% Ca into 10 atomic% Ce substituted system drives the FM state towards a more disordered one and when in place of 10 atomic% Ce, the substitution is of 5 atomic% Ce and 5 atomic% Ca, the system shows up to be far better FM ordered. In the series $La_{1-2x}Ce_xCa_xMnO_3$ no upturn is seen in resistivity but there is only a slight tendency of increase at ~30 K [Figure 1]. This would mean that in the Ce/Ca substituted samples, of the two competing factors – decreasing scattering with lowering of temperature leading to reduction in resistivity and spin polarized tunneling leading to enhancement of resistivity - the factor of decreasing scattering overtakes. In insulating regions of all the samples, at temperatures above the M – I transition points, conduction is controlled by variable range hopping and at higher temperatures small polaron hopping mechanism is operative [1]. Values of activation energy are much smaller those reported in other substituted manganites [2]. The magnetoresistance (MR), plot shown in Fig. 1 as a function of temperature, is observed to be negative and large. For all the three samples, under 5 T field it is as high as ~40% at temperatures close to I – M transition and under 14 T the maximum is ~68% for LCeCaM05. At 300 K and under 5 T field it is close to 15% for all the samples.

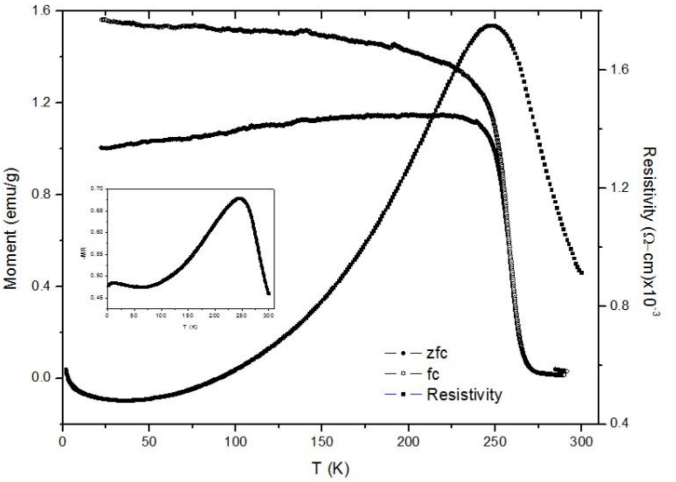


Fig. 1. Temperature dependent magnetization and resistivity (inset show MR plot) of 5 atomic % Ce and 5 atomic % Ca substituted sample.

References

[1] P. Raychaudhuri et. al., *Phys. Rev. B* **59,** 13919 (1999).
[2] Arita Banerjee et. al., *J. Chem. Phys.* **115**, 1550 (2001).

PS1-22-79

Studies of GdZn compound magnetic properties using PAC spectroscopy with ^{140}Ce and ^{111}Cd as probe nuclei

B.Bosch-Santos[1], **G.A. Cabrera-Pasca**[2], **A.W. Carbonari**[1]

[1]*Instituto de Pesquisas Energéticas e Nucleares, IPEN, São Paulo, Brasil*
[2]*Instituto de Física Universidade de São Paulo*

In this work, we have investigated magnetic properties of the ferromagnetic GdZn compound by perturbed γ-γ angular correlation (PAC) spectroscopy using $^{140}La \rightarrow ^{140}Ce$ ($t_{1/2}$ = 3.4 ns, and g-factor 1.014) and $^{111}In \rightarrow ^{111}Cd$ ($t_{1/2}$ = 85 ns, and g-factor 0.306) as probe nuclei. The study of magnetic properties of rare earth and zinc (RZn) compounds is interesting because rare earth elements present a localized magnetism associated with 4*f* electrons, and these electrons do not participate in chemical bonds, as a consequence the RZn magnetic properties originate from the 4*f* electrons of rare earth. The compound GdZn exhibits the cubic CsCl structure and the Curie temperature is 268 K. The saturation moment at 4.2 K lies along the [101] and the value is 7.30 μ_B.

The PAC spectroscopy provides information about the hyperfine interaction between nuclear external fields and nuclear moments of a probe nucleus at a certain atomic site in a crystalline structure, and consequently allows extracting information of the involved hyperfine parameters, as well as the characterization of phase transitions of the crystal. This technique is based on the emission of two gamma radiations in a cascade as a result from the decay of the excited states of the probe nucleus. $^{140}La(^{140}Ce)$ probe is very interesting because show low quadrupole moment (Q), what allows only measurements of the magnetic hyperfine field (mhf). ^{140}La (^{140}Ce) probe were obtained by the irradiation of natural La at the IPEN research reactor with a neutron flux around 3 x 10^{13} ncm^{-3}/s.

The compound GdZn (Gd = 99.9% e Zn = 99.999% purity) was prepared by arc-melting the constituent elements. ^{140}La nuclei were added to the samples by arc-melting them again along with a small piece of irradiated natural La followed by a thermal treatment. ^{111}In was diffused into the samples which was sealed in vacuum and annealed at 800 ºC. Samples have been characterized by X-ray diffraction, and it was observed a major fraction corresponding to the phase of the GdZn.

In the case of ^{111}Cd-GdZn measurements it was observed one frequency which corresponds to the probe nucleus replacing a position of one atom in the cubic structure of GdZn. The hyperfine parameters at 10 K were $\nu_M = 74.819\ MHz$, $\nu_Q = 1.573\ MHz$ and $\delta = 0.51\%$. The results shows that the temperature dependence of magnetic field can be fitted by the Brillouin function for $J = 7/2$.

In the case of ^{140}Ce-GdZn measurements showed a sharp deviation from an expected standard Brillouin function. The major fraction with magnetic frequency $\nu_M = 767.293\ MHz$ and $\delta = 0.84\%$ at 10 K ,which corresponds to probe nucleus replacing a position of one Gd atom in the cubic structure of GdZn.

PS1-23-93

$DyNi_2Mn$ – Magnetisation and Mössbauer Spectroscopy

J.L. Wang[1,2], S.J. Campbell[1], S.J. Kennedy[2], S.X. Dou[3] and G.H. Wu[4]

[1]*School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, The Australian Defence Force Academy, Canberra ACT 2600, Australia*
[2]*Bragg Institute, ANSTO, Lucas Heights, NSW 2234, Australia*
[3]*Institute for Superconductivity and Electronic Materials, University of Wollongong, Wollongong, NSW 2522, Australia*
[4]*Institute of Physics, Chinese Academy of Science, Beijing 100190, P. R. China*

We have investigated the physical properties of $DyNi_2Mn$ doped with ^{57}Fe by magnetisation (10 – 300 K) and ^{57}Fe Mössbauer spectroscopy measurements (5 – 300 K). X-ray diffraction analysis indicates that RNi_2Mn compounds crystallize in the $MgCu_2$-type (C-15-type) cubic structure (space group: Fd 3m) [1-2] even though the ratio of rare earth atoms to transition metal atoms is 1:3 as confirmed by energy dispersive spectroscopy [1]. The $DyNi_2Mn$ ordering temperature has been derived to be $T_C = 95$ K - much higher than those of the corresponding $DyNi_2$ ($T_C \sim 22$ K) and $DyMn_2$ ($T_C \sim 35$ K) compounds [1].

Our detailed analyses of isothermal M-H curves and the related Arrott plots confirm that the magnetic phase transition at T_C for $DyNi_2Mn$ is second order. The magnetic entropy change around T_C has been found to be 4.0 J/kg K for a magnetic field change of 0 T to 5 T. The Mössbauer spectra below T_C were fitted with three sub-spectra representing three inequivalent local magnetic environments while two doublets were used to fit the paramagnetic Mössbauer spectra. Mean values of the ^{57}Fe hyperfine interaction parameters of $DyNi_2Mn(^{57}Fe)$ have been determined from the Mössbauer spectra (e.g. Fig. 1).

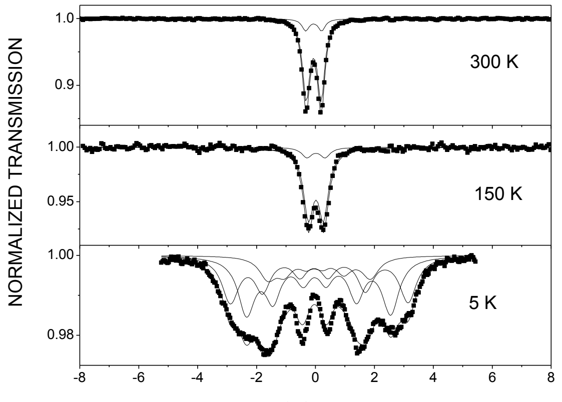


Fig. 1. ^{57}Fe Mössbauer spectra and fits for $DyNi_2Mn(^{57}Fe)$ over the temperature range 5–300 K. Examples of the subspectral components are shown.

References

[1] J.L. Wang, C. Marquina, M.R. Ibarra and G.H. Wu, Phys. Rev. B **73,** 94436 (2006)
[2] D.D. Jackson, S.K. McCall, S.T. Weir, A.B. Karki, D.P. Young, W. Qiu and Y.K. Vohra, Phys. Rev. B **75** 224422 (2007)

PS1-24-109

Magnetic Hyperfine Interaction of ^{59}Fe in Nickel

Suguru Muto,[1] **Susumu Ohya**[2], **Takashi Ohtsubo**[2], **Takuji Izumikawa**[3], **and**
Katsuhiko Nishimura[4]

[1] *Neutron Science Laboratory, KEK, 1-1 Oho, Tsukuba 305-0801, Japan, suguru.muto@kek.jp*
[2] *Department of Physics, Niigata University, 2-8050 Ikarashi, Niigata 951-2181, Japan*
[3] *Radioisotope Center, Niigata University, 1-757 Asahimati, Niigata 951-8510, Japan*
[4] *Faculty of Engineering, University of Toyama, 3190 Gofuku, Toyama 930-8555, Japan*

The nuclear magnetic resonance on oriented nuclei (NMR-ON) is a powerful method for investigating the hyperfine interactions of probe nuclei in ferromagnetic metals. A systematic study of the hyperfine fields gives us very important information on the electronic structures of the elements in ferromagnetic host metals. Previously, we reported successful measurement hyperfine field of ^{59}Fe in iron host [1], and nuclear spin-lattice relaxation time [2]. We measured the hyperfine field and nuclear spin-lattice relaxation time of ^{59}Fe in nickel host using β-ray detected NMR-ON method.

The sample of ^{59}Fe*Ni* was produced by irradiation of ^{58}Fe*Ni* foil with thermal neutrons. After irradiation the sample was annealed at 800°C in vacuum for 1 hour. The NMR-ON experiment was performed by ^{3}He/^{4}He dilution refrigerator at Niigata University. The sample was cooled down to about 10mK. The asymmetry of β rays was monitored by two Si detectors mounted at 0° and 180° with respect to the orientation axis. The resonance spectra were measured at external field B_0 = 0.1, 0.2, 0.4, and 0.6 T. From the linear shift of resonance frequencies with external field B_0, we obtained ν_0 = 48.34(1) MHz. The magnetic moment of ^{59}Fe was reported as μ = -0.3358(4) μ_N [1]. Using this value and neglecting a possible Knight shift, the hyperfine field of Fe*Ni* was deduced to be B_{HF} = -28.33(5) T, which is in good agreement with the previously reported value of 28.2(2) T [3]. The nuclear spin-lattice relaxation time was also measured by turning FM on and off at the center of the resonance frequency. The further data analysis is in progress.

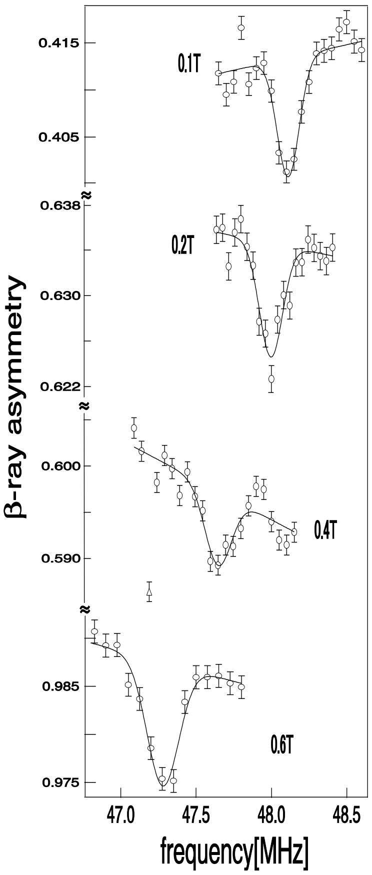


Fig. 1. NMR-ON spectra of ^{59}Fe*Ni* for B_0 = 0.1, 0.2, 0.4, and 0.6 T.

References

[1] T. Ohtsubo, D.J. Cho, Y.Yanagihashi and S. Ohya, Phys. Rev. C**54**, 554 (1996).
[2] T. Ohtsubo, D.J. Cho, Y.Yanagihashi, K. Komatsuzaki, K. Mizushima, S. Muto and S. Ohya, Proceedings of the 10th International Conference on Hyperfine Interactions; Hyperfine Interactions (C), 577 (1996).
[3] V.G. Bhide and G. K. Shenoy, J. Phys. Soc. Japan **21**, 625 (1966).

PS1-25-116

Magnetoelectric $AgCrO_2$: A new local insight given by PAC

G.N.P.Oliveira[1,2], **A.M.L.Lopes**[1], **T.M.Mendonça**[2], **J.P.Araújo**[2], **J. Agostinho Moreira**[2], **A. Almeida**[2], **V.S.Amaral**[3], **J.G.Correia**[4]

[1]CFNUL, Centro de Física Nuclear, Universidade de Lisboa, Portugal, e-mail: goliveira@fc.up.pt
[2]IFIMUP & IN- Instituto de Nanociência e Nanotecnologia, Depto Física e Astronomia da Fac. Ciências daUniversidade do Porto
[3]Departamento de Física e CICECO, Universidade de Aveiro
[4]ITN, Instituto Tecnológico e Nuclear, Sacavém, Portugal

Systems exhibiting coupling between ferroelectric (FE) and (anti)ferromagnetic (AFM/FM) orders, are suitable for new magnetoelectric memories, which allow to write electrically information and to read it magnetically (or vice-versa) [1-3].

This work is focused in the delafossite type compound $AgCrO_2$, which has gave rise a recent renewed interest due to its magnetoelectric properties [3]. Single-phase polycrystalline samples were prepared through the standard solid-state reaction method, using O_2 flow. The phase purity was checked [3] through Rietveld XRD powder analysis. The temperature dependence of the magnetization and of the dielectric constant exhibits the expected behavior near the AFM and FE ordering temperature (T_N =21 K). Furthermore, the temperature dependence of the magnetic susceptibility below T=100 K shows a peculiar behavior, generally attributed to the development of 2D short-range magnetic correlations (SRMC), due to strong frustration, coming from the AFM exchange interactions in a triangular spin lattice [4].

We have studied in detail the temperature dependence of the electric field gradient (EFG) at the Cr site via perturbed angular correlation measurements with the ^{111}In probe. We have evidence that a second EFG emerges below 100 K and remains down to 10 K. In addition, the relative abundance of these two EFG varies linearly extrapolating to 50% at T=0 K.

Taking into account the strong interplay between magnetic and electric degrees of freedom present in $AgCrO_2$, the SRMC can facilitate the onset of a second EFG (EFG_2) ~~that~~ having a relatively close frequency to the first one (EFG_1), but with a different asymmetry parameter (η_2). A possibility that could explain our data is connected with ion polar displacements that would start below 100 K. A-site displacements were in fact suggested to occur in $LiCrO_2$[5]. Moreover, a distortion of the Cr triangular lattice was claimed below T_N in $CuCrO_2$ [6]. In this way, our results suggest that the observed EFG_2 might be associated with a precursor effect of the FE/AFM phase transition.

References:

1. Y.H. Chu, L.W. Martin, et al, *Nature Materials* **7**, 478 (2008).
2. M. Bibes and A. Barthélémy, *Nature Materials* **7**, 425 (2008).
3. S. Seki et al, *Phys. Rev. Lett.* **101**, 067204-1, (2008)
4. Y. Oohara, et al, *Journal of the Physical Society of Japan*, **63** (3):847–850, 1994.
5. J. Sugiyama, et al, *Physical Review B*, **79** (18):184411, 2009.
6. K. Kimura, et al, *Journal of the Physical Society of Japan*, **78** (11), 113710, 2009

PS1-26-121

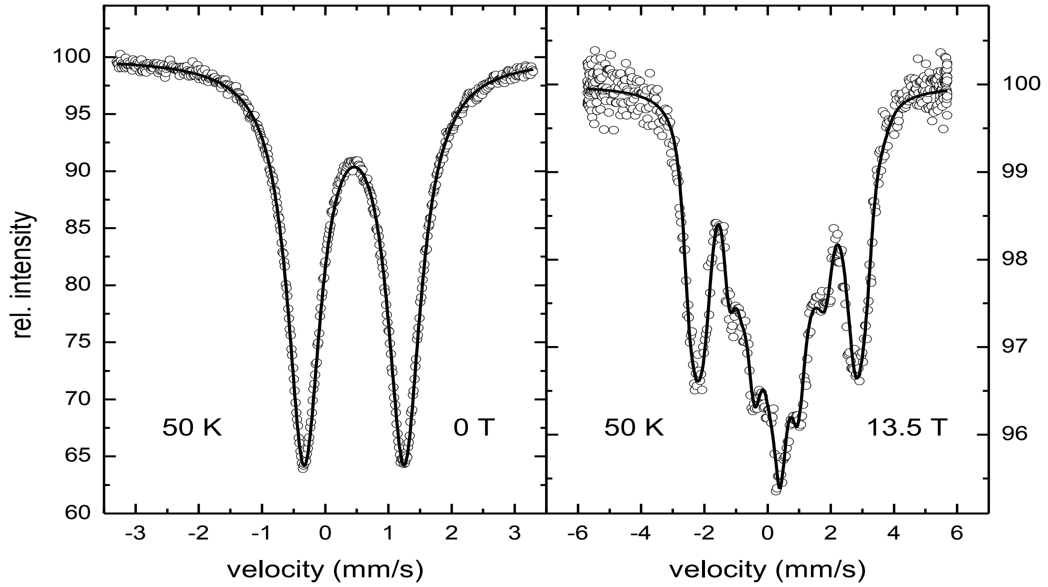
Investigations on $FeSb_2$ by high field ^{57}Fe Mössbauer spectroscopy

M.Reissner,[1] **A.Farhan**[1], **R.Bliem**[1], **A.Leithe-Jasper**[2], **W.Steiner**[1]

[1] *Institute of Solid State Physics, Vienna University of Technology, Vienna A-1040, AUSTRIA,*
reissner@ifp.tuwien.ac.at
[2] *Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany*

$FeSb_2$ has gained much interest in recent years, because of its potential as a thermoelectric material. It is a nearly ferromagnetic small gap semiconductor with a semiconductor-metal transition above 80 K [1]. It crystallizes in the marcasite structure, where Fe has only one crystallographic site, surrounded by distorted Sb-octahedra [2]. These octahedra are corner shared in the *ab*-plane and edge sharing along the *c*-axis. With decreasing temperature the distortion of the octahedra increases, showing a maximum around 100 K [3]. At low temperatures the material is diamagnetic. With increasing temperature a paramagnetic-like behavior is observed. The aim of this work is to get more information about the magnetic state of the iron atom in this compound. We report on ^{57}Fe Mössbauer investigations in zero and in applied fields up to 13.5 T at temperatures between 4.2 K and RT on polycrystalline $FeSb_2$ samples enriched with Fe-57. The spectra were analysed by solving the full Hamiltonian, taking into account both electrostatic and magnetic interactions, as well as the sample thickness.

The zero field spectra can be fitted by only one subspectrum, with a quadrupole splitting which increases with decreasing temperature, reaching a maximum at about 50 K. In contrast to this the in-field spectra are extremely complex. Several models were tested to explain the spectra. At least 5 subspectra is necessary with line widths for some of them indicating that this is only a minimum number. Common to all models is that the mean values for quadrupole splitting and center shift fit well to the zero-field results.



References

[1] A.V. Lukoyanov et al., *Eur.Phys.J. B* **53**, 205 (2006).
[2] F. Hullinger, *Struct. Bonding* (Berlin) **4**, 83 (1967).
[3] C. Petrovic et al., *Phys.Rev.B* **72**, 045103 (2005).

PS1-27-123

Structural, electronic and magnetic properties of Ho substituted $BiFeO_3$ as a function of temperature

D. Naidoo[1], **M. Ncube**[1], **D.R. Sahu**[1], **K. Bharuth-Ram**[2,3], **W.N. Sibanda**[1], **H. Masenda**[1], **R.M. Erasmus**[1], **S.K. Pradhan**[4] **and B.K. Roul**[4]

[1]*School of Physics, University of the Witwatersrand, WITS 2050, South Africa.*
Deena.Naidoo@wits.ac.za
[2]*School of Physics, University of KwaZulu-Natal, Durban 4001, South Africa.*
[3]*iThemba LABS, P.O. Box 722, Somerset West 7129, South Africa.*
[4]*Institute of Materials Science, Bhubaneswar-751013, India.*

There is renewed interest in bismuth ferrite, $BiFeO_3$, due to its special multiferroic properties at and above room temperature (RT) [1, 2]. It is therefore important to investigate the structural, electronic and magnetic properties of doped $BiFeO_3$ systems such as $BiHoFeO_3$ using a suite of spectroscopic methods. Here we present results of ^{57}Fe-Mössbauer spectroscopy (MS) studies on Ho substituted $BiFeO_3$. The MS measurements were performed in standard transmission geometry with a ^{57}Co(Rh) source, at 90 K and on the as-synthesized sample, and at room temperature after annealing the sample at temperatures between 373 K and 1123 K in argon for 18 hours. Selected Mössbauer spectra are shown in Figure 1. The spectra at 90 K, for the as-synthesized sample and after annealing at $T_A \leq 673$ K are very similar and are generally characterized by two Zeeman sextets and two quadrupole split doublets. The isomer shifts and hyperfine fields of the sextets are close to those observed for $BiFeO_3$; the quadrupole splitting of the sextets are much larger. However, at $T_A > 673$ K, the recorded spectra exhibit collapsing magnetic fields and pronounced growth of the central regions are observed at higher annealing temperatures and this is tentatively assigned to paramagnetic spectral components. Raman spectroscopy, X-Ray Powder Diffraction and magnetization data will be presented to confirm the findings obtained from the Mössbauer results.

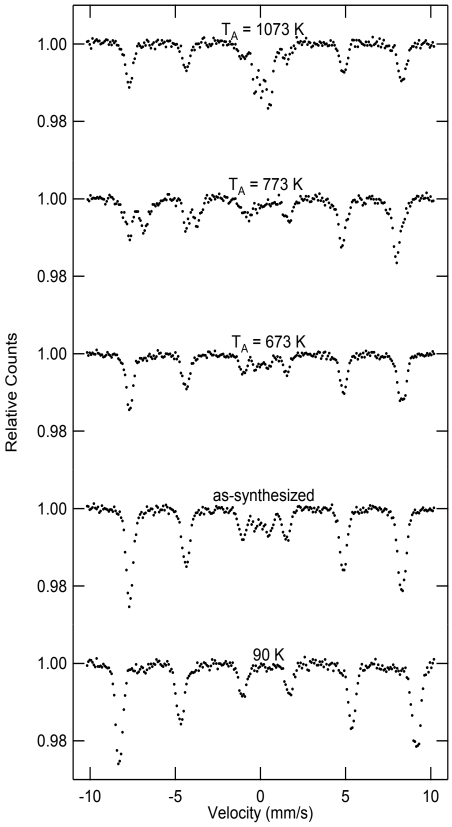


Figure 1: Selected Mössbauer spectra as a function of temperature.

References
[1] A. Palewicz *et. al.*, *Acta Cryst.* (2007) B **63**, 537-544.
[2] A. Palewicz *et. al.*, *Solid State Communications* **140** (2006) 359-363.

PS1-28-125

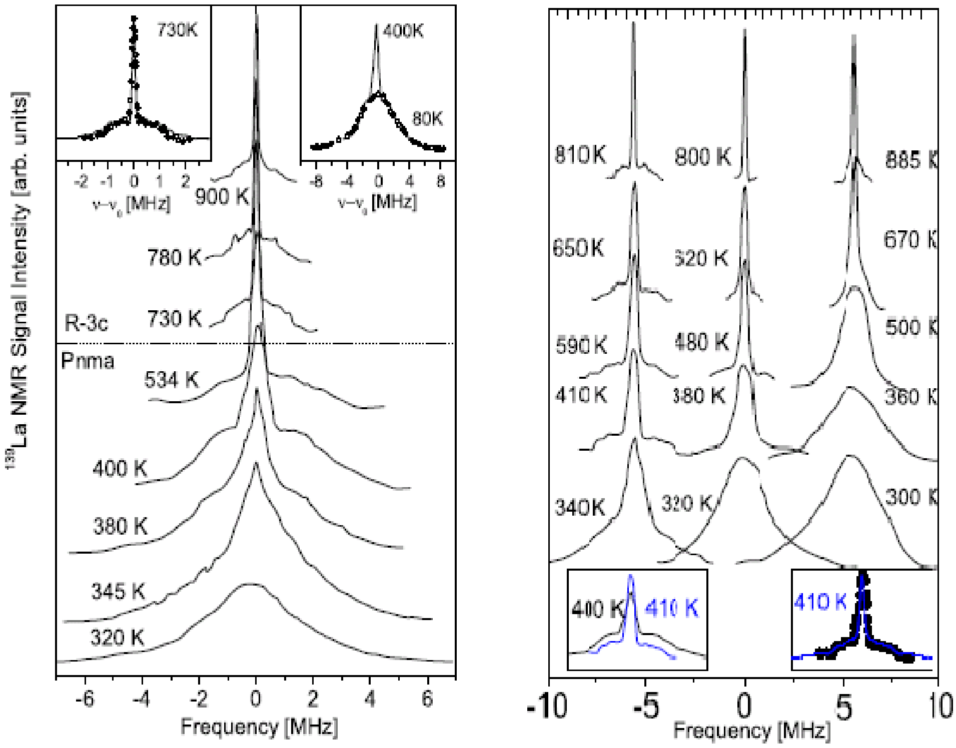
A high temperature NMR study in optimally doped manganites

N. Panopoulos, D. Koumoulis, M. Fardis, M. Pissas, and G. Papavassiliou

Institute of Materials Science, NCSR Demokritos, 152 10 Aghia Paraskevi, Attiki, Greece,

e-mail:panon@ims.demokritos.gr

Understanding the complex glassy phenomena, which accompany polaron formation in optimally doped manganites (ODM) is a cumbersome issue, which remains still unanswered. Here, on the basis of ^{139}La and ^{55}Mn NMR measurements, performed in the temperature range 80 K – 900 K we show that glass freezing, observed in the Paramagnetic phase of ODM $La_{0.67}Ca_{0.33}MnO_3$, is not a random uncorrelated process due to quenched disorder, but the signature of a collective spin-glass state, which for $T<T_c$ consolidates with the Ferromagnetic state in a new thermodynamic phase. Comparison with NMR measurements on $La_{0.77}Ca_{0.23}MnO_3$, $La_{0.59}Ca_{0.41}MnO_3$, and $La_{0.70}Sr_{0.30}MnO_3$, indicates that the key parameter is the magnitude of short range correlated polaronic distortions, which control (i) the stability of the spin glass phase component and (ii) the kind (first or second order) of the Paramagnetic to Ferromagnetic phase transition.



^{139}La spectra for LCMO(0.33, 0.23, 0.41) and LSMO(0.30) in 9.4 T external magnetic field.

PS1-29-126

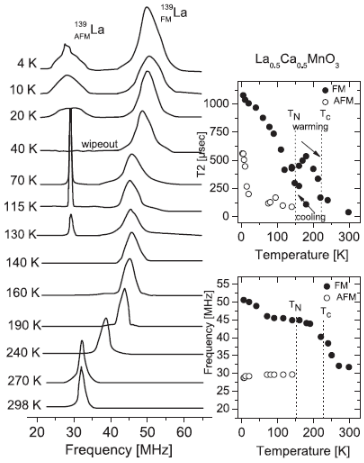
Incommensurate modulated spin order and NMR wipeout effect in electron-doped manganites probed by ^{139}La NMR

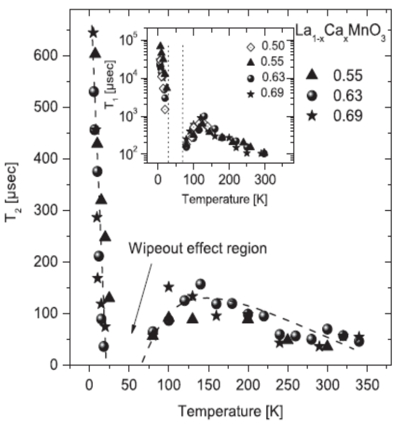
D. Koumoulis,[1,2] **N. Panopoulos**[1], **M. Fardis**[1], **M. Pissas**[1] **and G. Papavassiliou**[1]

[1] *Institute of Materials Science, NCSR, Demokritos, 153 10 Aghia Paraskevi, Athens, Greece,*
[2] *School of Chemical Engineering, National Technical University of Athens, 157 80 Athens, Greece, e-mail: dimkoumoulis@ims.demokritos.gr*

Hole doped transition metal oxides are famous due to their extraordinary charge transport properties, such as high temperature superconductivity (cuprates) and colossal magnetoresistance (manganites). Astonishing, the mother system of these compounds is a Mott insulator, whereas important role in the establishment of the metallic or superconducting state is played by the way that holes are self-organized with doping. Experiments have shown that by adding holes the insulating phase breaks into antiferromagnetic (AFM) regions, which are separated by hole rich clumps (stripes) with a rapid change of the phase of the background spins and orbitals. However, recent experiments in overdoped manganites of the $La_{1-x}Ca_xMnO_3$ (LCMO) family have shown that instead of charge stripes, charge in these systems is organized in a uniform charge density wave (CDW).

Nuclear Magnetic Resonance (NMR) has been a powerful local probe for a static and dynamic investigation of magnetic states due to the distribution of local magnetic fields in the sample via hyperfine interactions. In ^{139}La NMR the lanthanum nucleus (I=7/2) directly exhibits the magnetic state (FM or AF) of the nearest manganese ions neighbors. Here, by using ^{139}La NMR we provide direct evidence that the ground state of overdoped LCMO is indeed solitonic. By lowering temperature the narrow NMR spectra observed in the AFM phase are shown to wipe out, while for $T < 30$ K a very broad spectrum reappears, characteristic of an incommensurate (IC) charge and spin modulation. Remarkably, by further decreasing temperature, a relatively narrow feature emerges from the broad IC NMR signal, manifesting the appearance of a solitonic modulation as $T \rightarrow 0$.





References

[1] D. Koumoulis et al., *Physical Review Letters* **104**, 077204 (2010).
[2]G. Papavassiliou et al., *Physical Review Letters* **87**, 177204 (2001).

PS1-30-144

Magnetism in $CaFe_2As_2$ and Phase Separation in Superconducting $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ Single Crystals: A Mössbauer Study

D. R. Sánchez[1], **M. Alzamora**[2], **J. Munevar**[2], **S. L. Bud'ko**[3], **P. C. Canfield**[3], **G. F. Cheng**[4] **and E. M. Baggio-Saitovitch**[2]

[1]Instituto de Física, Universidade Federal Fluminense, Av. Milton Tavares de Souza, s/n –Campus da Praia Vermelha. 24210-346 Niterói. Rio de Janeiro, Brazil, e-mail: dalber@if.uff.br
[2] Centro Brasileiro de Pesquisas Fisicas. Rua Xavier Sigaud 150. Urca. CEP 22290-180. RJ, Brazil, e-mail: elisa@cbpf.br
[3]Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, e-mail:budko@ameslab.gov
[4]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, Peoples Republic of China

The ternary $A_{1-x}M_xFe_2As_2$ (A=Ca, Sr, Ba and Eu; M=K and Na) were found to have similar structural, magnetic and superconducting properties with the related $RFeAsO_{1-x}F_x$ [1]. The Ca_2Fe_2As undergoes a first-order high-temperature h-T tetragonal to low-temperature l-T orthorhombic phase transition at T_S~170K [2]. Concomitant with the structural transition the Fe moments order in a commensurate AFM structure [3]. This compound becomes superconducting either under moderate applied pressure and or Na-doping [4,5]. The $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ are superconductors with Tc ~37 K and ~35 K, respectively. μSR measurements have shown a coexistence of superconductivity and phase separated static magnetic order in these compounds [6].

Mössbauer spectroscopy have been used to investigate the magnetic and structural phase transition of $CaFe_2As_2$ as well as the occurrence of phase separation in superconducting $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ single crystals. A mosaic of single crystal plates, with the *c* axes parallel to γ-ray direction, were built to perform the Mössbauer transmission measurements. Room temperature measurements revealed that the main component of electric field gradient V_{zz} is along *c* axis for these ternary compounds. For the non superconducting $CaFe_2As_2$ an abrupt increase of the magnetic hyperfine field B_{hf} below T_N~170K was observed indicating a first-order magnetic transition. Low temperature spectra fits lead to $V_{zz} > 0$ with Fe moments lying in the (*a*,*b*) plane. The quadrupole splitting ΔE_Q values have a discontinuity at ~170K confirming that structural and magnetic transition occurs concomitantly. The Mössbauer spectra of $Ba_{0.5}K_{0.5}Fe_2As_2$ and $Sr_{0.5}Na_{0.5}Fe_2As_2$ have a unique crystal site for Fe at room temperature, however at 4.2K the presence of two phases is clearly seen. For $Ba_{0.5}K_{0.5}Fe_2As_2$ ~ 51% of Fe is in a paramagnetic state while the remaining is in a magnetic phase with small magnetic moments (~$0.15\mu_B$). For $Sr_{0.5}Na_{0.5}Fe_2As_2$ only ~12% of Fe are paramagnetic, the remaining Fe are in a magnetic state with magnetic moments of the order of ~$0.57\mu_B$.

[1]C. Krellner, et al., Phys. Rev B 78 (2008)100504.
[2] N. Ni, et al., Phys. Rev. B 78 (2008) 014523.
[3] A. I. Goldman, et al., Phys. Rev B 78 (2008) 100506.
[4] M. S. Torikachvili, et al., Phys. Rev Lett. 101 (2008) 057006.
[5] P. M. Shirage, et al., Appl. Phys. Express 1 (2008) 081702.
[6] T. Goko, et al., Phys. Rev B 80 (2009) 024508.

PS1-31-153

Magnetic and Electric Properties of Cadmium Films Containing Nanometer Size Clusters of Iron

William Trujillo[1] **Pablo Munayco**[1], **Elisa Baggio-Saitovitch**[1,] **F. Jochen Litterst**[2]

[1] *Brazilian Center for Research in Physics (CBPF), Brazil*
e-mail: william@cbpf.br
[2] *IPKM, TU Braunschweig, Germany*

Dilute magnetic impurities in non-magnetic metallic matrices have been intensively studied in for investigating single ion Kondo effect and the development of spin glassy behavior upon increasing magnetic interactions with dopant concentration. Here we report on an investigation of magnetic iron nano-clusters formed in non magnetic hosts with low solubility for iron. We will concentrate on films of cadmium in comparison with our earlier studies on silver films. Nanometer size clusters of iron can be formed in films containing iron in the range from 0.1 to several at% via vapor co-deposition. Characterization of samples was performed via X-ray diffraction, resistivity, magnetization, susceptibility, and Mössbauer spectroscopic measurements at various temperatures and applied magnetic fields. Up to concentrations of about 2 at% Fe the iron clusters are well defined as distinguished from their distinct hyperfine parameters.

Spin-freezing is traced from Mössbauer and magnetization data with freezing temperatures ranging from below 4 K up to about 15 K depending on cluster concentration. Models for describing the dynamic hyperfine spectra in this temperature range will be presented taking into account different mechanisms for cluster-cluster interactions.

Above the freezing temperature we can derive average cluster magnetic moments from magnetization data and also from the field dependence of the magnetic hyperfine fields at Fe obtained in applied external fields. Both macroscopic and local magnetic data are in good agreement yielding moments on the order of 15-20 μB for iron clusters in Cd films, compared with 35-40 μB found for Ag films. I.e., in both cases the clusters comprise only few atoms. The hyperfine spectra taken in applied field indicate a reduction of the iron moments at low temperatures which can be interpreted with moment compensation via conduction electron scattering. A competition between Kondo effect and the magnetic coupling of clusters via conduction electron polarization interaction could be clearly traced from the resistivity data of the silver films.

Whereas in films with iron concentrations up to about 2 at% we have controlled formation and growth of small clusters, this is no more the case for higher concentrations. Strong irreversibility in magnetization is found extending up to 100 K. The hyperfine data prove the presence of the same kinds of clusters as found for lower concentration yet with much bigger sizes.

PS1-32-156

Hyperfine local probe study of alkaline-earth manganites $BaMnO_3$ and $SrMnO_3$

J. N. Gonçalves[1], V. S. Amaral[1], J. G. Correia[2], H. Haas[2], A. M. L. Lopes[3], J. P. Araújo[4], P. B. Tavares[5]

[1] *Departmento de Física and CICECO, Universidade de Aveiro, 3810-193 Aveiro, Portugal*
[2] *Instituto Tecnológico e Nuclear, E.N. 10, 2686-953 Sacavém, CFNUL, Av. Prof. Gama Pinto 2, P-1699 Lisboa, Portugal*
[3] *Departamento de Física and IFIMUP, Universidade do Porto, 4169-007 Porto, Portugal*
[4] *Departamento de Química and CQ-VR, Universidade de Trás-os-Montes e Alto Douro, 1013, 5001-801 Vila Real, Portugal*

We report perturbed angular correlations (PAC) and first-principles calculations with ^{111m}Cd/^{111}Cd and ^{111}In/^{111m}Cd probes, implanted at the ISOLDE-CERN laboratory, in the compounds/polymorphs $BaMnO_3$-6H and $BaMnO_3$-15R and $SrMnO_3$-4H. Magnetic and structural studies were also performed.

The experiments are complemented with calculations of the electric field gradient (EFG), with density functional theory, by the LAPW method (Wien2k code [1]). Calculations consider different magnetic states, and for the case of $BaMnO_3$ the results from different polymorphs are analyzed. Comparison with the experimental results requires considering supercells with diluted Cd impurities, to account for the presence of the radioactive probe in the host material (ppm). The results of the calculations are checked for convergence with increasing dilution of Cd probes, corresponding to increasing size of the supercell. Based on the calculations, the assignment of the sites for the ^{111m}Cd and ^{111}In probes at the Ba (for $BaMnO_3$-6H) and Sr (SrMnO3-4H) sites gives good agreement for most cases. The EFG shows no visible changes with temperature in $BaMnO_3$-6H and $SrMnO_3$-4H, in the range 20-700 C, as shown in the figure). The PAC spectra of BaMnO3 in the two polymorphs reveal different frequencies. The results on $BaMnO_3$ using ^{111}In/^{111m}Cd, show an additional interaction frequency in comparison with Cd.

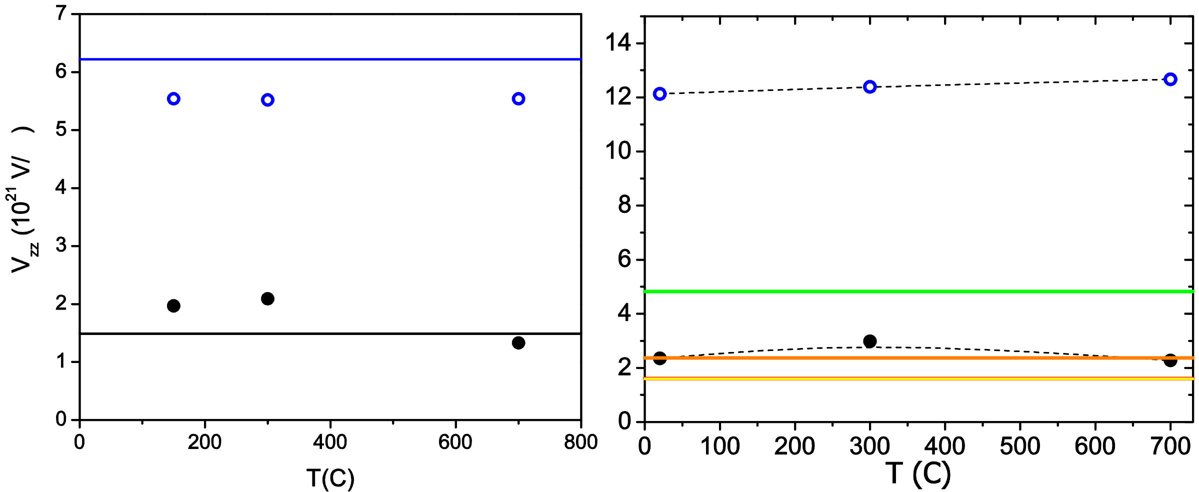


Fig.1. Experimental ^{111m}Cd PAC measured EFG (Vzz component) as a function of temperature (circles) and calculated EFG (horizontal lines). For $SrMnO_3$-4H(left) the two Sr sites are probed while for $BaMnO_3$-6H (right), only one of the Ba sites is probed. The (minoritary) higher frequency has no assignment and is probably associated with a defect.

[1] Blaha P. et al, WIEN2k, Technische Universitat Wien (ISBN 3-9501031-1-2), (2001).

PS1-33-161

Effect of deposition conditions on the characteristics of the thin films obtained by using Pulsed Laser Deposition

J. J. Dolo, **H.C. Swart, E. Coetsee, JJ Terblans and OM Ntwaeaborwa**

Department of Physics, University of Free State, P.O Box 339, Bloemfontein 9300, South Africa, e-mail: dolojj@qwa.ufs.ac.za

There has been extensive research on how the deposition conditions parameters (substrate temperature, background pressure, laser energy, laser fluency, laser repetition rate/number of pulses etc.) affect the characteristics (such as crystal structure and surface morphology) of the films grown. However the influence of deposition conditions on luminescence properties of films has not yet been extensively studied because it is a secondary effect and results mainly because of the change in crystal structure and the surface morphology of the films. This paper presents the effect of substrate temperature and oxygen partial pressure on the crystal structure, surface morphology and the luminescence characteristics of the $Gd_2O_2S:Tb^{3+}$ thin films grown using PLD. It was observed that oxygen pressure affects the structural properties of the $Gd_2O_2S:Tb^{3+}$ thin film and high quality layers can only be prepared in the narrow range of oxygen pressure between 100 and 200 mTorr. The oxygen pressure has a major effect on the film morphology. The films deposited at 100mTorr are very smooth and dense. The films deposited at 300mTorr are very rough with numerous cracks on their surface and display a porosity. These differences in film morphology is explained by the decrease of the kinetic energy of the deposited species with increasing oxygen pressure. Thin film deposited at 100 mTorr was found to be the best in terms of the PL intensity of the $Gd_2O_2S:Tb^{3+}$ emission, and thereafter the PL intensity decreased dramatically as the oxygen partial pressure increased. The main emission peak due to the $^5D_4$-$^7F_5$ transition is at a wavelength of 545 nm. The PL of the films grown at a higher substrate temperature was generally also more intense than those that were grown at a lower substrate temperature.

PS1-34-166

Tin, Manganese doped chromium iron oxides of composition α-$Sn_{0.2}Cr_{1.8-x}Fe_xO_3$ and α-$Mn_{0.2}Cr_{1.8-x}Fe_xO_3$

Mbela Kalengay,[1] **T Moyo**[1], **J Z Msomi**[2]

[1] *School of Physics, University of KwaZulu-Natal, Durban 4000, South Africa*
Mbelak@ukzn.ac.za
[2] *Department of Physics, University of Free State, Phuthaditjhaba 9866, South Africa*

We have investigated single phase formation in a series of (Sn, Mn)$_{0.2}$Cr$_{1.8-x}$Fe$_x$O$_3$ produced by low temperature synthesis based on hydrothermal process in a reflux system and in a stirred pressure reactor. The evolution of the properties is investigated by X-ray diffraction (XRD) and by magnetic measurements. Evidence of successful Sn or Mn incorporation into the corundum structure is obtained. ^{57}Fe Mössbauer spectra show the materials to be paramagnetic for Fe concentration $x \leq 0.5$ and in ordered magnetic state at higher concentration. Rietveld structure refinement of the XRD spectra is employed in the analysis.

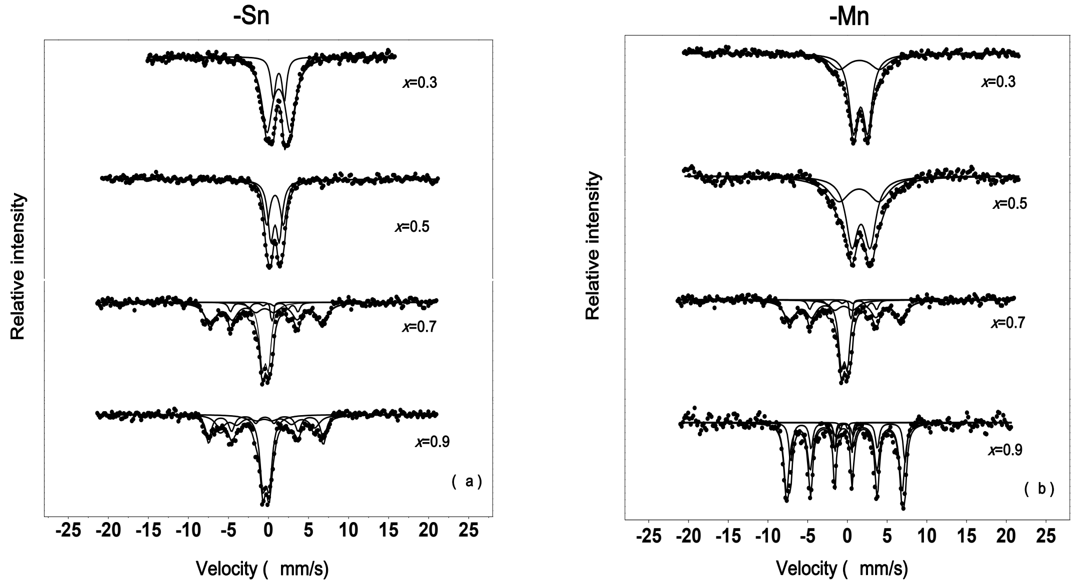


Fig. 1. Room-temperature transmission Mössbauer Spectra for (a) $Sn_{0.2}Cr_{1.8-x}Fe_xO_3$, and (b) $Mn_{0.2}Cr_{1.8-x}Fe_xO_3$.

References

[1] R. A. Young (Eds.), The Rietveld Method, Oxford University Press, New York, 1993.
[2] F. J. Berry, C. Greaves, M. Mortimer, J. G. Mc Manus, and G. Oates, *J. Solid State Chem.*, 1997, 130, 272.

PS1-35-77

Paramagnetism in Mn/Fe implanted ZnO

H. P. Gunnlaugsson[1], T. E. Mølholt[2], R. Mantovan[3], H. Masenda[4], D. Naidoo[4], W. B. Dlamini[5], R. Sielemann[6], K. Bharuth-Ram[5,7], G. Weyer[1] K. Johnston[8], G. Langouche[9] , S. Ólafsson[2], H. P. Gíslason[2], Y. Kobayashi[j10], M. Fanciulli[3,11] , ISOLDE Collaboration[8].

[1] *Department of Physics and Astronomy, Aarhus University, DK-8000 Århus C, Denmark,e-mail: hpg@phys.au.dk,* [2]*Science Institute, University of Iceland, IS-107 Reykjavík, Iceland,* [3]*Laboratorio MDM, IMM-CNR, Via Olivetti 2, 20041 Agrate Brianza (MB), Italy ,*[4]*School of Physics, University of the Witwatersrand, WITS 2050, South Africa,* [5]*School of Physics, University of KwaZulu-Natal, Durban 4001, South Africa,* [6]*Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany,* [7]*iThemba LABS, P.O. Box 722, Somerset West 7129, South Africa,* [8]*PH Dept, ISOLDE/CERN, 1211 Geneva 23, Switzerland,* [9]*Instituut voor Kern-en Stralings fysika, University of Leuven, B-3001 Leuven, Belgium,* [10]*The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-0198, Japan,* [11]*Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy.*

Prompted by the generally poor understanding [1,2] of the nature of magnetic phenomena in 3d-metal doped ZnO, we have undertaken on-line ^{57}Fe Mössbauer spectroscopy at the ISOLDE facility at CERN on ZnO single crystal in an external magnetic field of 0.6 T, following implantation of radioactive $^{57}Mn^+$ ($T_{½}$ = 1.5 min.) ions at room temperature. The Mössbauer spectra of the dilute Fe impurities are dominated by sextets whose angular dependence rules out an ordered magnetic state, but are well accounted for on the basis of Fe^{3+} paramagnetic centres with long relaxation times.

Mössbauer spectra are shown in Fig. 1, obtained under the conditions indicated. The spectra have been analyzed in terms of a superposition of three sextets originating from the three Kramers doublets belonging to the $S_Z = \pm 5/2$, $\pm 3/2$ and $\pm 1/2$ crystal field states [3]. In addition, doublets assigned to substitutional Fe^{2+} (D2) and interstitial Fe (D3) are included [4]. The disappearance of the $\Delta m_I = 0$ nuclear transition for a $S_Z = \pm 3/2$ electronic state in the $\theta = 0°$ measurements evidences that these sextets originates from Fe^{3+} in a paramagnetic state with unusually long spin-lattice relaxation times. This is attributable to the weak coupling of the spherical ^{6}S ground state of Fe^{3+} to the lattice. Fe^{2+}, shows fast relaxation, and is observed as a quadrupole split doublet. The results provide direct insight in the charge states of the Fe ions and their lattice sites.

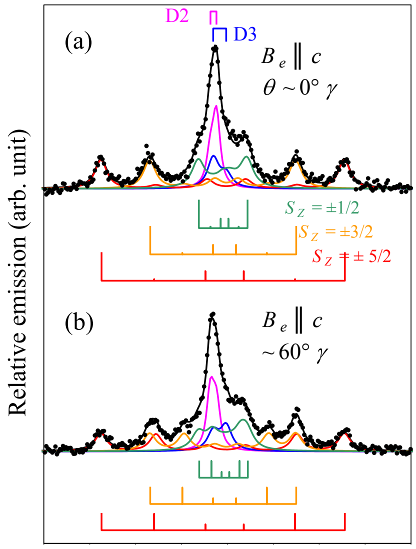


Fig. 1. Room temperature Mössbauer spectra obtained in B_e = 0.6 T applied parallel to the *c*-axis and at two different emission angles (θ) relative to the *c*-axis as indicated.

References

[1] A. Koji, *Science* **312**, 1883 (2006).
[2] Ü. Özgür, Ya. I. Alivov, C. Liu, A. Teke, M.A. Reshchikov, S. Doğan, V. Avrutin, S.J. Cho, and H. Morkoç, *J. Appl. Phys.* **98**, 041301 (2005).
[3] H. H. Wickman, and G. K. Wertheim, *Phys. Rev. B* **148**, 211 (1966).
[4] G. Weyer, H. P. Gunnlaugsson, R. Mantovan, M. Fanciulli, D. Naidoo, K. Bharuth-Ram, and T. Agne, *J. Appl. Phys.* **102**, 113915 (2007).

PS1-36-40

Absence of room temperature ferromagnetism in transition metal doped ZnO nanocrystalline powders from PAC spectroscopy

Rakesh Dogra[1], Moacir R. Cordeiro[2], Artur W. Carbonari[2], Rajendra. N. Saxena[2]

[1]*Beant College of Engineering & Technology, Gurdaspur-143 521, India.*
[2]*Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN, São Paulo, SP, Brazil.*

An extensive research efforts have been carried out worldwide on searching for room temperature ferromagnetism in transition metal doped ZnO, especially in Mn- and Co-doped ZnO, for its potential use in future spintronic devices. However, the results are not consistent: some studies reported observation of room-temperature ferromagnetism in Mn- and Co-doped ZnO whereas others reported absence of ferromagnetism. The effect of Cu co-doping, a possible pathway for inducing ferromagnetism has also been observed in transition-metal-doped ZnO. It is therefore still questionable whether transition metal doped ZnO is really a ferromagnetic at room temperature!

In the present work, the local structural and electronic environment around ^{111}In probe atoms in pure ZnO, transition metal doped $Zn_{1-x}T_xO$ (T=Mn and Co; x=0.01, 0.02, 0.05) and Cu co-doped $Zn_{1-x}Co_xCu_{0.01}O$ (x=0.01-0.04) nanocrystalline powders have been monitored on an atomic scale by a perturbed angular correlation (PAC) spectroscopy. For these measurements, the single phase nanocrystalline powders were synthesized at low annealing temperature by sol-gel Pechini method. Phase purity and structure refinement done by means of the Rietveld analysis technique showed that the dopants substitute properly into Zn cation sites. The PAC measurements (Figure 1) exhibited the well known oscillations corresponding to the electric quadrupole interaction only (ν_Q~31 MHz) which have been attributed to the substitutional incorporation of the ^{111}In probe atoms at the cation sites of ZnO lattice. The present measurements did not reveal any evidence of magnetic ordering down to 77 K in pure or doped ZnO nanocrystalline powders. These results are consistent with the recent observation of paramagnetic behavior in transition metal doped ZnO with synchrotron based studies [1,2].

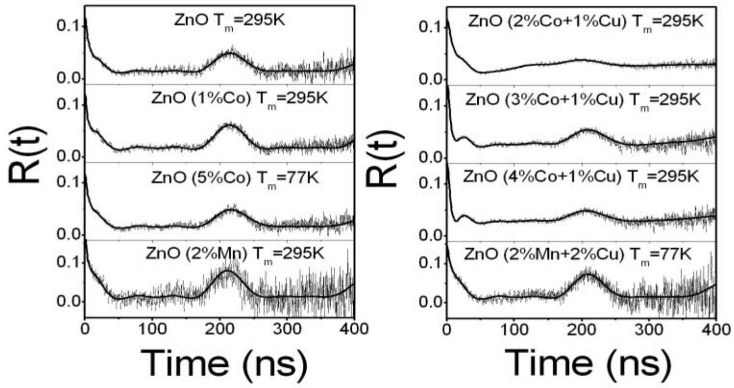


Figure 1: Least squares fitted PAC spectra for pure and doped ZnO with ^{111}In probes.

[1] A. Ney, et al., Phys. Rev. Lett. 100, 157201 (2008).
[2] N R S Farley, et al., New Journal of Physics 10, 055012 (2008).

PS1-37-52

X-ray absorption and magnetic circular dichroism characterizations of $Mo_{1-x}Fe_xO_2$ (x = 0 – 0.05) thin films grown by pulsed laser ablation

<u>P. Thakur</u>[1], J. C. Cezar[1], N. B. Brookes[1], R. J. Choudhary[2], D. M. Phase[2], K. H. Chae[3], and Ravi Kumar[4]

[1]European Synchrotron Radiation Facility, BP220, 38043 Grenoble cedex, France, e-mail: thakur@esrf.fr
[2]UGC-DAE Consortium for Scientific Research, Indore 452001, India
[3]Nano Analysis Centre, Korea Institute of Science and Technology (KIST), Seoul 136-791, Korea
[4]Centre for Materials Science and Engineering, National Institute of Technology, Hamirpur 177005 (H.P), India

In the several last years, molybdenum oxide has attracted attention because of its potential applications in gas sensing devices, optically switchable coatings, catalysis, etc. Besides the above-mentioned attractive physical and optical applications, if another degree of dimensionality in terms of magnetic properties could be induced in the system by doping some magnetic impurity, the resulting device would be a boost to the existing MoO_x based technology. This is the aim of this study.

Well characterized thin films of undoped and Fe (0–5 at. %) doped MoO_2 were grown on *c*-plane sapphire single crystal substrates by pulsed laser ablation technique [1,2]. The near edge X-ray absorption fine structure (NEXAFS) measurement at O K, Mo $M_{3,2}$, Fe $L_{3,2}$-edges, and X-ray Magnetic Circular Dichroism (XMCD) at Fe $L_{3,2}$-edges have been carried at the ID08 beam line of the European Synchrotron Radiation Facility to understand the electronic structure changes, relative stability of cation distributions and the responsible magnetic interactions at room temperature. The O *K*-edge NEXAFS spectra reveal that the intensity of O 2*p*–Mo 4p hybridized states changes with the Fe dilution and can be interpreted in terms of competition between hybridization of Mo 4p and Fe 3d with O 2p orbitals. The Mo M-edges exhibit a signature of mixed valance Mo^{4+}/Mo^{5+} ions. The Fe $L_{3,2}$ absorption spectra shows a similar spectral profile; on the other hand, the XMCD spectra show the characteristic fine structure with ferromagnetic ordering at room temperature. These differences are attributed to the variety of 3d electron configuration of Fe ions (Fe^{2+}/Fe^{3+}) and the local symmetry (tetrahedral/octahedral) [3]. The cation distributions at different sites exhibit a significant variation with the change in iron concentration indicating the strong correlations between charge and spin of the electrons.

References:

[1] R. Prakash, D. M. Phase, R. J. Choudhary, and R. Kumar, J. Appl. Phys. **103**, 043712 (2008).
[2] P. Thakur, J. C. Cezar, N. B. Brookes, R. J. Choudhary, R. Prakash, D. M. Phase, K. H. Chae, and Ravi Kumar, Appl. Phys. Lett. **94**, 062501 (2009).
[3] J.-Y. Kim, T.Y. Koo, and J.-H. Park, Phys. Rev. Lett. **96**, 047205 (2006).

PS1-38-29

Features of Structural Transformations in $La_{1-x}Ca_xMn_{0.98}Fe_{0.02}O_{3+\delta}$ (x = 0.05 – 0.50)

Vera Sedykh,[1] **Vyacheslav Rusakov**[2]

[1] *Laboratory of Structural Investigations, Institute of Solid State Physics, Russian Academy of Sciences, Instutute str. 2, Chernogolovka, Moscow district, 142432, Russia*
e-mail: sedykh@issp.ac.ru
[2] *Moscow State University, Russia*

The lanthanum manganite compounds doped with a divalent impurity are the materials with colossal magnetoresistance and widely used in different fields of modern engineering. In lanthanum manganites manganese has a mixed valence: Mn^{3+} and Mn^{4+}. Mn^{3+} is the Jahn-Teller ion with a degenerated orbital state of electrons. The main feature of the compounds with Jahn-Teller ions is strong correlation between lattice and electron subsystems. These compounds are characterized by strong lattice distortions.

The features of structural transformations in $La_{1-x}Ca_xMn_{0.98}Fe_{0.02}O_{3+\delta}$ (x = 0.05 – 0.50) as a function of Ca concentration have been studied by Mössbauer spectroscopy and X-ray diffraction analysis. For x = 0.05 and 0.10 the rhombohedral phase (space group R-3c) has been shown to be synthesized. Beginning from x = 0.20 the structure of the origin synthesized samples is orthorhombic (space group Pnma). Varying the heat treatment conditions it is possible to transit from one phase to another. The phases are subsequently suppressed with an increase in a Ca concentration. For Ca concentrations less than 20% all set of the phases with reversible structural transitions PnmaII ↔ PmnaI ↔ R-3c can be obtained under heat treatment like in the Ca-undoped compound $LaMn_{0.98}Fe_{0.02}O_{3+\delta}$. The rhombohedral phase is suppressed for x = 0.20. When a Ca concentration higher than 20%, the PnmaII phase is suppressed, as a result, only the PnmaI phase remains which is stable under any heat treatment.

Mössbauer spectra for the PnmaI and R-3c phases have relatively narrow lines and were processed by single doublet. Spectra for the PnmaII phase represent strongly broadened quadrupole-splitting (QS) doublets. A large QS value is related to the strong lattice distortion due to the Jahn-Teller effect. Since the spectra for the PnmaII phase have a smooth shape, they were processed by the QS distribution.

Doping with divalent Ca occupying trivalent La positions generates vacant oxygen sites in the lattice. Therefore already during synthesis a part of Jahn-Teller Mn^{3+} ions transfers to Mn^{4+} and oxygen coming with Mn^{4+} should occupy first of all these oxygen sites. Under oxidation (annealing in air) the Mn^{4+} ion concentration increases and excess oxygen will now occupy interstitial positions.

Based on the analysis of the obtained experimental data it is possible to suppose that the reversibility of the phase transitions is possible only when excess oxygen is in interstitial positions in the lattice. If excess oxygen occupies only vacant sites in the lattice, the phase transitions are absent.

The features of the phase formation in the basic undoped compound $LaMnO_{3+\delta}$ and in the Ca-doped compound $La_{1-x}Car_xMn_{0.98}Fe_{0.02}O_{3+\delta}$ are compared.

The work was supported by the Russian Foundation for Basic Research (project no. 09--02--00767) and by the Program of Russian Academy of Sciences "Physics of Condensed Media".

PS1-39-17

Experimental and theoretical study of the σ-phase in Fe-Cr and Fe-V alloys

Jakub Cieslak,[1] **Janusz Tobola,**[1] **Stanislaw M. Dubiel**[1]

[1] *Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Krakow, Poland*
e-mail: cieslak@novell.ftj.agh.edu.pl

Mössbauer spectra of a series of a σ-phase Fe-V and $Fe_{53.8}Cr_{46.2}$ alloys in the paramagnetic state were analysed using electronic structure calculations by the KKR technique as shown in details in [1]. A wide spectrum of various nearest neighbour atomic configurations, within the complex thirty atom tetragonal unit cell with five sublattices, was taken into account in order to obtain isomer shift parameters for the five lattice sites. Quadrupole splitting values were estimated on the basis of an extended point charge model. The predicted values (IS, ΔIS and QS) combined with the measured probabilities of Fe occupancy allowed to successfully fit the Mössbauer spectra, using only five adjustable parameters [2]. The resulting average IS-values for the Fe-V σ-phase subspectra are found to be more negative then the corresponding ones of the Fe-Cr system. The QS-values for the latter are similiar to the former system, except two values, were they are significantly smaller. The overall shape of the Mössbauer spectrum is also influenced by the different Fe occupation parameters and, consequently, relative subspectra intensities.

The spin-polarized charge self-consistent KKR method was applied to the σ-$Fe_{53.8}Cr_{46.2}$ and the results obtained have been applied to analyze the magnetic structure of the sample at 0K. They enabled determination of Fe and Cr atoms magnetic moments for all five sublattices, which were found oriented opposite. Also the magnetic structure of the unit cell has been revealed and will be discussed. The calculated average magnetic moment per unit cell is equal to 15.6mB, and that per atom to 0.52mB. Corresponding experimental values determined from magnetization measurements are 4.3mB and 0.14mB i.e. smaller by a factor of 4 [3]. For that reason and because of symmetry analysis predictions, the antiferromagnetic-like ordering was proposed and analysed. The discrepancy between the calculated and the measured values has been significantly reduced - the calculated average magnetic moment per unit cell decreased to 6.0mB, and that per atom to 0.20mB, which is comparable to the measured values.

References

[1] A. Bansil, S. Kaprzyk, P.E. Mijnarends and J. Tobola, Phys. Rev. B, 60 13396 (1999)
[2] J. Cieslak, J. Tobola, S.M. Dubiel, S. Kaprzyk, W. Steiner and M. Reissner, J. Phys.: Condens. Matter 20 235234 (2008)
[3] J. Cieslak, M. Reisner, W. Steiner and S. M. Dubiel, Phys. Stat. Sol. (a) , 205 1794 (2008)

PS1-40-141

Detection of sub-lattice magnetism in sigma-phase Fe-V compounds by zero-field NMR

S.M. Dubiel[1*], **J.R. Tozoni**[2], **J. Cieślak**[1], **D.C. Braz**[2], **R. Oliveira-Silva**[2], **E.L.G. Vidoto**[2], **T.J. Bonagamba**[2]
Dubiel@novell.ftj.agh.edu.pl

[1]*Faculty of Physics and Computer Science, AGH University of Science and Technology, PL-30-059 Kraków, Poland*
[2]*Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, São Carlos, 13560-970, São Paulo, Brazil.*

A sigma-phase can be produced by a solid-state reaction in some alloy systems in which at least one constituent is a transition element. It has a tetragonal crystallographic structure and its unit cell contains 30 atoms that are distributed over five different crystallographic sites A, B, C, D and E. Because of a high coordination numbers (12-15), the phase belongs to a family of the so-called Frank-Kasper phases. Among over 50 binary alloys in which the sigma-phase was found, only that in the Fe-Cr and Fe-V alloys has well evidenced magnetic properties [1-6]. Despite first magnetic investigations of the sigma-phase were carried out over 40 years ago [2,3], its magnetism, which is usually termed as weak and low temperature, is not well understood, which prompts and justifies further studies. The first successful measurements of a sub-lattice magnetism with ^{51}V zero-field NMR techniques in the sigma-phase $Fe_{100-x}V_x$ alloys with x = 34.4, 39.9 and 47.9 are shown in Figure 1.

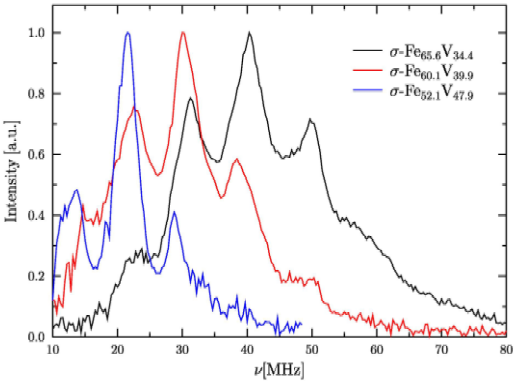


Fig. 1: ^{51}V NMR spectra recorded at 4.2 K for samples with Fe-contents *(1-x)* equal to 65.6, 60.1 and 52.1.

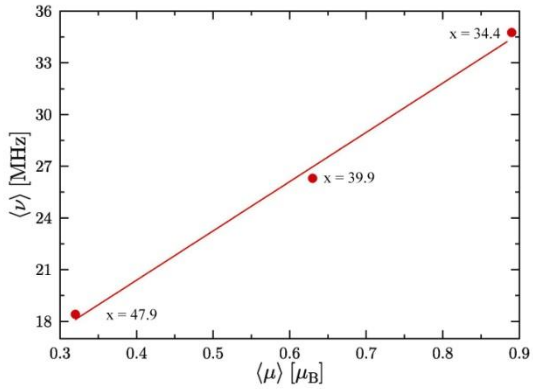


Fig. 2 The average frequency of the spectra versus the average magnetic moment per Fe atom, $<\mu>$.

Despite not being magnetic, Vanadium atoms, which were revealed to be present on all crystallographic sites [7], produce magnetic resonance signals due to the transferred magnetic field produced by the neighboring ^{57}Fe atoms. Their magnetic properties are characteristic of a given site, and for a given site they intensely depend on the composition. The strongest magnetism exhibit sites A and the weakest one sites D. The estimated average magnetic moment per V atom decreases from 0.36 μ_B for x = 34.4 to 0.20 μ_B for x = 47.9. As displayed in Fig. 2, the magnetism revealed at V atoms is linearly correlated with the magnetic moment of Fe atoms, which implies that the former has been induced by the latter.

References

[1] E. O. Hall and S. H. Algie, Metall. Rev., **11**, 61 (1966)
[2] D. A. Read and E. H. Thomas, IEEE Trans. Magn., MAG-**2,** 415 (1966)
[3] D. A. Read, E. H. Thomas and J. B. Forsythe, J. Phys. Chem. Solids, **29,** 1569 (1968)
[4] J. Cieślak, M. Reissner, W. Steiner and S. M. Dubiel, J. Magn. Magn. Mater., **272-276,** 534 (2004)
[5] J. Cieślak, M. Reissner, W. Steiner and S. M. Dubiel, Phys. Stat. Sol (a), **205,** 1794 (2008)
[6] J. Cieślak, B.F.O. Costa, S.M. Dubiel, M. Reissner and W. Steiner, J. Magn. Magn. Mater., **321**, 2160 (2009)
[7] J. Cieślak, M. Reissner, S. M. Dubiel, J. Wernisch and W. Steiner, J. Alloys Comp., **205,** 20 (2008)

Poster session II
Tuesday 14th September 2010
15:40 – 17:00

Mezzanine

PS2-1-26

Search for ferromagnetic ordering in Pd doped wide band gap semiconductors GaN and ZnO

P. Kessler[1], K. Müller[1], Th. Geruschke[1], H. Timmers[2], A. P. Byrne[3], R. Vianden[1]

[1] *Helmholtz – Institut für Strahlen- und Kernphysik, 53115 Bonn, Germany, e-mail:* kessler@hiskp.uni-bonn.de

[2] *School of Physical, Environmental and Mathematical Sciences, The University of New South Wales at the Australian Defence Force Academy, Canberra ACT 2600, Australia*

[3] *Department of Nuclear Physics, Research School of Physics and Engineering, The Australian National University, Canberra ACT 0200, Australia*

GaN and ZnO are candidates for dilute magnetic semiconductors with Curie temperatures above room temperature [1]. Doping with transition metals (TM) like Co, Mn or Fe is a simple way to create such systems. The PAC probe ^{100}Pd/^{100}Rh is isoelectronic to cobalt and therefore a perfect tool to investigate the incorporation of TM´s into these compounds as well as the influence of other impurities onto the internal magnetic fields. (0001) and (1010) oriented ZnO single crystals samples, freestanding GaN films and GaN thin films on 6 µm thick sapphire substrates were recoil-implanted with the ^{100}Pd/^{100}Rh probe as described in detail elsewhere [1]. The probe was produced using the fusion evaporation reaction ^{92}Zr(^{12}C,4n)^{100}Pd at a beam energy of 70 MeV. After recoil implantation PAC spectroscopy was performed at room temperature. The samples were measured as-implanted, and following isochronal annealing for 10 min at increasing temperatures. First results without and with an applied external magnetic field (Fig. 1) are indicative of a strongly disturbed lattice vicinity of Pd impurities in both hosts. No signs of spontaneous ferromagnetic ordering were observed.

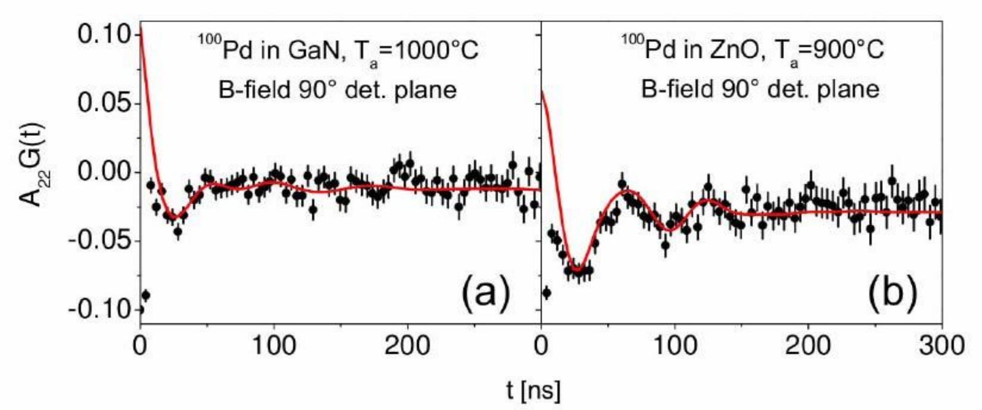


Figure 2 Measured ratio functions for (a) GaN and (b) ZnO placed in a 0.5 T external magnetic field. In both cases the influence of the external field can be seen from the oscillation of the function at a frequency much higher than that observed without magnetic field.

References

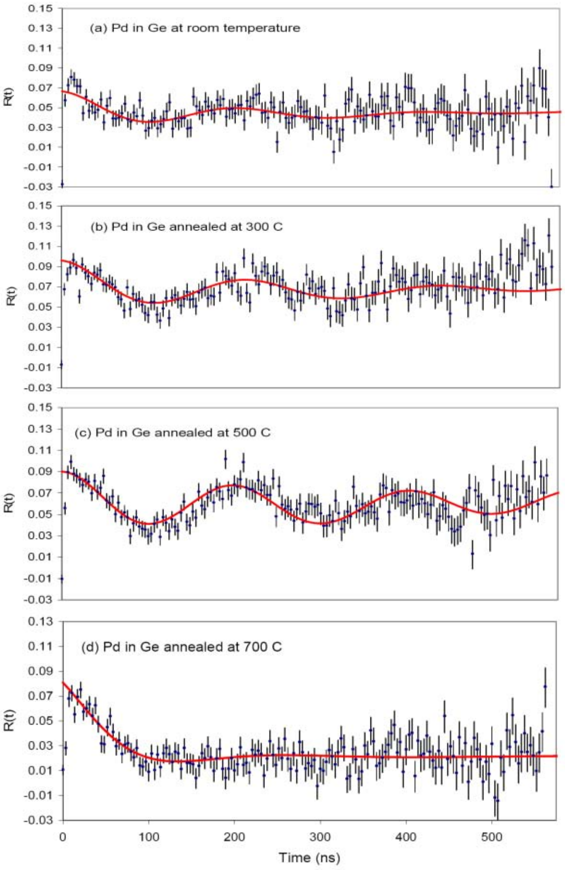
[1] T. Dietl, *Science*, **287**, 1019 (2000).
[2] E. Bezakova, *Ph.D. thesis*, Australian National University, Canberra, (1998).

PS2-2-28

Evidence of defect pairing for Pd-atoms in Germanium

H. Timmers[1], W. Kemp[1], A. P. Byrne[2], M.C. Ridgway[2], R. Vianden[3], P. Kessler[3]

[1] *School of Physical, Environmental and Mathematical Sciences, University of New South Wales at the Australian Defence Force Academy, Canberra, Australia*
e-mail: H.Timmers@adfa.edu.au
[2] *Research School of Physics and Engineering, Australian National University, Canberra, Australia*
[3] *Helmholtz – Institut für Strahlen- und Kernphysik, 53115 Bonn, Germany*



The relevance of germanium in current transistor technology is rising. An example is the addition of a germanium layer between an active silicon and a relaxed SiGe layer to create a p-type metal-oxide-semiconductor field effect transistor with enhanced hole mobility. Using the probe nucleus ^{100}Pd/^{100}Rh the local defect dynamics of Pd-atoms in germanium has been studied with time differential perturbed angular correlation spectroscopy (TDPAC). In addition to Pd, results may inform on the behaviour of isoelectronic atoms, such as cobalt. The effect of codoping with Ga, As and In atoms on Pd-related defects has also been explored.

The ^{100}Pd/^{100}Rh probe was recoil-implanted at the 14UD accelerator in Canberra into germanium single crystal samples and samples, pre-implanted with 10^{16} ions/cm^2 of Ga, As and In, respectively. The probe ($t_{1/2}$ = 3.6 d) was produced using the fusion evaporation reaction ^{92}Zr(^{12}C,4n)^{100}Pd at a beam energy of 70 MeV [1]. After recoil-implantation TDPAC spectroscopy was performed at room temperature. The samples were measured as-implanted and following isochronal annealing in vacuum for 20 min at 300°, 500°, 600°, and 700°C.

The figure displays measured ratio functions and fits for ^{100}Pd/Rh in germanium. The measurement on the as-implanted germanium shown in (a) indicates a low frequency modulation of the ratio function. The amplitude of this modulation increases with increasing annealing temperature. The modulation is most pronounced in the ratio function obtained after annealing at 500 °C. Further annealing at 700 °C removes the effect as shown in (d). A similar result has been obtained for ^{100}Pd/Rh in silicon, where the probe pairs with vacancy defects [2].

The observed effect appears to persist in germanium pre-implanted with Ga, As or In. TDPAC spectroscopy of the same samples using the probe ^{111}In/^{111}Cd is underway.

References

[1] E. Bezakova, 1998, *Ph.D. thesis*, Australian National University, Canberra.
[2] Dogra R., Byrne A.P., Ridgway M.C., 2009, Journal of Electronic Materials, Vol. **38**, No. **5**.

PS2-3-42

Oxygen ordering in the $HgBa_2CaCu_2O_{6+\delta}$ high-T_C superconductor

Tania M. Mendonca,[1] **Joao G. Correia**[2], **Heinz Haas**[2], **Philippe Odier**[3], **Pedro B. Tavares**[4], **Armandina M.L. Lopes**[5], **Joao Pedro Araujo**[1], **Manuel R. da Silva**[5], **Celine Darie**[3]

[1] *IFIMUP and IN – Institute of Nanosciences and Nanotechnology, Dep. De Física da Faculdade de Ciências da Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto, Portugal, e-mail: tania.de.melo.mendonca@cern.ch*
[2] *Instituto Tecnológico e Nuclear, E.N.10, 2686-953 Sacavém, Portugal*
[3] *Institut Néel, CNRS, Av. des Martyrs 25, F-38042 Grenoble CEDEX 9, France*
[4] *Centro de Química – Vila Real, Departamento de Química, Universidade de Trás-os-Montes e Alto Douro, 5001-911 Vila Real, Portugal*
[5] *Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto 2, 1649-002 Lisboa, Portugal*

Lattice sites and collective ordering of oxygen atoms in $HgBa_2CaCu_2O_{6+\delta}$ (Hg-1212) were studied using the Perturbed Angular Correlation technique. The electric field gradients (EFG) at ^{199m}Hg nuclei have been measured allowing a full characterization of the Hg neighborhood charge distribution as function of the oxygen doping on the Hg planes. The experiments have been performed at different annealing conditions, under argon flow or oxygen pressure up to 152 bars. In comparison with the data and calculations obtained for oxygen and fluorine doping in Hg1201, the analysis hints that at high concentrations oxygen atoms order in a different way than the reported previously. Furthermore, the experimental results show that a local scale there is a non-uniform oxygen distribution.

A series of ab-initio calculations, simulating different oxygen doping configurations, is also presented. Several $Hg_mBa_{2m}Ca_{m-1}Cu_mO_{6m+n}$ supercells, for different nominal oxygen concentrations, have been constructed. The simulated results are further compared with the experimental ones. Moreover, the possibility of the existence of oxygen dumbbell molecules, instead or coexisting with single atoms in the center of the Hg mesh is discussed. Atomic stripe-like oxygen configuration and the location of oxygen atoms in the $(0, \pm 1/2, z_{Hg})$ position are experimentally excluded.

PS2-4-53

Perturbed γ-γ angular correlation studies of indium containing 211-MAX phases

Daniel Jürgens[1]*, Michael Uhrmacher*[1]*, Hans Hofsäss*[1]*, Ulrich Vetter*[1]*,*
Jose Mestnik-Filho[2] *and Michel Barsoum*[3]

[1] *II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1 37077 Göttingen, Germany. Presenting Author e-mail: djuerge@gwdg.de*
[2] *Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil*
[3] *Dep. Material Science and Engineering, Drexel University, Philadelphia, PA 19104, USA*

The $M_{n+1}AX_n$ (MAX) phases, where n is 1, 2 or 3, are nanolaminated layered hexagonal carbides and nitrides, which feature an unusual set of attributes of both metals and high-performance ceramics. Theses intermetallic compounds can be good electrical and thermal conductors, behave elastically stiff as well as high thermal shock resistant and damage tolerant.

To investigate the local structure of these phases, the technique of perturbed angular correlation (PAC) was used for material characterization beside X-ray diffraction and electron microscopy. Radioactive ^{111}In ions were implanted at 400 keV into the samples, sensing as spies their local environment via hyperfine interactions.

The PAC technique was applied to the 211-MAX phases Ti_2InC, Zr_2InC and Nb_2InC to determine strength and symmetry of the electric field gradients (EFG) as a fingerprint for probe atoms on the A-site. In each material an axially symmetric EFG was found with a characteristic quadrupole coupling constant ν_Q varying between 200 MHz and 350 MHz. Regarding to the question of lattice location we demonstrate that the In-probes occupy the A-site since In is the self-atom on the unique A-site in these phases and by comparing the experimental results with *ab initio* DFT calculations using the FP-LAPW+LO method implemented in the WIEN2k package..

PS2-5-55

Perturbed γ-γ angular correlation studies of indium free 211-MAX phases

Daniel Jürgens[1], *Michael Uhrmacher*[1], *Hans Hofsäss*[1], *Ulrich Vetter*[1],
Jose Mestnik-Filho[2] *and Michel Barsoum*[3]

[1] *II. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1 37077 Göttingen, Germany. Presenting Author e-mail: djuerge@gwdg.de*
[2] *Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil*
[3] *Dep. Material Science and Engineering, Drexel University, Philadelphia, PA 19104, USA*

Nanolaminated layered ternary carbides and nitrides, the so called $M_{n+1}AX_n$ phases where M is an early transition metal, A an A-group element (mostly IIIA and IVA), X either carbon and/or nitrogen and n = 1-3, have attracted great attention recently. By now over 60 compounds are known which feature a unique combination of the best attributes of both metals and high-performance ceramics. This class of materials possesses for instance good electrical and thermal conductivities as well as considerable damage tolerance and high temperature oxidation resistance.

The method of perturbed angular correlation (PAC) was chosen for material characterization complementary to X-ray diffraction and electron microscopy. The PAC technique was applied in extension to previous experiments on In-containing Ti_2InC and Zr_2InC (see first abstract) for the first time to Nb_2AlC, Nb_2AsC, Ti_2AlN and Cr_2GeC. R(t) spectra were taken after different annealing steps to determine strength and symmetry of the electric field gradients (EFG) as a fingerprint for probe atoms on a specific lattice site and local surrounding. Each material showed axially symmetric EFGs similar to the ones found in the indium containing phases. Consequently we assume that these EFGs are due to probes occupying the A-site. This assumption is supported by ab initio DFT calculations using the FP-LAPW+LO method implemented in the WIEN2k package. During the course of annealing in some of the MAX phases, other smaller EFGs appeared which might be explained by probes on the M-site. To verify this prediction further calculations are needed and planned for the near future.

PS2-6-61

Experimental and ab initio study of Ta-doped ZnO semiconductor

E. L. Muñoz[1], D. Richard[1], P.D Eversheim[2], and M.Rentería[1]

[1]*Departamento de Física and Instituto de Física La Plata (IFLP, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina, emails:munoz@fisica.unlp.edu.ar, richard@fisica.unlp.edu.ar*

[2]*Helmholtz-Institut für Strahlen- und Kernphysik (H-ISKP), Universität Bonn, Nussallee 1416, 53115 Bonn, Germany.*

In the last years, *ab initio* calculations performed in the framework of the Density Functional Theory (DFT) have been successfully applied to the study of doped oxide semiconductors. The Full-Potential Augmented Plane Wave plus local orbitals (FP-APW+lo) method enables to determine the Electric-Field-Gradient tensor (EFG) at impurity sites localized in cation sites of the host structure with very good precision. From an *ab initio* - experimental study, the electronic structure and structural relaxations produced by the inclusion of the Perturbed Angular Correlation (PAC) tracers in the host system can be determined [1,2,3] .

In this work, we present PAC results in polycrystalline ZnO semiconductor implanted with (^{181}Hf→)^{181}Ta probes. The FP-APW+lo calculations in Ta-doped ZnO were carried out using the supercell method and varying self-consistently the charge state of the impurity. Ta is a triple donor impurity with respect to Zn^{2+} in ZnO and thus it can loose 1, 2 or 3 donor electrons under certain circumstances. The comparison between the experimental EFG results and our *ab initio* predictions suggests that the Ta impurity may be in a completely ionized charge state, i.e., with the 3 donor electrons removed from the impurity.

References

[1] L.A. Errico et al., *Phys. Rev. Lett.* **89**, 55503 (2002).
[2] L.A. Errico et al., *Phys. Rev. B* **67**, 144104 (2003).
[3] G. N. Darriba et al., *Phys. Rev. B* **79**, 115213 (2009).

PS2-7-66

An In-defect complex as a possible explanation for high luminous efficacy of InGaN and AlInN based devices

Patrick Keßler[1], Katharina Lorenz[2], Sérgio M. C. Miranda[2], João G. Correia[2], Karl Johnston[3], Reiner Vianden[1], ISOLDE collaboration

[1] *Helmholtz-Institut für Strahlen-und Kernphysik, 53115 Bonn, Germany,*
e-mail: kessler@hiskp.uni-bonn.de
[2] *Instituto Tecnólogico e Nuclear, P-2686-953 Sacavém, Portugal*
[3] *Technische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany*

InGaN based LEDs show a high luminous efficacy despite a high defect concentration. These defects, mainly threading-dislocations that form during the growth of GaN films would normally lead to nonradiative recombination of excitons. However, it seems that such non-radiative recombination is efficiently suppressed in In-containing alloys.

The role of indium in GaN and AlN films is investigated with the method of the perturbed angular correlation (PAC) using PAC probe ^{111}In. In addition to In on substitutional Ga sites we observe an In-Nitrogen-vacancy (V_N) defect complex, that could be a competing exciton trap and may be involved in the processes leading to the high efficacy.

The observed In-V_N complex is stable up to high temperatures, but is masked above 400 K [1]. This can be explained by assuming that the Cd-V_N complex which is formed after the electron capture (EC) decay of ^{111}In to ^{111}Cd disintegrates during the time the nucleus spends in the 417 keV level preceding the PAC cascade. The same complex was observed in AlInN where the characteristic signal is even more pronounced than in GaInN.

To rule out the possible influence of an after effect and to confirm the assumption that nitrogen vacancies are not bound to substitutional Cd impurities, additional measurements with ^{111m}Cd and ^{117}Cd were performed at the ISOLDE facility. An after effect can occur, when after the EC a hole remains in the electron shell. Additional electron-gamma measurements are presented, to confirm the nonexistence of such an effect. The PAC measurements are complemented by Rutherford backscattering/channeling and X-ray diffraction to investigate the lattice site location of the implanted probes and the recovery of implantation damage by thermal annealing.

References

[1] K. Lorenz et al., *J. Appl. Phys.* **80**, Nr. 24, 4531 (2002)

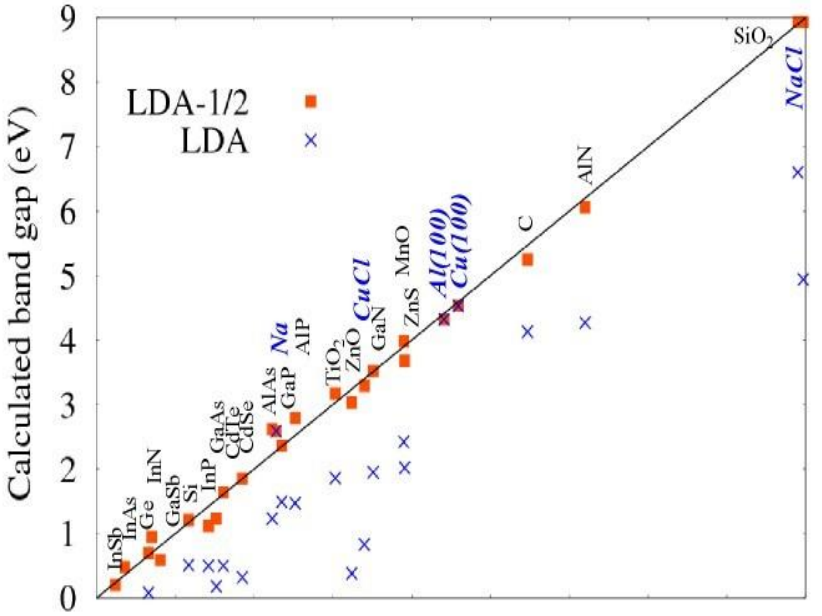
PS2-8-68

Precise calculation of semiconductor band gaps by means of the LDA-1/2 method

Luiz G. Ferreira,[1] **Lara K. Teles**[2]**, Marcelo Marques**[2]

[1] *Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970 São Paulo, Brazil, guima00@gmail.com* [2] *Instituto Tecnológico de Aeronáutica, 12228-900 São José dos Campos, SP, Brazil, lkteles@gmail.com and marcmarq@gmail.com*

The LDA-1/2 method [1] has been very successful in the calculation of semiconductor band gaps. The figure below shows the extent of its success. Despite of that, the method has no parameter to be arbitrarily adjusted. Its only parameter is obtained by the maximization of the band gap. In the oral presentation we intend to show its theory, from the old Slater's transition state and Janak's theorem, to the definition of the "self-energy potential", showing the necessity of the introduction of a parameter to cut the Coulomb potential tail, proving that it should maximize the gap, comparing the method to Perdew and Zunger's self-interaction. Although the method is parameter free, some choices must be made. For example, in atoms and good insulators one cannot run the self-consistent loops after adding the self-energy perturbation potential. In the other extreme, for the calculation of work functions of metals, the method does not differ from standard LDA. For example, for the group IV semiconductors the procedures are slightly different. The method clearly points to the interpretation that hole states in solids are described by square integrable wave functions, not Bloch functions.



References

[1] L. G. Ferreira, M. Marques, L. K. Teles, Phys. Rev B **78**, 125116 2008

PS2-9-69

Study of annealing behavior of HfO_2 fiber by hyperfine interaction technique.

<u>D. Banerjee</u>[1], S. K. Das[1], P. Das[2]

[1] *Radiochemistry Laboratory, Variable Energy Cyclotron Centre,*
Bhabha Atomic Research Centre, 1/AF Bidhan nagar, Kolkata 700064, India
dbanerjee@vecc.gov.in
[2] *Variable Energy Cyclotron Centre, Kolkata 700064, India*

The thermal behavior of hafnium oxide fiber has been investigated with the help of Time Differential Perturbed Angular Correlation (TDPAC) technique along with XRD and SEM measurements. The HfO_2 fiber of diameter 6-7μm and density 1.21 gm/cc was neutron-irradiated to produce the indigenous probe $^{181}Hf/^{181}Ta$ for TDPAC measurement, annealed at different temperatures and then counted on a TDPAC set-up [1] at RT. A typical TDPAC spectrum for HfO_2 fiber annealed at 1673K is shown in fig1. TDPAC parameters, shown in table-1, remain almost same in all the cases indicating the structural identity. Only a meager increment in δ-values indicates a little loss in crytallinity in the samples annealed at higher temperature. The TDPAC parameters for HfO_2 fiber are also in good agreement with that for bulk HfO_2. XRD spectra also remain same except a little broadening of the peaks at 1673K. It indicates that the fiber can retain its physical integrity almost intact even at 1673K. SEM measurement of the fiber indicates that the diameter of the fiber is not changed up to 1673K.

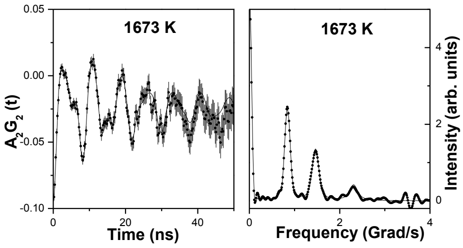


Fig. 1: TDPAC spectra for HfO_2 fibers

HfO_2 fiber	V_{ZZ} x 10^{17} (VCm^{-2})	η	δ(%)
Unannealed	13.08 (1)	0.35(1)	2.6(2)
Annealed at 1173K	13.01 (1)	0.36(1)	3.0(1)
Annealed at 1673K	13.08 (1)	0.35(1)	3.2(2)
HfO_2 bulk [a]	13.06 (1)	0.34(1)	1.0(1)

[a] For comparison with fiber

Table 1: TDPAC parameters for different HfO_2 samples

Hence the HfO_2 fiber has high thermal stability and stable lattice structure up to 1673 K. The porosity of the material and hence the diffusion-efficiency of the fiber are also not hampered even at 1673 K.This indicates the suitability of this material to be used as the target material for Radioactive Ion Beams [2]. However, a small increase in the frequency distribution may be attributed to the minor structural change with temperature. Literature [3] indicates a phase transformation from monoclinic to tetragonal HfO_2 taking place above 1443 K. However in this present work we could not find any structural change up to 1673 K. It implies that either it has not undergone any phase transition or the phase transition is reversible.

References

[1] S. K. Das etal, Journal of Physics and Chemistry of Solids 70 (2009) 778–781.
[2] D. Bhowmick etal., Nuclear Instruments and Methods in Physics Research A 539 (2005) 54–62.
[3] F. Cardarelli, Material Handbook (Springer, London, 2000).

PS2-10-70

Zr-doped Rutile TiO_2: A Quadrupole Interaction Study

D. Banerjee[1], S. K. Das[1], P. Das[2], S. V. Thakare[3], T. Butz[4]

[1] *Radiochemistry Laboratory, Variable Energy Cyclotron Centre,*
Bhabha Atomic Research Centre, 1/AF Bidhan nagar, Kolkata 700064, India
dbanerjee@vecc.gov.in
[2] *Variable Energy Cyclotron Centre, Kolkata 700064,India*
[3]*Radiopharmaceutical Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[4]*Universität Leipzig, Fakultät für Physik und Geowissenschaften,*
Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

Rutile TiO_2 has a tetragonal structure with space group P42/mnm. In this, the Ti atom is surrounded by eight O atoms as the nearest neighbors in an octahedral geometry. In the next layer there are eight Ti atoms in the corner of the tetragon. In the TDPAC measurement, the $^{181}Hf/^{181}Ta$ used as the probe is expected to replace the Ti atom in the lattice. The resultant EFG arises due to the interaction between the probe and the surrounding O and Ti atoms. When the probe concentration is on a trace level, there are no two probe atoms nearby to influence each other. In the present work, we investigated the role of Zr atoms, belonging to the same group of Ti & Hf, on the quadrupole interaction of ^{181}Ta in the rutile modification of TiO_2. Zr doped (up to 10 atom %) TiO_2 was prepared by following the method described elsewhere [1]. Co-precipitation of Ti-hydroxide along with Zr and ^{181}Hf tracer was carried out by the addition of ammonium hydroxide to the solution containing Ti^{+4} and the desired amount of Zr^{+4} along with the tracer ^{181}Hf. Data acquisition was carried out by the coincidence setup based on CAMAC electronics [2]. A_2G_2 spectra and their cosine transforms for a typical 5% Zr-doped sample are shown in Fig1. Table 1 shows the respective TDPAC parameters for different samples. The quadrupole frequency (ω_Q) and η remain almost the same in all the samples except for the increase in δ with increasing the at% of Zr. This indicates that the contribution to the interaction between probe and the O atom is predominant and the statistical fluctuation arising due to the presence of the randomly distributed Zr atoms in the next neighboring layer is of minor importance.

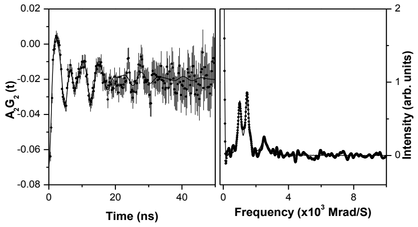


Fig 1. TDPAC spectrum of 5% Zr-doped sample

Samples	ω_Q (Mrad/S)	η	δ (%)
Pure rutile[a]	130.07(9)	0.56(1)	0.0
1% Zr/rutile	127.04(4)	0.55(1)	0.0
5% Zr/rutile	126.2(3)	0.58(1)	8.3(9)
10% Zr/rutile	127.44(7)	0.55(3)	12.8(5)

[a] Ref 2

Table 1: TDPAC parameters of different samples

The thermal analysis along with the XRD measurement is also under progress. Theoretical calculations with super cells containing statistically distributed Zr-atoms are under way.

References

[1] Seung baek Ryu et al., *Physical Review B* **77**, 094124 (2008).
[2] S K Das et al., *Journal of Physics and Chemistry of Solids* **70**, 778-781 (2009).

PS2-11-73

Search for "After-Effects" in Cd-doped ZnO semiconductor: PAC experiments supported by ab initio results

E. L. Muñoz[1], **M. E. Mercurio**[2], **L.F. Pereira**[2], **A. W. Carbonari**[2], **J. Mestnik-Filho**[2] **and M. Rentería**[1].

[1]*Departamento de Física e Instituto de Física La Plata (IFLP, CCT La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina, e-mail:munoz@fisica.unlp.edu.ar*

[2] *Instituto de Pesquisas Energéticas y Nucleares-IPEN-CNEN/SP, São Paulo, Brazil.*

During the last 25 years, several Time-Differential Perturbed-Angular-Correlation (PAC) experiments have observed dynamic hyperfine interactions when the probe isotope ^{111}Cd, obtained after the electron-capture (EC) decay of its parent ^{111}In was used in certain semiconductor and insulating oxides. In the eighties of the previous century the group from La Plata proposed that these dynamic interactions were originated in the electronic relaxation of the probe atom, usually called "after-effects" (AE) that follows the electron capture decay of the ^{111}In isotope. This relaxation must occurs during the time-window of the intermediate sensitive nuclear state of the γ-γ cascade used to measure the hyperfine interaction at the probe nucleus. It was believed that the ECAE can only be detected if the probe atom was an impurity in the system under study.
In order to check this necessary condition, the only binary oxide where ^{111}Cd is not an impurity is CdO, and ECAE where also not reported in this system and the observed electric-field gradient (EFG) is null due to the high symmetry (a regular octahedron) of the coordination of the cation site with the nearest oxygen neighbors. Following these ideas, we present here results of PAC experiments performed in an oxide, ZnO, were the ^{111}Cd probe atom is not an impurity, at least from the nominal valence point of view of the involved cations (Cd and Zn). But this time the observed non-null EFG behavior will be analyzed under the light of *ab initio* calculations of the (EFG) as a function of the charge state of the Cd atom.
PAC experiments carried out on ^{111}In-diffused polycrystalline ZnO have been performed in order to measure the EFG at (^{111}In (EC)$\rightarrow$) ^{111}Cd nuclei located at the cation site of the ZnO crystal structure. The PAC experiments were performed in a large temperature range. The absence of dynamic hyperfine interactions were verified fitting the spectra with a perturbation factor based in the Bäverstam and Othaz model [2,3]. The experimental results were compared with *ab initio* calculations performed with the Full-Potential Augmented Plane Wave plus local orbital (FP-APW+lo) method. The FP-APW+lo calculations were performed in the framework of the Density Functional Theory (DFT), using the Wien2K code. The dependence of the EFG at the Cd sites as a function of the charge state of the calculated supercell (i.e. the charge state of the *impurity* atom) was determined. From the *ab initio*-experimental comparison we can explained why we do not observe dynamic hyperfine interactions in the ZnO:Cd system.

References

[1] J. Desimoni, A.G. Bibiloni, C.P. Massolo and M. Rentería, Physical Review B **41**, 1443 (1990).
[2] U. Bäverstam, R. Othaz, N. De Sousa and B. Ringström, Nucl. Phys. **A186**, 500 (1972).
[3] A. Abragam and R. V. Pound, Phys. Rev. **92,** 943 (1953).

PS2-12-78

APW+lo and TDPAC study of the Electric-Field Gradient at the cation sites of the (^{44}Ti(EC)→)^{44}Sc-doped Sc_2O_3 Semiconductor

D. Richard[1], **E. L. Muñoz**[1], **T. Butz**[2], **L. A. Errico**[1,3] , **and M. Rentería**[1]

[1]*Departamento de Física and Instituto de Física La Plata (IFLP, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina, email: richard@fisica.unlp.edu.ar.*

[2]*Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstrasse 5, 04103 Leipzig, Germany.*

[3]*Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, 2700 Pergamino, Buenos Aires, Argentina.*

We report on an *ab-initio* study of the Electric-Field-Gradient tensor (EFG) at both inequivalent Sc sites in the semiconductor Sc_2O_3. This semiconductor crystallizes in the bixbyite structure with two six-fold coordinated cation sites called C and D. The first is highly asymmetric whereas the second is axially symmetric. The calculations were performed applying the Full-Potential Augmented-Plane Waves plus local orbitals (FP-APW+lo) method, in the framework of the Density Functional Theory (DFT), that allows us to treat the electronic structure and the atomic structural position refinements in a fully self-consistent way. Our results are compared with experimental data determined by Time-Differential γ-γ Perturbed-Angular Correlation (TDPAC) spectroscopy using the Leipzig 6-detector TDPAC spectrometer with $LaBr_3$(Ce) scintillators with the first excited $I=1^-$ state of the ^{44}Ti(EC)→ ^{44}Sc isotope as radioactive tracer. There is excellent agreement between experiment and the present *ab-initio* calculations. It is clear from the comparison of the experimental electric-field gradients and the Point-Charge Model (PCM) that the PCM can not describe even approximately the measured electric-field gradients at cation sites in pure scandium sesquioxide. In this simple situation, where the ^{44}Sc probe atom is not an impurity in the material under study, the tracer does not introduce structural distortions that are usually not taken into account in the PCM when an impurity is concerned and that does not introduce impurity levels in the band gap of the semiconductor, which are usually critical for the origin of the electric-field gradient. Nevertheless, in this simple case, the PCM seems to fail. This can be only due to a poor description of the electronic distribution around the probe atom, which is not taken into account with the Sternheimer antishielding factor that is proposed in the PCM to describe the polarization of the core electrons of the probe atom. We also found an experimental site preference for the ^{44}Ti impurity which can be understood by performing *ab-initio* calculations for the impurity system using super-cells.

PS2-13-81

Electronic and structural properties of the α-Fe_2O_3:Ta semiconductor. Experimental EFG determination and ab initio calculations.

G.N. Darriba[1], **E.L Muñoz**[1], **P.D. Eversheim**[2], **M. Rentería**[1]

[1]*Departamento de Física e Instituto de Física La Plata (IFLP, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina, email:*
darriba@fisica.unlp.edu.ar
[2]*Helmholtz-Institut für Strahlen- und Kernphysik (H-ISKP), Universität Bonn, Nussallee 1416, 53115 Bonn, Germany*

In this work we present results from Time-Differential Perturbed-Angular Correlations (PAC) experiments in α-Fe_2O_3 singlecrystals (in their *corundum* structure) implanted with ^{181}Hf(→^{181}Ta) ions at the ion accelerator facility of the H-ISKP at the Bonn University. The magnitude, asymmetry and orientation of the EFG were determined measuring the spin-rotation curves as a function of the singlecrystal orientation (for three different configurations of the sample) with respect to the laboratory system. The PAC experiments were carried out at 973 K in order to have only the electric-quadrupole interaction in the spectra, since above the Neel temperature (T_N=955 K) the system has a paramagnetic behaviour.

The experimental results are compared with *ab initio* calculations performed in the framework of the Density Functional Theory (DFT) and with predictions of the Point Charge Model. The *ab initio* calculations were carried out with the FP-APW+lo method (embodied in the WIEN2K code) with an impurity dilution of 1:12 (with respect to the cations).

This theoretical and experimental study enables to determine the structural relaxations introduced by the impurity in the host lattice, and the charge state of the impurity in the band gap of the system under study. The Ta impurity introduces a double donor level in α-Fe_2O_3, which seems to be partially ionized at 973 K, supported by the good agreement between the experimental EFG and the *ab initio* prediction for this charge state of the impurity.

We discuss here the validity to compare the *ab initio* calculations carried out at 0 K (where the system has an antiferromagnetic behaviour) with the experimental results taken at 973 K (where the system has a paramagnetic behaviour).

PS2-14-82

Observation of iron impurities diffusion in silicon under bending stress by Mössbauer spectroscopy

K. Suzuki[1], Y. Yoshida[2], K. Hayakawa[2], K. Yukihira[2], M. Ichino[2], and K. Asahi[1]

[1] *Tokyo Institute of Technology, Oh-okayama Meguro-ku Tokyo 152-8551, Japan,*
e-mail: suzuki.k.bd@m.titech.ac.jp
[2] *Shizuoka Institute of Science and Technology, Toyosawa Fukuroishi Shizuoka, Japane*

Semiconductor devices contain different types of lattice mismatch at boundaries, causing internal stresses in the silicon matrix. The strain field has a strong influence on impurity diffusion due to a change of the atomic interactions between the impurity and the host atoms [1], and therefore, yields a different segregation behavior of the impurities atoms. Among the impurities, iron is often connected to a degradation of the silicon devices. In the present experiments, external stress fields are applied to a ^{57}Fe-doped Si wafer by an Instron-type tensile testing machine, and simultaneously, Mössbauer spectra are measured as function the external stress.

N-type float zone silicon wafer was cut into a rectangular disk with 20×10×0.53 mm, and a 3 nm thick layer of ^{57}Fe was deposited on Si sample. The Si sample was annealed at 1273 K for one week to let ^{57}Fe diffuse into a Si matrix. The Si sample was fixed between a pair of alumina blocks in a tensile testing machine. By applying compressive stresses along the [011] direction, the Si wafer was bent, resulting in a tensile strain on one side and a compressive strains on the other side of the wafer. The transmission Mössbauer spectra of ^{57}Fe were obtained at room temperature under the stress up to 40 MPa when the tensile/compressive strains were applied on a ^{57}Fe deposited side.

After the annealing at 1273 K, the spectrum is well fitted with three components; substitutional Fe, interstitial Fe^0 and interstitial Fe^+ (from the left to the right side of the upper spectrum in Fig.1) When the external stresses are applied, the spectrum largely changes as is shown in Fig.1. The resonance area and the line width of interstitial Fe^0 increase. The line broadening appears to be due to a fast diffusion of interstitial Fe^0 under the external stress. The diffusion coefficient is estimated to be of the order of 10^{-9} cm^2/s, which is 6 orders of magnitude higher than that reported for a crystal Si [2]. In addition the resonance area of the substitutional Fe decreases with increasing the stress, suggesting that the interstitial Fe atoms are newly formed from substitutional Fe atoms by the external stresses.

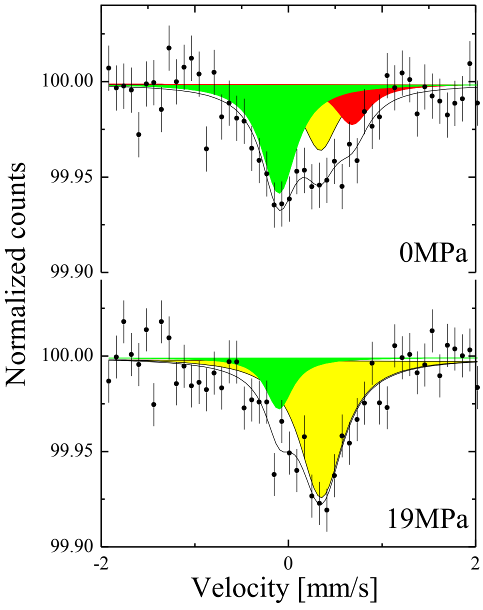


Fig. 1 Mössbauer spectra for the ^{57}Fe-doped silicon when compressive strain is applied on ^{57}Fe deposited side

References

[1] K. Suzuki, Y. Yoshida, T. Kamimuram, M. Ichino, K. Asahi, Physica B 404 (2009) 4678.
[2] E. R. Weber, Appl. Phys. A 30 (1983) 1.

PS2-15-94

Observation of long lived Fe^{3+} paramagnetic states in ZnO following the implantation with non-3d elements

R. Mantovan[1], H. P. Gunnlaugsson[2], K. Bharuth-Ram[3,4], M. Fanciulli[1,5], K. Johnston[6], G. Langouche[7], D. Naidoo[8], S. Ólafsson[2], R. Sielemann[9], G. Weyer[2], and the ISOLDE Collaboration[6]

[1]Laboratorio MDM, IMM-CNR, Via Olivetti 2, 20041 Agrate Brianza (MB), Italy , [2] Department of Physics and Astronomy, Aarhus University, DK-8000 Århus C, Denmark, [3]School of Physics, University of KwaZulu-Natal, Durban 4001, South Africa, [4]iThemba LABS, P.O. Box 722, Somerset West 7129, South Africa [4]Science Institute, University of Iceland, IS-107 Reykjavík, Iceland, ,[4]School of Physics, University of the Witwatersrand, WITS 2050, South Africa [5]Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy, [6]PH Dept, ISOLDE/CERN, 1211 Geneva 23, Switzerland, [7]Instituut voor Kern-en Stralings fysika, University of Leuven, B-3001 Leuven, Belgium, [8]School of Physics, University of the Witwatersrand, South Africa, [9]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany.

We have performed on-line ^{57}Fe Mössbauer spectroscopy following implantation of ^{57}Mn ($T_{1/2}$ = 1.5 min.) at the ISOLDE facility at CERN, in order to elucidate the role of the implantation process at room temperature in determining the magnetic properties of ion-implanted ZnO. We have recently demonstrated that dilute Fe^{3+} showing magnetically-split spectra in ZnO are due to Fe^{3+} long-lived paramagnetic states (LLPS) [1].

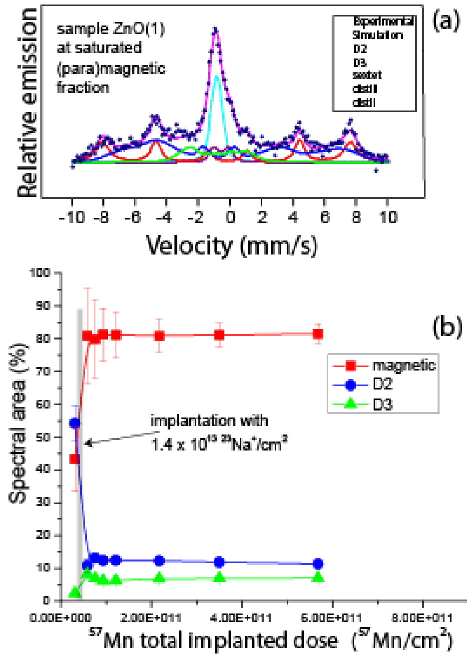


Fig. 1 (a) Mössbauer spectrum of ZnO(1) at saturated (para)magnetic contribution; (b) dose dependence in ZnO(2)

In this contribution, we describe implantation experiments in two ZnO crystals ZnO(1) and ZnO(2). ZnO(1) is implanted with $^{57}Mn^{+}$ ions, and a series of Mössbauer spectra are recorded during the consecutive implantation process. ZnO(2) is implanted with $^{57}Mn^{+}$ before and after an implantation with stable $^{23}Na^{+}$ ions (dose: ~1.4 x 10^{14} ions/cm^2). For the lowest implanted doses, the Mössbauer spectra of both samples are dominated by the presence of a quadrupole split component (D2) due to isolated . The consecutive ^{57}Mn implantation into ZnO(1) causes a dose dependence in the building up of a magnetic-type Mössbauer signal. [2].

Figure 1(b) shows the change of the spectral areas as a function of the total ^{57}Mn implanted dose in ZnO(2). Surprisingly, the same fraction of Fe atoms is observed in LLPS upon the implantation of ZnO with stable $^{23}Na^{+}$ ions. Our results show that the observation of Fe^{3+} LLPS in ZnO at the saturation level is intimately related to the implantation process and not necessarily connected to the 3d character and/or the radioactive nature of the implanted species.

References

[1] G. Weyer, H. P. Gunnlaugsson, R. Mantovan, M. Fanciulli, D. Naidoo, K. Bharuth-Ram, and T. Agne, *J. Appl. Phys.* **102**, 113915 (2007). [2] H. P. Gunnlaugsson *et al.*, In prep.

PS2-16-100

TDPAC study of the phase transitions in $PbTi_{1-x}Hf_xO_3$

R. E. Alonso, and A. López-García

Departamento de Física e Instituto de Física La Plata (IFLP, CONICET-UNLP), Facultad de Ciencias Exactas,
Universidad Nacional de La Plata, Casilla de Coreo 67, 1900 La Plata, Argentina.
e-mail: alonso@fisica.unlp.edu.ar

In this work we present a study of the phase transitions by means of the variations of the Electric Field Gradient (EFG) as a function of temperature at ambient pressure on powder samples of $PbTi_{1-x}Hf_xO_3$ for x= 0.25, 0.50 and 0.75. For the EFG determination Perturbed Angular Correlation Spectroscopy (TDPAC) was employed. ^{181}Ta were used as probes atoms, which were obtained by neutron capture activation of ^{180}Hf naturally present in the sample. The obtained experimental results are also compared with previous ones obtained by Impedance Spectroscopy (IS).

PS2-17-104

Fitting TDPAC Spectra with Stochastic Models: PolyPacFit

M. O. Zacate[1] **and W. E. Evenson**[2]

[1] *Dept. of Physics and Geology, Northern Kentucky University, Highland Heights, KY 41099, USA, e-mail: zacatem1@nku.edu*
[2] *Dept. of Physics, Utah Valley University, Orem, UT 84058, USA, e-mail: bill@evenson.ch*

PolyPacFit is an advanced fitting program for time-differential perturbed angular correlation (TDPAC) spectroscopy that incorporates stochastic models and provides robust possibilities for customization of fits. Notable features of the program include support for (1) fits to stochastic models of hyperfine interactions, (2) user-defined constraints among model parameters, and (3) fits to multiple spectra simultaneously. Another feature of PolyPacFit is that it is platform-independent.

The current version of PolyPacFit is limited to polycrystalline spectra, as the program name suggests. The program supports nuclear probes of any spin. It allows users to specify electric quadrupole, magnetic dipole, and mixed hyperfine interactions. Finally, PolyPacFit provides support for *ad hoc* line-shape parameters for dynamic damping and for inhomogeneous broadening. Examples showing the application of PolyPacFit will be presented.

This work is funded in part by NSF grant DMR 06-06006 (Metals Program) and computational resources were provided in part by KY EPSCoR grant RSF 012-03.

PS2-19-117

Fluctuating Hyperfine Interactions: Computational Implementation

M. O. Zacate[1] and W. E. Evenson[2]

[1] *Dept. of Physics and Geology, Northern Kentucky University, Highland Heights, KY 41099, USA, e-mail: zacatem1@nku.edu*
[2] *Dept. of Physics, Utah Valley University, Orem, UT 84058, USA, e-mail: bill@evenson.ch*

We report the creation of a library of computational routines to assist in the analysis of stochastic models of hyperfine interactions. We call this library the stochastic hyperfine interactions modeling library (SHIML). It provides routines written in the C programming language that (1) read a text description of a model for fluctuating hyperfine fields, (2) set up the Blume matrix, upon which the evolution operator of the system depends, and (3) find the eigenvalues and eigenvectors of the Blume matrix so that theoretical spectra of experimental techniques that measure hyperfine interactions can be calculated. The optimized vector and matrix operations of the BLAS and LAPACK libraries are utilized; however, there was a need to develop supplementary code to find an orthonormal set of (left and right) eigenvectors of complex, non-Hermitian matrices. Examples will be presented to illustrate the use of SHIML to generate perturbed angular correlation spectra for the special case of polycrystalline samples when anisotropy terms of higher order than A_{22} can be neglected.

This work is funded in part by NSF grant DMR 06-06006 (Metals Program) and computational resources were provided in part by KY EPSCoR grant RSF 012-03.

PS2-20-139

Study of hyperfine interactions in CeO_2 nanoparticle by PAC spectroscopy using ^{111}Cd

M.S. Costa[1], J. M. Ramos[1], A. W. Carbonari[1], G. A. Cabrera-Pasca[1], R. N. Saxena[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, IPEN, São Paulo, Brasil*

Cerium dioxide (CeO_2) is quite important for the high-technology industry with various applications such as in automotive industry, medicine, oxygen sensors, and protectors of the radiation and so on. This material has been studied recently using a variety of techniques. A case of special interest is that Co-doped Ceria is very attractive for multifunctional spintronic applications. In this work we have used PAC technique to measure the hyperfine interactions in a pure nanostructured CeO_2 as well as the one doped with *3d* transition metal Co. The samples of pure and Co-doped CeO_2 were prepared by the Pechini sol-gel method from pure Ce and Co elements. The samples were characterized by X-ray Diffraction (XRD) Scanning Electronic Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS). The radioactive probe nuclei ^{111}In-^{111}Cd was introduced during the sample preparation in all cases. To better study the contribution to the ferromagnetism of the samples due to the effect of vacancies in the structure or the presence of dopant transition metal ion, several different experiments were carried out with pure and doped CeO_2 which were prepared and annealed at different temperatures between 380°C and 700°C in air and nitrogen. The PAC measurements were performed at different temperature between 15 K and 1130 K. For instance, in Ceria pure with annealing at 500 °C, it was found at 400 K three quadrupole frequency $\nu_{Q1} = 106$ MHz with $f_1 = 58$ %, $\nu_{Q2} = 144$ MHz with $f_2 = 22$ % and $\nu_{Q3} = 14$MHz with $f_3 = 20$ %. This result is also a strong indication that f_1 should be assigned to 111Cd in Ce sites while f_2 in oxygen vacancy and f_1 is possible nuclei probe in grain surface.

PS2-21-140

First-principles study of magnetic hyperfine field at Cd probe in Co-doped ZnO semiconductor

L.F.D. Pereira[1], **E.L Muñoz**[2], **A.W. Carbonari**[1], **M. Rentería**[2], **R.N. Saxena**[1], **J. Mestnik-Filho**[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares IPEN-CNEN/SP, Lineu Prestes 2242, São Paulo and CEP:04180-070, Brazil, e-mail: lpereira@ipen.br*
[2] *Departamento de Física e Instituto de Física La Plata (IFLP, CCT La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina.*

Diluted magnetic semiconductor systems (DMS) have been widely studied in last years by different experimental techniques as well as by ab-*initio* calculations in an attempt to clarify the origin of the ferromagnetic order which is observed in several experiments. In general, magnetic order in samples of wide band-gap semiconductor oxides doped with transition metal elements is more likely to occur when they show structural defects, and such magnetism is claimed to be mediated by them. Among these systems, Co-doped ZnO has been intensively investigated and many experiments observed magnetic ordering in samples of this compound whereas many other did not.

One experiment, in particular, demonstrated unambiguously a magnetic hyperfine field (mhf) at ^{111}Cd probe nuclei substituting Zn sites in $Zn_{0.9}Co_{0.1}O$ bulk samples [1]. The experiment was performed by means of Perturbed gamma–gamma Angular Correlation spectroscopy (PAC) which is able to observe local fields with an atomic scale.

The aim of this work is to search for possible magnetic mechanisms which can originate a magnetic hyperfine field at Cd ion located in Zn site of Co-doped ZnO matrix by means of first-principles calculations. Our ab-*initio* calculations were developed under Density Functional Theory (DFT) framework using Linearized Augment Plane Waves method (LAPW) embodied within WIEN2k code [2].

The calculations were performed with some different ZnO supercells with diluted Co and/or Cd ions. For the exchange and correlation functionals, both the LDA and GGA approximations were tested. We have verified that calculated mhf and electric field gradient at Cd probe located in cation site of ZnO-Co supercell are in good agreement with the experimental values reported in reference [1]. Furthermore, results at Cd ion neighborhoods show that magnetic moments are transferred from Co ions towards Cd ions, by means of a super-exchange effect, which is mediated by Oxygen ions.

References

[1] M.E. Mercúrio, A.W. Carbonari et al., J. Magn. Magn. Mater. **322**, 1195 (2010).
[2] Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz, J.: WIEN2K, an Augmented Plane Wave plus Local Orbitals Program for Calculating Cristal Properties. Karlheinz Schwarz, Techn. Universität Wien, Austria. ISBN 3-9501031-1-2 (2001).

PS2-22-142

Electric quadrupole interactions in nano-structured SnO_2 as measured with PAC spectroscopy

J. M. Ramos,[1] **A. W. Carbonari**[1]**, M. S. Costa**[1]**, R. N. Saxena**[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, São Paulo, SP, Brasil, e-mail: emrjmr@superig.com.br*

The search for diluted magnetic semiconductors with ferromagnetic ordering at room temperature has attracted a great deal of interest in the last years. In this search several wide band-gap semiconductor oxides such as ZnO, TiO_2, and SnO_2 have been doped with transition metals in an attempt to create magnetic properties without significantly affecting the physical properties of the host. Among these materials, SnO_2 is a good candidate to successfully exhibit intrinsic magnetic ordering when doped with transition metal because of native oxygen vacancies occurrence, once it has been reported that such vacancies play an important role in the ferromagnetic order of semiconductor oxides.

In the present work electric quadrupole interactions in Tin dioxide (SnO_2) samples have been measured with perturbed gamma-gamma angular correlation (PAC) spectroscopy using ^{111}In (^{111}Cd) as a nuclear probe. Single phase nanocrystalline powder samples of SnO_2 were produced by the sol-gel Pechini method. At the sol step, the solution was separated in two parts. Probe nuclei were introduced in one of these parts which along with the other one were annealed at different temperatures under nitrogen atmosphere. The samples without ^{111}In were characterized by Scanning Electron Microscopy (SEM) measurements as well as X-ray Diffraction. The results showed nanometric particles homogeneously distributed, with particle diameter in the range of 15 – 60 nm.

PAC measurements were carried out in the temperature range from 10 K to 1123 K and the results show that the temperature dependence of the electric quadrupole frequency depends on the annealing temperature. In all measurements it was observed two different electric quadrupole interactions. One of them with $\nu_Q \sim 115$ MHz, $\eta \sim 0.1$, and $\delta \sim 12$ %, which changes very little with temperature has been assigned to ^{111}Cd at Sn sites in SnO structure. The second interaction is characterized by a wider distributed frequency that changes with temperature with values in the range of 120-160 MHz and asymmetry parameter varying from 0.4 to 1. This interaction was associated with ^{111}Cd probes tapped in defects near the surface of the nanoparticles.

PS2-23-143

Study of the electronic structure and electric field gradient at Cd probe in Co-doped ZnO matrix by first principles calculations

L.F.D. Pereira[1], E.L Muñoz[2], A.W. Carbonari[1], M.R. Cordeiro[1], M.E. Mercúrio[1], M. Rentería[2], R.N. Saxena[1], J. Mestnik-Filho[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares IPEN-CNEN/SP, Lineu Prestes 2242, São Paulo and CEP:04180-070, Brazil, e-mail: lpereira@ipen.br*
[2] *Departamento de Física e Instituto de Física La Plata (IFLP, CCT La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina.*

The investigation on wide-band gap semiconductors doped with transition metals (TM) has attracted a considerable interest in last years, mostly because of its possible applications in the spintronic field. Among these materials, cobalt-doped zinc oxide (Co-doped ZnO) has been one of the most investigated systems. Despite the focus on the magnetic aspect in these compounds in order to reach ferromagnetic ordering at room temperature, there is still enough space for some interesting questions regarding electronic structure that might be investigated.

The study of the possible changes in the electronic structure caused by the introduction of a TM, is a question of great interest, especially if it is necessary to introduce large quantities of TM and carriers.

One of the quantities that can be used in order to observe the differences in the electronic structure of a given crystalline site, is the electric field gradient (EFG), since is a very sensitive parameter that may reveal even small changes occurring in an atomic scale.

In this way, in the reference [1] it is presented PAC results at ^{111}Cd probe inserted in pure ZnO and 5% Co-doped ZnO. Two measurements on pure compound were performed; one with a commercially available sample and the other one was prepared at our laboratory together with the Co-doped sample utilizing sol-gel methodology. It was observed that the perturbation spectra are practically identical for all of the three situations, with Cd quadrupole frequency (ν_q) assuming values within the 31-32 MHz range.

Yet in another work [2], it was developed a systematic PAC study with the ^{111}Cd probe focusing on the concentration variation of cobalt dopant in ZnO within the 5 – 15 % Co range. These samples have a single ZnS-type phase and presented a same major fraction of sites with a very similar quadrupole frequency ν_q in the range between 31.1 – 33.1 MHz.

In the present work we try to explain which electronic phenomena could be occurring when Co-doped ZnO do not generate any change at Cd efg. For this purpose we used first principles electronic structure calculations, carried out within the Density Functional Theory (DFT) framework using Linearized Augment Plane Waves methods (LAPW) embodied at the WIEN2k code [3].

In our calculations, several ZnO cells were set up with Cd and/or Co ions and then, different Cd neighborhoods were simulated. The electric field gradient at Cd, the density of states (DOS) and charge density distributions were analyzed. The resulted EFG at Cd are in agreement with the experimental values [2]. By means of DOS it was observed that both the Co and Zn electronic structure are very similar.

References

[1] M.E. Mercurio, A.W. Carbonari et al., J. Magn. Magn. Mater. **322**, 1195 (2010).
[2] M.E. Mercurio, A.W. Carbonari, oral communication. To be published.
[3] Blaha, P., Schwarz et al: WIEN2K, an Augmented Plane Wave plus Local Orbitals… . Karlheinz Schwarz, Techn. Universität Wien, Austria. ISBN 3-9501031-1-2 (2001).

PS2-24-148

TDPAC study of a solid-state reaction doping process of ^{181}Hf($\rightarrow^{181}$Ta) impurities in the Ho_2O_3 semiconductor

D. Richard[1], **E.L. Muñoz**[1], **G.N. Darriba**[1], **L.A. Errico**[1,2], and **M. Rentería**[1]

[1] *Departamento de Física-IFLP (CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina*
[2] *Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, 2700 Pergamino, Buenos Aires, Argentina*

Nuclear methods and, in particular, the time-differential perturbed-angular correlation (TDPAC) spectroscopy have been extensively applied to study materials to elucidate at a subnanoscopic scale the environment of impurities or constituent atoms of solids (see, e.g., Ref. 1). In the case of TDPAC, a suitable probe isotope, generally an impurity in the system under study, is used and the information provided, at this probe site, is given as a product of a nuclear and an extra nuclear quantity. In the case of electric-quadrupole interactions, the nuclear quantity is the nuclear quadrupole moment (Q), characteristic of a given nuclear state, which interacts with the electric-field gradient (EFG) acting on the site of the probe atom. Since the EFG mostly originates in the non-spherical electronic charge density close to the impurity nucleus, the TDPAC technique can be used as a powerful tool in order to study the electronic structure (and related structural, electronic or magnetic properties) in the close neighborhood of the probe.

The probe can be introduced in the host material by different methods: thermal diffusion, chemical methods, neutron activation, or ionic implantation. In this work we study an alternative doping method: ball-milling-assisted solid-state reaction between neutron-activated m-HfO_2 and the system under study (in the present case, the bixbyite Ho_2O_3). In order to follow the doping process of ^{181}Hf donor impurities in the semiconductor Ho_2O_3 and to elucidate the effect of each variable involved in the process (milling time, temperature, ball to powder ratio, etc.), TDPAC experiments were carried out after each step of the doping process. The obtained hyperfine parameters were compared to those of m-HfO_2, to those expected for Ho_2O_3 using a well established EFG systematics for ^{181}Ta in bixbyte sesquioxides, and to TDPAC results obtained in Ho_2O_3 samples doped by ion implantation of ^{181}Hf($\rightarrow^{181}$Ta).

As we will show, we can determine the effect played by the milling and the thermal treatments, showing the capability of the TDPAC technique to follow the doping process and to give information about the inter-diffusion processes. We also demonstrate the excellent efficiency of the ball-milling-assisted solid-state reaction process to locate Hf donor impurities at the defect-free cationic sites of the Ho_2O_3 semiconductor, quantifying directly the amount of impurities doped after each step of the process.

References

[1] L.A. Errico, G. Fabricius, M. Rentería, P. de la Presa, M. Forker, Phys. Rev. Lett. **89** (2002) 55503; L.A. Errico, G. Fabricius, M. Rentería, Phys. Rev. B **67** (2003) 144104, and references therein.

PS2-25-160

PAC study of the Si-HfO_2 system subjected to high energy ball milling

Chain, C.Y.[1], Damonte L. C.[1,3], Ferrari S. [1,3], Martinez J. L. [1,2], Rodríguez Torres C. E.[1,3], Pasquevich A. F. [1,2]

[1]*Departamento de Física, IFLP, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata, Argentina, e-mail: yamil@fisica.unlp.edu.ar*
[2]*Comisión de Investigaciones Científicas- Provincia de Buenos Aires (CICPBA), Argentina*
[3] *Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina*

The nanotechnological interest in reducing the dimensions of Si complementary metal-oxide-semiconductor devices has led to a need of replacing the SiO_2 gate insulator with high-k dielectric oxides. Among many candidates, HfO_2 and its alloys with SiO_2 have attracted the attention due to their high permittivity and thermodynamic stability concerning solid- state reactions with Si subtrate. This fact makes the study of the solid-state reactions between Si and HfO_2 of main interest. The Perturbed Angular Correlations (PAC) method is a powerful tool for the determination of electric field gradients at atomic sites in solids. In this way, it is possible to characterize different compounds and phases.

The aim of this article is to characterize high-energy ball milled equimolar mixture of HfO_2 and crystalline silicon powder by PAC technique complemented with X-ray diffraction analysis. In order to better analyze the results of the milling treatments, pure hafnium oxide was milled in the same conditions and measured subsequently.

PAC results from pure hafnium oxide revealed that the well-known monoclinic phase of HfO_2 is strongly disrupted with 2 hours of high- energy ball milling. A new hyperfine interaction, rather asymmetric, must be proposed to give account of the experimental results. The damage does not increase so much as the milling treatment progresses.

The structure of *m*-HfO_2 seems to be less perturbed in the milled mixtures HfO_2-Si if compared with the same milling times in pure HfO_2. The same new interaction observed in milled HfO_2, but more asymmetric and distributed, must be considered to give account of the experimental results. The results are compared with previous PAC studies on milled HfO_2-SiO_2 [1].

References

[1] C.Y. Chain et al., *Journal of Alloys and Compounds* **495**, 527 (2010)

PS2-26-162

Thermal Evolution of Short Range Order in Cu-Hf-Based Amorphous Alloys

L. Damonte,[1] **A. F. Pasquevich**[1], **L. A. Mendoza Zelis**[1]

[1] *UNLP, Argentina,*
e-mail: damonte@fisica.unlp.edu.ar

Cu-based ternary metallic glasses are promising for practical applications since they joint together interesting mechanical properties like strong glass-forming ability, high strength, ductility and low cost. For the Cu-Zr(Hf)-Ti system, Ti addition increases the glass forming ability of the alloy while diminishes its glass transition temperature, Tg, but improves its mechanical properties. From the point of view of the glass forming ability, it is important not only the structural characterization of the starting amorphous alloys but the stable and metastable crystalline phases formed at each crystallization step as well. In this sense, we are interested in look forward a relationship between short range order, i.e different crystalline phases, and mechanical properties.

We present here a Perturbed Angular Correlation (PAC) study on these amorphous alloy series, prepared by melt-spinning, with different copper and titanium content.
The electric field gradient (EFG) thermal evolution is analyzed in order to characterize the intermediate and final phases.

PS2-27-164

Dimensionless Coordinates for Simulations and Theory of Hyperfine Interactions in Materials

W. E. Evenson[1] **and M. O. Zacate**[2]

[1] *Dept. of Physics, Utah Valley University, Orem, UT 84058, USA, e-mail: bill@evenson.ch*
[2] *Dept. of Physics and Geology, Northern Kentucky University, Highland Heights, KY 41099, USA, e-mail: zacatem1@nku.edu*

For problems involving simulations or theory of hyperfine interactions in materials, it would be convenient to work in dimensionless coordinates of reasonable magnitude. The length scale should be approximately a lattice parameter. The time scale should be approximately an inverse hyperfine frequency. The energy scale should be approximately a hyperfine splitting energy. The scale for electric charge should be approximately the elementary electronic charge. The scale for electric field gradients (EFGs) should be approximately as observed in materials (e.g. 10^{19} to 10^{21} V/m^2). Similarly for magnetic hyperfine fields.

There are too many constraints here to allow for an ideal, universal dimensionless unit system. Nevertheless, we can define a useful "natural" dimensionless unit system that simplifies point-charge approximations, scaling between different crystal structures, scaling charges of various defects in materials, and other computations involving hyperfine interactions. We present the proposed system with examples of its use for data analysis as well as in simulations and theory. We also show concretely the connections between the dimensionless units and experimental quantities.

This work is funded in part by NSF grant DMR 06-06006 (Metals Program).

PS2-28-165

Defects studies in pure and doped In_2O_3 single crystals by PAC

R Quille Ramos[1], Y. Chain[1], L. Damonte,[1] A. F. Pasquevich[1], L. A. Mendoza Zelis[1]

[1] *UNLP, Argentina,*
e-mail: yamil@fisica.unlp.edu.ar damonte@fisica.unlp.edu.ar

The indium oxide electronic properties, pure or impurity doped, as massive material or thin films, irrespective of its morphology, i.e. nanoparticles or nanowires, are of high interest due to their potential technological applications. Perturbed Angular Correlations (PAC) measurements on pure and doped In_2O_3 using ^{111}In as radioactive probe are presented.

Already the first paper on the application of the PAC technique to an oxide found the electron capture after-effects (AE) for ^{111}In/^{111}Cd probes in In_2O_3. The ^{111}In isotope decays via EC to the 7/2+ state of ^{111}Cd and after 170 ps the first γ quanta of the PAC cascade is emitted. The EC-decay caused a hole in the K-shell, which is filled by X-ray and/or Auger transitions. Within 0.01 ps further Auger processes produce additional holes in higher shells. Therefore, the ^{111}Cd-atom is highly ionized after its creation and electrons are needed to stabilize its electron shell. It depends strongly on the properties of the matrix (metal, semiconductor, and insulator) whether enough electrons are available in time or not. In metals the missing electrons are fast supplied and no AE is observed. But in semiconductors or insulators the relaxation time of the excited electron shell may be longer than the mean lifetime of the hyperfine-sensitive intermediate state in ^{111}Cd ($\tau \approx 122$ ns), leading to time-dependent (fluctuating) EFGs and damped PAC perturbation functions $G_{22}(t)$

Many different experiments have proven that the EC after-effect is, without doubts, the origin of this damping of the R(t) functions. Implantations at ISOLDE/CERN of the 48 min isotope ^{111m}Cd into different bixbyite oxides showed no aftereffect, the same was observed in the PAC-experiments with the ^{181}Hf/^{181}Ta. In both cases, no EC-decay can distort the probe's electron shell and no additional electron is needed.

The existence of these aftereffects depends on the oxide purity. In this communication are presented results obtained with indium oxides samples contaminates with different impurities. An equimolar mixture of OCd and In_2O_3 doped with ^{111}In and overnight calcinated at 1273 K in normal air atmosphere, results in In_2O_3 doped with Cd impurities. Additionally, In_2O_3 doped with C was made: a mixture of indium metal and carbon, in a porcelain crucible, loosely cover was overnight calcinated at 1273 K. In this way crystals of In_2O_3 grew on the walls and cover of the crucible. Later the crystals were doped with ^{111}In. PAC spectra of both samples were studied as a function of temperature. The obtained results show pronounced differences, which can be ascribed to the donor or acceptor character of the impurities.

PS2-29-60

Hyperfine parameters of Fe atoms in superconducting FeSe as function of temperature, pressure and magnetic field.

V. Ksenofontov[1], G. Wortmann[2*], T. Gasi[1], S. Medvedev[1,3,]
T.M. McQueen[4], R.J. Cava[4], and C. Felser[1]

[1]*Institut Anorg. Analyt. Chemie, Universität Mainz, D-55099 Mainz, Germany*
[2]*Department Physik, Universität Paderborn, D-33095 Paderborn, Germany*
[3]*Max-Planck-Institute for Chemistry, D-55128 Mainz, German*
[4]*Department of Chemistry, Princeton University, Princeton NJ 08544, USA*

A pressure and temperature effect was studied in the Fe partial phonon density of states by ^{57}Fe nuclear resonant inelastic scattering (NIS) in the superconducting $Fe_{1.01}Se$. We found i) no pronounced changes across the tetragonal – orthorhombic phase transition and ii) a hardening of the phonon spectrum as a function of pressure in the superconducting phase. We conclude that the strong increase of T_c in $Fe_{1.01}Se$ with pressure [1] cannot be described in the framework of classical electron-phonon coupling, for instance, in the McMillan formalism. This result suggests the importance of both lattice and spin fluctuations in the observed superconductivity [2].
Mössbauer spectroscopic studies were done at ambient and high pressure. Temperature dependence of the Mössbauer-Lamb factor in $Fe_{1.01}Se$ was measured across the tetragonal-orthorombic structural phase transition at ca. 95 K. It has been shown that the orthorhombic phase is slightly softer that the tetragonal one. Among other factors which could be responsible for T_c enhancement in $Fe_{1.01}S$ under pressure is the behavior of electronic density of states at the Fermi level. Indirectly the information about the electronic density at the Fe sites bears the isomer shift on ^{57}Fe nucleus. We observe a decrease in the isomer shift in the tetragonal phase of $Fe_{1.01}Se$ which corresponds to increase in s electron density at Fe nucleus under pressure. We discuss several mechanisms by which core electron contribution can be altered by pressure.
Mössbauer measurements in the external magnetic field below the transition to the superconducting state revealed zero electron spin density on Fe atoms in $Fe_{1.01}Se$ and $FeSe_{0.5}Te_{0.5}$. Interpretation of Mössbauer spectra of $Fe_{1.01}Se$ and $FeSe_{0.5}Te_{0.5}$ in the Shubnikov phase will be discussed [3].

References

[1] S. Medvedev, T.M. McQueen, I. Trojan, T. Palasyuk, M.I. Eremets, R.J. Cava, S. Naghavi, F. Casper, V. Ksenofontov, G. Wortmann, C. Felser, Nature Mater. 8, 630 (2009).
[2] V. Ksenofontov, G. Wortmann, A.I. Chumakov, T. Gasi, S. Medvedev, T.M. McQueen, R.J. Cava, and C. Felser, Phys. Rev. B (accepted).
[3] V. Ksenofontov, G. Wortmann, T. Gasi, J. Deisenhofer, V. Tsurkan and C. Felser (in preparation).

PS2-30-12

Beta-NMR Measurements of ^{58}Cu in Si

M. Mihara,[1] **K. Matsuta**[1], **D. Nishimura**[1], **T. Izumikawa**[2], **T. Nagatomo**[3], **T. Moriguchi**[4], **Y. Ito**[4], **D. Nagae**[4], **H. Ueno**[5], **A. Yoshimi**[5], **K. Yamada**[5], **M. Takechi**[5], **Y. Ichikawa**[5], **M. Fukuda**[1], **S. Momota**[6], **Y. Hirayama**[7], **T. Ohtsubo**[8], **S. Suzuki**[8], **T. Kubo**[8], **Y. Namiki**[8], **A. Ozawa**[4], **Y. Ishibashi**[4], **H. Oishi**[4], **K. Suzuki**[9], **I. Hachiuma**[10], **K. Namihira**[10], **D. Horikawa**[6], **T. Minamisono**[11], **T. Yamaguchi**[10], **T. Kuboki**[10], **T. Suzuki**[10], **K. Sato**[10], **Y. Kobayashi**[5], **K. Asahi**[9], **K. Matsukawa**[12], and **K. Shirai**[13]

[1] *Dept. Physics, Osaka University, Toyonaka, Osaka 560-0043, Japan, e-mail: mihara@vg.phys.sci.osaka-u.ac.jp*
[2] *Radioisotope Center, Niigata University, Niigata 951-8510, Japan*
[3] *International Christian University, Mitaka, Tokyo 181-8585, Japan*
[4] *Dept. Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan*
[5] *RIKEN Nishina Center for Accelerator-Based Science, Wako, Saitama 351-0198, Japan*
[6] *Faculty of Engineering, Kochi University of Technology, Tosayamada, Kochi 782-8502, Japan*
[7] *Institute of Particle and Nuclear Studies, KEK, Tsukuba, Ibaraki 305-0801, Japan*
[8] *Departmement of Physics, Niigata University, Niigata 950-2181, Japan*
[9] *Dept. Physics, Tokyo Institute of Technology, Meguro-ku, Tokyo 152-8550, Japan*
[10] *Dept. Physics, Saitama University, Saitama 338-8570, Japan*
[11] *Dept. Applied Nuclear Technology, Fukui University of Technology, Fukui 910-8505, Japan*
[12] *Renesas Technology Corp., Itami, Hyogo 664-0005, Japan*
[13] *ISIR, Osaka University, Ibaraki, Osaka 567-0047, Japan*

Contamination of silicon with copper impurities has been a longstanding problem in processing devices, which causes degradation of their performance because of the fast diffusivity and formation of deep levels in the band gap [1]. β-NMR studies with a short lived nucleus ^{58}Cu($I^{\pi} = 1^{+}$, $T_{1/2} = 3.2$ s) as a microscopic probe should be able to provide unique information on the mechanism of Cu diffusion and behavior of Cu-dopant complex (ex. Cu-B pair) in Si. In this report we present the first result on the β-NMR measurements of ^{58}Cu in silicon.

A spin polarized ^{58}Cu beam was produced through the charge exchange reaction of ^{58}Ni with a Be target, using a 63*A*-MeV ^{58}Ni beam provided by the K540 RIKEN Ring Cyclotron. The ^{58}Cu nuclei emitted at angles in between 0.75° and 4.1° were separated by RIPS and implanted into a catcher sample of single crystalline Si (B doped) at 15 K. The β-ray yield from ^{58}Cu was ~10^3 counts/s. The finite polarization of about 0.2% was observed and then the β-NMR spectrum for ^{58}Cu in Si was obtained as shown in Fig. 1. The magnetic moment of ^{58}Cu was determined to be $(0.46 \pm 0.03)\mu_N$ which is in agreement with the recent results on the laser spectroscopy [2]. The spin lattice relaxation rate $1/T_1 = (0.7 \pm 0.6)$ s^{-1} for ^{58}Cu in Si(B) was also obtained at 15 K. The present result has shown that the ^{58}Cu nucleus is promising as a nuclear probe for the microscopic study of copper impurities in silicon.

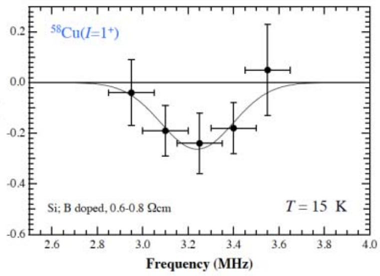


Fig. 1. Beta-NMR spectrum of ^{58}Cu in Si.

References

[1] E.R. Weber, *Appl. Phys.* **A 30**, 1 (1983).
[2] N.J. Stone et al., *Phys. Rev.* **C 77**, 067302 (2008), T.E. Cocolios et al., *Phys. Rev.* **C 81**, 014314 (2010).

PS2-31-32

Temperature dependence of the hyperfine fields of ^{111}In in sapphire (Al_2O_3) single crystals

Michael Steffens,[1] **Jakob Penner**[1], **Hassan Kamleh**[2], **Reiner Vianden**[1]

[1] *Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Nußallee 14-16, 53115 Bonn,*
e-mail: steffens@hiskp.uni-bonn.de
[2] *Department of physics, Faculty of Sciences, University of Damascus, Syria*

The decay of ^{111}In to ^{111}Cd via electron capture, accompanied by Auger electrons, leaves the outmost atomic shell of the Cadmium in a highly ionized state.

In PAC measurements, this so called "electron capture after effect" leads to a significant loss of anisotropy and can be associated with a highly fluctuating electric field gradient (EFG).

The recovery of the ^{111}Cd shell by electronic recombination depends on the concentration and the mobility of charge carriers in the material. For insulators, the recombination timescale lies in the nanosecond regime, the generic timescale of hyperfine interaction processes as investigated by the PAC method.

In previous measurements the fraction of undisturbed probe atoms showed a strong and reversible dependence on the sample temperature [1].

Our current approach is to determine and alter the conditions under which electrons are sufficiently available to suppress the "after effect".

Sapphire single crystals were ion implanted with ^{111}In at the mass separator in Bonn. After rapid thermal annealing the samples were held at temperatures up to 1000 K. To alter the recombination characteristics and to study the influence of acceptor and donator levels, the samples were additionally doped with several concentrations of Si, Cr and P.

References

[1] J. Penner and Reiner Vianden, *Hyperfine Interactions* **158**, 389 (2004)

PS2-32-84

Nuclear electric quadrupole interactions of ^{111}Cd in the heavy-fermion compound CeCoIn$_5$

M. Forker[1], P. R. J Silva[1], E. Baggio-Saitovitch[1], H. Saitovitch[1], S. Ramos[1], R. E Alonso[2], L. A. Errico[2,3], M. A. Taylor[2]

[1] *Centro Brasileiro de Pesquisas Física , 22290-180 Rio de Janeiro, Brasil , e-mail: elisa@cbpf.br*
[2] *Departamento de Física & Instituto de Física La Plata (IFLP, CCT-La Plata, CONICET-UNLP), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Argentina,*
email: errico@fisica.unlp.edu.ar
[3] *Universidad Nacional del Nordeste Bonaerense (UNNOBA) CP 2700, Buenos Aires, Argentina*

The nuclear electric quadrupole interaction of the probe nucleus ^{111}Cd on In sites of the heavy-fermion compound CeCo(In$_{1-x}$Sn$_x$)$_5$; x = 0.01 has been investigated in the temperature range $15 \leq T \leq 290$ K by perturbed angular correlation spectroscopy. Single crystals of CeCo(In$_{1-x}$Sn$_x$)$_5$ grown from an In flux by combining stoichiometric amounts of Ce and Co with excess In [1] were doped with the PAC probes ^{111}Cd by diffusion at 700 K of radioactive ^{111}In from a carrier-free solution of ^{111}InCl$_3$ into the host lattice.

Apart from a sizeable fraction of non-reacted In metal, the PAC spectra contain contributions of two In-sites related to the CeCoIn$_5$ structure, an axially symmetric and an asymmetric site. The ^{111}Cd electric field gradient (EFG) of these sites differs substantially from the two EFG values determined by NQR measurements for the probe ^{115}In on sites 1*c* and 4*i* of CeCoIn$_5$, both with respect to symmetry and strength ratio. For insight into the mechanism leading to these differences, an a*b initio* study of the structural and electronic properties of ^{111}Cd on In sites of CeCoIn$_5$ is under way.

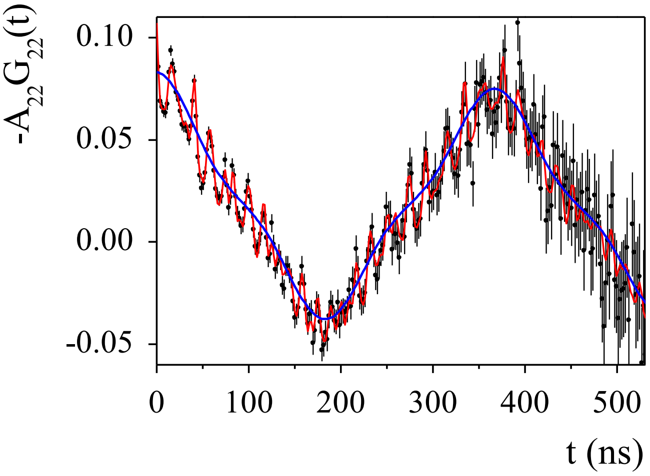


Fig. 1: PAC spectrum of ^{111}Cd in a single crystal sample of CeCo(In$_{1-x}$Sn$_x$)$_5$; x = 0.01 at 290 K.

References

[1] C. Petrovic, P. Pagliuso, M. Hundley, R. Movshovich, J. Sarrao, J.Thompson, Z. Fisk, and P. Monthoux, J. Phys.: Condens. Matter **13**, L337 (2001)

PS2-34-16

A User-friendly Fully Digital TDPAC-Spectrometer

Tilman Butz[1], Markus Jaeger[1], Kornelius Iwig[2]
[1] *University of Leipzig, Germany, e-mail: butz@physik.uni-leipzig.de*
[2] *MSC-Technik GmbH Halle, Germany*

The new user-friendly fully digital TDPAC spectrometer consists of 6 detectors (38 mm diameter x 38 mm height $LaBr_3(Ce)$ scintillators mounted on XP2020URQ photomultipliers; energy resolution DE/E = 3% at 662 keV) arranged in a cube (see fig.1), a PXI system with 3 digitizer cards of the type AC240 (each card has 2 channels and one FPGA, see fig.1), and a single PC with a special PCI card to communicate with the PXI system.

Each digitizer channel runs with a sample rate of 1GS/s and for every digitizer channel there is an independent data stream. These 6 data streams are fed into 3 FPGAs. The task of the FPGA is to process the data streams by real parallel digital hardware. The FPGA has 2 main tasks: (i) search for pulses and calculate the pulse area for the energy histogram (takes 265 ns); (ii) search for pulses and calculate their timestamps by the CFD method (takes 1354 ns).

To calculate a timestamp in the FPGA a 5 stage pipelined digital circuit is used: 1) Detection of pulse by a threshold comparison in order to filter uninteresting data. 2) Summation of the digitized data stream for the energy determination. 3) Classification of the pulses by the calculated energy area from stage 2. This is done by a comparison with a given energy window. 4) Fitting a polynomial of degree 3 by 4 points around the CFD level. 5) Finding the CFD timestamp with a binary search algorithm by comparing the CFD level with the values of the polynomial.

After stage 5 the calculated timestamp is saved into a FIFO inside the FPGA. The FIFO is built by FPGA internal BRAMs. Stage 5 is the bottleneck with a throughput of 1.05 million timestamp per second. The spectrometer creates a timestamp data stream of 8.4 MByte/s per channel, i.e. a 50.4 MByte/s data stream from the digitizers to the PC. In a typical application we have a pulse rate of 5 kHz per channel, i.e. a data stream of only 240 kByte/s from the digitizers to the PC.

The PC with Windows XP executes the spectrometer software which collects the datasets from the digitizers via PCI DMA transfers (85 MByte/s).

The software runs on an Intel Core2Duo CPU with 1.8GHz. For the time spectrum the software executes a coincidence search, the critical part of the spectrometer software. The coincidence search has a throughput of 7 million timestamp comparisons per second.

analog electronics and cable delays Right: 3 digitizer cards AC240 replacing all conventional hard

Fig.1 Left: 6-detector cube with conventional analog electronics and cable delays. Right 3 digitizercards AC240 replacing all conventional hardware.

References

[1] N.V. Unknown et al., *Journal Title* **49**, 6187 (2005) and references therein.
[2] J.W. Blabla et al., *Journal Title* **186-187**, 1658 (1989).

PS2-35-21

Methodology of Quantitative Analysis in Mossbauer Spectroscopy

S.M.Irkaev[1], **V.G.Semenov**[2], **V.V.Panchuk**[2]

[1] *Institute for Analytical Instrumentation RAS, Rishgski pr.26, 192000 St.Petersburg, Russia, sobir_irkaev@mail.ru*
[2] *Dept. Chemistry, St.Petersburg State University Universitetskii pr.26, 198504 St.Petersburg, Russia mail: val_sem@mail.ru*

The Mössbauer spectroscopy technique belongs to few methods of defining the phase state or crystallographic sites of substance. The Mössbauer spectra bear information on various hyperfine interactions, many of which are indirectly related to the chemical nature of the Mössbauer atom and its nearest environment. Determination of parameters of hyperfine interactions that can be extracted from Mössbauer spectra and used for qualitative analysis is a routine task. The nice description of calculation the most important parameters from experimental spectra are given in excellent reviwes [1-2].

In present work we studied the influence of main factors on experimental errors encountered in quantitative defining the phase composition or site populations of the substance under study. Such as measurements geometry, Lamb - Mössbauer coefficients, absorber thickness, efficiency and dead time of the detection system and spectral line shape. The absolute f measurements were made with "black" absorber method. Mössbauer measurements were carried out under carefully controlled of background intensities. Since the accuracy of f evaluation is directly depend on the measurement of background. The influence of a non-uniformity of samples on results of the quantitative analysis is discussed. Data analysis we divided into two parts: removal of instrumental artifacts by folding and baseline correction and deconvolution to extract hyperfine parameters of individual local environments [3-5].

In our approach calibration graphs were drawn by measuring the spectra of a series of analogous samples having different known concentrations. For the same purpose, internal standard method also was used. Experimental data are presented for phase analysis of different industrial samples.

References

E.Kuzmann, S.Nagy, A.Vertes. Pure Appl.Chem., (2003), **75** (6), 801.
R.E. Vandenberghe, E.De Grave, P.M.A. De Bakker. Hyperfme Interactions, (1994), **83**, 253
M.C.D.Ure, P.A.Flinn. in Mossbauer Effect Methodology, New York, London: Plenum Press, (1971), **7**, 245
T.M.Lin, R.S. Prenston. in Mossbauer Effect Methodology, New York, London: Plenum Press, (1975), **7**, 20
D.G.Rancourt. Nuclear Instruments and Methods in Physics Research **B**, (1989), **44**(2), 199

PS2-36-57

Lattice location of beryllium and boron, measured by thermal-neutron-induced emission channeling measurements

Ulli Koester,[1] **Etienne Bustarret**[1], **J. G. Correia**[3], **C. Granja**[4], **Jan Jakubek**[4], **J. Uher**[4], **Jiri Vacik**[5], **U. Wahl**[3]

[1] *Institut Laue Langevin Grenoble, France*
e-mail: koester@ill.fr
[2] *Institut Néel, CNRS Grenoble, France*
[3] *Instituto Tecnológico e Nuclear Sacavém, Portugal*
[4] *Czech Technical University Prague, Czech Republic*
[5] *Nuclear Physics Institute, Czech Academy of Sciences, Řež, Czech Republic*

Emission-channeling (EC) is a powerful experimental technique to pin down the exact site of atoms in a crystal lattice [1]. For EC typically radioactive isotopes are implanted that subsequently emit alpha or low-energy beta particles or conversion electrons. Unfortunately several elements have no radioisotope with suitable half-life and charged particle energies. However, if the element in question has an isotope with high cross-section for thermal neutron-induced proton or alpha emission, these charged particles can be produced by exposing the sample to an intense neutron flux. This technique was explored already 30 years ago by Biersack *et al.* at Institut Laue Langevin [2,3]. However, then the 2D particle detector covered only a fraction of the solid angle of the EC pattern and a measurement of a total EC pattern required the lengthy separate measurement and subsequent overlay of tens of spectra.

Today, modern silicon pixel detectors can cover the entire EC pattern in a single measurement. We will present results of the first use of the TimePix detector for thermal neutron induced charged particle emission channeling measurements. The semiconductor pixel detector TimePix (256 x 256 pixels) is a successor of the Medipix2 device. Timepix pixels can be operated in the so-called Time-over-Threshold (TOT) mode allowing direct measurement of the energy deposited in each pixel [4].

We observed EC patterns with bulk LiF crystals (with 6Li at its natural isotopic composition of 7.5%) and in highly ^{10}B doped diamond. The latter samples become superconducting at a T_c of several K [5].

Today intense ^{7}Be beams can be produced at ISOLDE-CERN, allowing the doping of samples with several 1015 atoms of ^{7}Be within few hours [6]. We also studied the EC patterns of ZnO implanted with ^{7}Be at ISOLDE.

Clear EC patterns could be observed for all these samples.

Prospects for lattice location studies of beryllium and boron by neutron-induced charged particle EC in a variety of materials will be discussed.

References

[1] U. Wahl, Phys. Rep. 280, 146 (1997).
[2] J.P. Biersack et al., Nucl. Instr. Meth. 149, 93 (1978).
[3] J.P. Biersack et al., Nucl. Instr. Meth. 188, 411 (1981).
[4] J. Jakůbek et al., Nucl. Instr. Meth. A560, 143 (2006).
[5] E. Bustarret et al., Phys. Rev. Lett. 93, 237005 (2004).
[6] U. Köster et al., Nucl. Instr. Meth. B204, 343 (2003).

PS2-37-112

Advantages of resonant detecting in hyperfine structure investigation by Moessbauer spectroscopy

Vitaly Panchuk,[1] **Valentin Semenov**[1]**, Sobir Irkaev**[2]

[1] *St. Petersburg State University, Department of Chemistry, St. Petersburg, Russia,*
e-mail: vitpan@mail.ru
[2] *Institute for Analytical Instrumentation, Russian Academy of Sciences, St. Petersburg, Russia*

Nowadays the investigations of nanostructures and nanomaterials by various physical techniques are of great interest. Mössbauer spectroscopy is one of not numerous methods, which allows determining of physicochemical state of the substance, its structure, electrical and magnetic properties. However, Mössbauer spectra of nanoparticles generally possess a complicated, poorly resolved, hyperfine structure with low signal-to-noise ratio. It should be noted, that same situation may be observed when metalloorganic substances and biological objects or after-effects of nuclear transformations are investigated. So that, when such materials are under investigation, a problem arises to refine resolution and sensitivity of Mössbauer spectroscopy technique. The most effective way to resolve the problem is application of resonance detectors. On advantage of resonant detectors over usual nuclear physics detectors is that they possess high selectivity with regard to resonant radiation and allow raising considerably the method's sensitivity when working in the transmission mode. In addition, when investigating the after-effects of nuclear transformations in the emission mode, there is no need to use spectral line analyzers, and the value of the resonant effect can be as high as several hundred percent. It is well known that resonant nucleus de-excitation after absorption of the Mössbauer radiation is realized by several ways. Interaction of incident radiation with a medium leads to reemitted gamma radiation, secondary X-rays, conversion electrons and Auger electrons. Registration of secondary radiation, preferably secondary electrons, is the base of manufacturing of resonance counter. As the counter of secondary radiations any nuclear physics counters can be used. But experimental investigations show, that the best one is a gas proportional microfoil counter. Up to date among all Mössbauer isotopes we can find only two effective resonance counter, namely for ^{119}Sn and ^{151}Eu experiments. For tin experiments there are two effective converters – $CaSnO_3$ and $BaSnO_3$ with f-factor equal to 0,5 and natural line width. For europium it is possible to use the EuF_3 compound. Searches for resonant pairs for the most widespread isotope ^{57}Fe led to the selection of double ferrocyanide (2PFC) $K_2MgFe(CN)_6$, whose spectral line coincides almost completely with the source line for Co(Cr) (δc = 0,3 mm/s), however for 2PFC the f-factor is only 0,3. The best parameters for iron experiments show the compounds $Fe_{50}Al_{50}$ and $FeGe_2$, which have natural line width and f-factor ~ 0,6. Unfortunately spectral lines of these compounds do not coincide with any sources used in experiment. We offer the optical scheme of versatile Mössbauer spectrometer, which will allow expanding considerably a number of Mössbauer isotopes to which the principle of resonance registration can be applied. The scheme of such spectrometer contains two strictly synchronized motions. In this work, the particulars of applying resonance detection are described and its advantages are demonstrated experimentally in comparison with conventional methods of detection.

PS2-38-152

POLAREX : Study of polarized nuclei - First measurement

<u>C. Gaulard,</u>[1] **L. Risegari L.**[1], **J.R. Stone**[2,3], **N.J. Stone**[2,4], **G. Audi**[1], **S. Cabaret**[1]

[1] *Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse, Bât 108, 91405 Orsay Campus, France, e-mail: gaulard@csnsm.in2p3.fr*
[2] *Department of Physics, University of Oxford, OX1 3PU Oxford, UK*
[3] *Department of Chemistry and Biochemistry, University of Maryland, College Park, MD20742, USA*
[4] *Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA*

POLAREX (POLARization of EXotic nuclei) is a new experiment for the study of the nuclear magnetic moments and spins of exotic nuclei [1]. The On-Line Nuclear Orientation (OLNO) method will be used to observe the decay of a spin-oriented ensemble of nuclei. The OLNO method associates on-line implantation of a radioactive beam of interest with the "Low Temperature Nuclear Orientation" (LTNO) technique [2]. The low temperature orientation is obtained with an OXFORD 400 ^{3}He-^{4}He dilution refrigerator which represents the main technical part of the system and that we inherited from TRIUMF (Fig. 1). The exotic nuclei are implanted into a ferromagnetic host foil held at a temperature of order 10 mK attached to the cold finger of the refrigerator.

The nuclear spins are oriented through the internal hyperfine field (10-100 T) and the ferromagnet fully magnetized by an external magnetic field (about 0.5 T). The aim of this experimental setup is to study neutron-rich nuclides produced at the ALTO facility (Linear Accelerator at Orsay Tandem) by fission induced by electrons from the linear electron accelerator (10-50 MeV, 10 μA) [3]. At the conference it will be presented the first "off-line" measurement achieved with this setup: anisotropy of ^{60}Cobalt on single crystal of cobalt. The aim of such measurement was to calibrate the apparatus. Then it will be also discussed the planning of the next studies and the evolution of this infrastructure.

Fig. 1. POLAREX dilution refrigerator

References

[1] http://csnwww.in2p3.fr/polarex/
[2] Low Temperature Nuclear Orientation, eds. N.J. Stone and H. Postma (North-Holland, Amsterdam) 1986
[3] http://ipnweb.in2p3.fr/tandem-alto/alto/

PS2-39-2

Air pollution studied by Mossbauer spectroscopy and synchrotron

G. L. Zhang, J. Lin, C. Jin, X. L. Li, Y. Li

Key Laboratory of Nuclear Analysis Techniques, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China

Air pollution is focused upon strongly nowadays because many diseases are caused by inhaled particulate matter (PM) in air such as pulmonary and trachea diseases as well as epidemiological diseases. The toxicity of PM to human health is not only related to its elemental concentration and particle size also to its chemical species. Mossbauer spectroscopy can be used to study that information from Fe [1]. Pb, Zn, Cu and Mn can be studied besides Fe by XANES on Synchrotron. In order to control the pollution to find the origin of pollution sources is also important. The synchrotron X-ray fluorescence microprobe (μ-SXRF) is a powerful tool to study that by analysis of individual aerosol particles combined with the pattern recognition technique [2].

In this paper we present the study of speciation of iron and other elements and their transformation in atmospheric particulate matter in Shanghai. The samples of PM_{10} (aerodynamic diameter<10μm) and $PM_{2.5}$ were collected from four sampling sites in Shanghai, China. They represent the iron and steel industrial district, commercial district and suburban district, respectively, as well as a special place i.e. tunnel where only for vehicles. The elemental concentrations were determined by ICP-MS.

The results showed that iron compounds in all samples consisted of Fe_2O_3, Fe_3O_4 , $Fe_2(SO_4)_3$ and Fe^{2+} high spin state but their proportions were different in different sampling sites, dependent of each environmental condition. The relative concentration of iron oxide in samples collected in the iron and steel industrial district is higher than the one in commercial and suburban districts, but the relative concentration of the iron sulfate is contrary to that case. In addition it was found that the concentrations of ferric sulfate in $PM_{2.5}$ are higher than those in PM_{10}. In order to study the transformation of iron compound the samples collected from different position in tunnel were measured. The transformation of Fe_3O_4 to Fe_2O_3 and the transformation of iron oxide to iron sulfate by SO_2 were found. Many results for iron were proved by XANES. Meanwhile speciation of Pb, Zn, Cu and Mn in PM is also presented

In addition a big amount of superparamagnetic particles with ~10 nm contained in PM was found by Mossbauer spectroscopy at 12 K, and their relative concentrations were related to the sampling sites. These nano-particles can reach alveoli directly.

The result of pollution source assignment shows that the most of analyzed PM_{10} and $PM_{2.5}$ particles were derived from vehicle exhaust, metallurgic emissions and power plants, and the mass concentration decreasing with year was found.

References

[1] Y. P Tong, et al. Environmental Science & Technology, 2001, 35(7): 1432 - 1436

[2] X. Li, et al. Nucl. Instr. and Meth. B 260 (2007) 336–342

PS2-40-101

^{57}Mn Implantation Mössbauer Spectroscopy of α-Al_2O_3 by Anticoincidence Method

Y. Kobayashi[1], **T. Nagatomo**[1,2], **Y. Yamada**[3], **M. Mihara**[4], **W. Sato**[5], **J. Miyazaki**[6], **S. Sato**[7], **A. Kitagawa**[7], **and M. K. Kubo**[2]

[1] Advanced Meson Science Lab., Nishina Center for Accelerator-Based Science, RIKEN, Wako, Saitama 351-0198, Japan; [2] Internatio nal Christian University, Mitaka, Tokyo 181-8585, Japan; [3] Dept. of Chemistry, Tokyo University of Science, Shijuku, Tokyo 162-8601, Japan; [4] Grad. School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan; [5] Dept. of Chemistry, Kanazawa University, Kanazawa, Ishikawa 920-1192, Japan; [6] College of Industrial Technology, Nihon University, Narashino, Chiba 275-8575, Japan; [7] National Institute of Radiological Science (NIRS), Inage, Chiba 263-8555, Japan.

Radioisotope (RI) beam can be applied as a Mössbauer probe to obtain the useful information about site occupations, dynamical behaviors, and exotic chemical states of extremely diluted atoms in materials. In the ^{57}Mn ($T_{1/2}$=1.45 min) implantation Mössbauer spectroscopy, a gas-filled resonant detector with an ^{57}Fe-enriched stainless-steel absorber was used exclusively to obtain Mössbauer spectra. The detector, so-called a parallel-plate avalanche counter (PPAC), can collect effectively a few numbers of Mössbauer γ-quanta by accumulating the conversion electrons emitted by Mössbauer effect. However, since ^{57}Mn nuclei decay to ^{57}Fe by emitting high-energy electrons, the β-rays penetrated to PPAC cause the background level of the spectrum to increase. We improved the detection system to reduce the noise level by using an anticoincidence method between the β–ray and the Mössbauer γ-ray originated from ^{57}Mn, and succeeded to obtain the spectra of a single-crystalline α-Al_2O_3 with sufficient the S/N ratios. Here, we discuss the final lattice sites and chemical states of ^{57}Fe arising from ^{57}Mn in α-Al_2O_3 based on the obtained Mössbauer parameters and the results of density functional calculation.

^{57}Mn was produced by projectile fragmentation of an ^{58}Fe beam on a Be target using the Heavy Ion Medical Accelerator (HIMAC) of NIRS. ^{57}Mn nuclei (~10^6 pps) were implanted into a single-crystalline α-Al_2O_3 after passing through energy degraders. A thin plastic scintillation counter was set between PPAC and the α-Al_2O_3 sample to reject the β-rays that induced high background.

The ^{57}Mn implantation Mössbauer spectra were measured at room temperature, 193 K, and 92 K. The obtained spectra could be analyzed by three components of doublets from the calculations of ORCA program. It was concluded that D1 (δ=0.43 mm/s, ΔE_Q=0.22 mm/s), D2 (δ=0.70 mm/s, ΔE_Q =1.31 mm/s), and D3 (δ =0.68 mm/s, ΔE_Q =2.43 mm/s) at R.T. were assigned to be substitutional Fe atoms on Al sites, interstitial Fe atoms with octahedral symmetry of oxygen, and substitutional Fe atoms with an oxygen deficiency. The temperature dependence of these components will be discussed.

PS2-41-92

Kramers-degenerated Spin Systems “NV+n^{13}C” in Diamond for Quantum Magnetometry: Spin-Hamiltonian and Quantum Chemistry Analysis

A.P. Nizovtsev[1], **S.Ya. Kilin**[1], **A.L. Pushkarchuk**[2], **S.A. Kuten**[3]

[1]*B.I. Stepanov Institute of Physics NASB, Nezavisimosti Ave., 68, 220072 Minsk, Belarus,*
e-mail: apniz@ifanbel.bas-net.by
[2]*Institute of Physical Organic Chemistry NASB, Surganova str., 13, 220072 Minsk, Belarus,*
[3]*Institute for nuclear problems, BSU, Bobruiskaya str., 11, 220050 Minsk, Belarus*

Spin systems consisted of single electronic spin S=1 of the NV center and few nearby isotopic ^{13}C nuclei spins I=1/2 in diamond lattice which can be used as a register of a quantum computer [1] or as a sensor of a magnetic field [2] are studied using spin Hamiltonian method. At odd number of ^{13}C nuclei the eigenstates of the spin system at zero external magnetic field are twofold (Kramers) degenerated due to the time reversal invariance of the spin Hamiltonian. This degeneracy is lifted only by external magnetic field regardless of any electric (crystal) field presented thus making such spin systems to be perspective for measurement of a local magnetic field by the NV-based single-spin quantum magnetometer [2].

Here (see also [3]) we have discussed spin properties of such spin systems using experimental data on hyperfine interactions obtained by observing electron paramagnetic resonance (EPR) on NV ensemble or by monitoring optically detected magnetic resonance (ODMR) spectra and spin echo modulation on single NV centers. Additionally, we used the density functional theory (DFT) to simulate the H-terminated carbon clusters hosting NV centers and calculate the hyperfine interaction matrices for ^{13}C nuclei in clusters. We have shown that our cluster simulations provide better correspondence to experimental data even for comparatively small clusters (the largest considered cluster was the $C_{84}H_{78}NV$ cluster) then the super-cell calculations [4] made using much larger super-cells. Moreover, for a first time we have calculated zero-field splitting parameters D and E for the NV center and found for the $C_{84}H_{78}NV$ cluster the values D=2837.23 MHz and E=2.12 MHz. For the simplest spin system “NV+1^{13}C” we got exact analytical expressions for energy levels and eigenstates. Available experimental data [5] on ODMR spectra and spin echo modulation obtained on “NV+n^{13}C” spin cluster are interpreted without fitting parameters.

Additionally, we have studied (see also [6]) the effects of a diamond surface on the NV spin properties depending on position and orientation in the NV center in cluster. The cases of non-passivated as well as H-, OH- and COOH- terminated surfaces (111) are considered. We have calculated hyperfine interaction constants as well as ZFS parameters D and E. All these characteristics have been found to be dependent on position and orientation of the NV center with respect of the surface as well as on the type of surface functionalization. Especially dramatically spin characteristics are changed (with respect to those for “bulk” clusters) for the NV center near non-passivated diamond surface.

References

[1] M.V. Gurudev Dutt et al., *Science,* **316**, 1312 (2007).
[2] J.R. Maze, et al., *Nature*, **455,** 644 (2008); G. Balasubramanian, et al., *Nature*, **455,** 648 (2008).
[3] A.P. Nizovtsev, et. al., *Optics and Spectroscopy*, **108**, 230 (2010);
[4] A. Gali, M. Fyta and E. Kaxiras, *Phys. Rev. B,* **77,** 155206 (2008).
[5] P. Neumann et al. *Science,* **320**, 1326 (2008).
[6] V.A. Pushkarchuk, et. al., *Optics and Spectroscopy*, **108**, 254 (2010).

Poster session III
Thursday 16th September 2010
15:40 – 17:00

Mezzanine

PS3-1-54

H/D Isotope Effect of ^{1}H MAS NMR Spectra and ^{79}Br NQR Frequencies in Piperidinium and Pyrrolidinium *p*-Bromobenzoate

Hisashi Honda[1,2], **Shinshin Kyo**[2], **Hiromitsu Terao**[3]

[1] *Graduate School of Nanobioscience, Yokohama City University, Kanazawa-ku, Yokohama, 236-0027, Japan, e-mail:hhonda@yokohama-cu.ac.jp*

[2]*Faculty of Sciences, Yokohama City University, Kanazawa-ku, Yokohama, 236-0027, Japan*

[3]*Facultyof Integrated Arts and Sciences, Tokushima University, Minamijosanjima-cho, Tokushima, 770-8502, Japan*

Piperidine and pyrrolidinium molecules form two kinds of O---H---N type hydrogen bonding with a *p*-bromobenzoic acid in each crystal. These crystals take the same space group of *Pbca* as piperidinium and pyrrolidinium *p*-chlrobenzoate (abbreviated to PIC(H) and PYC(H)) crystals[1-3]. Deuterium substitution samples of piperidinium and pyrrolidinium *p*-chlrobenzoate-d_2 (PIC(D) and PYC(D)) have shown anomalous H/D isotope effects: large shifts of ^{35}Cl NQR frequencies reaching to *ca*. 290 kHz have been recorded, although Cl atoms makes no hydrogen bond in the crystals. In addition, ^{1}H MAS NMR lines have displayed significant changes, while in contrast, little shifts of ^{13}C CP/MAS NMR signals have been obtained[1,2]. Since it is expected that anomalous H/D isotope effects are also detected in piperidinium and pyrrolidinium *p*-bromobenzoate, ^{79}Br NQR and ^{1}H MAS spectra measurements were carried out.

Piperidinium and pyrrolidinium *p*-bromobenzoate (PIB(H) and PYB(H)) were prepared by adding piperidinine and pyrrolidine to a hot benzene solution of *p*-bromobenzoic acid and by evaporating the solvent. The crude specimens obtained were recrystallized from benzene. PIB(D) and PYB(D) were prepared by crystallizing three times from a hot CH_3OD and recrystallization from dried benzene. Measurements of ^{79}Br NQR frequency were performed using a handmade super-regenerative spectrometer. Solid-state high-resolution ^{1}H MAS NMR experiments were carried out at a Larmor frequency of 600.13 MHz with a Bruker Avance 600 spectrometer. The samples were packed in a ZrO rotor with an outer diameter of 2.5 mm and the spinning rate was kept at 30 kHz through the acquisition of FID.

Temperature dependences of ^{79}Br NQR frequencies obtained for PIB(H) and PIB(D) are shown in Fig. 1. Small H/D isotope shifts of *ca*. 70 kHz were recorded although large ^{35}Cl NQR shifts have been detected for PIC[1]. Moreover ^{1}H MAS NMR spectra of PIB and PYB showed little changes by deuterium substitution. In order to reveal these differences between PIB, PIC, PYB and PYC, DFT calculations were carried out using the Gaussian 03w computer program. DFT estimation suggests that H/D changing of atomic arrangements contribute to EFG of Br atoms and shielding tensors of H atoms.

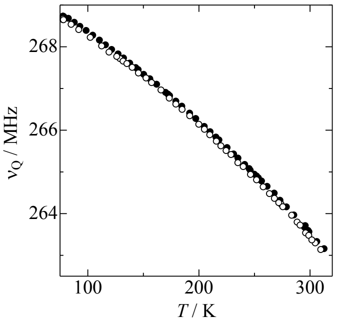


Fig. 1 Temperature dependences of ^{79}Br NQR frequency (ν_Q) of PIB(H) (●) and PIB(D) (○).

References

[1] R Nakano, H. Honda, T. Kimura, et. al., *Hyperfine Interactions*, **181**, 59-68 (2008).
[2] R Nakano, H. Honda, T. Kimura, et. al., *Bull. Chem Soc. Jpn.*, in press (2010).
[3] S. Kashino, Y. Sumida, M. Haisa, *Acta Cryst.*, **B28**, 1374(1972).

PS3-2-56

Variations of ^{57}Fe Hyperfine Parameters in Medicaments Containing Ferrous Fumarate and Ferrous Sulfate

M.I. Oshtrakh[1], **E.G. Novikov**[1,2], **S.M. Dubiel**[3], **V.A. Semionkin**[1,2]

[1] *Faculty of Physical Techniques and Devices for Quality Control and* [2] *Faculty of Experimental Physics, Ural State Technical University – UPI, Ekaterinburg, 620002, Russian Federation,*
e-mail: oshtrakh@mail.utnet.ru
[3] *Faculty of Physics & Computer Science, AGH University of Science & Technology, PL-30-059 Kraków, Poland*

^{57}Fe hyperfine parameters may be used to additionally characterize a quality of iron-containing pharmaceutical products. Therefore, we studied, using a high velocity resolution Mössbauer spectroscopy, several commercially available medicaments containing ferrous fumarate ($FeC_4H_2O_4$) and ferrous sulfate ($FeSO_4$) as a source of ferrous iron. It was shown earlier that Mössbauer spectroscopy with a high velocity resolution gives a better accuracy of hyperfine parameters evaluation, hence it enables revealing of small variations in their values [1, 2]. In this study, Mössbauer spectra of various samples were measured in 4096 channels at room temperature using a spectrometric complex described elsewhere [3, 4]. The spectra of the samples containing ferrous fumarate were presented for their analysis in 2048 channels by consequent summation of 2 neighboring channels, while those of other samples were analyzed in 4096 channels. As example, the spectrum of Sorbifer Durules ($FeSO_4$) is shown in Fig. 1. The analysis of the spectra recorded on the samples containing $FeSO_4$ revealed a presence of one main and two minor ferrous compounds, whose hyperfine parameters are shown in Fig. 2. It is interesting to observe small differences of the hyperfine parameters for the main component ($FeSO_4$). Similar differences in the hyperfine parameters of the main component ($FeC_4H_2O_4$) were found for the samples containing ferrous fumarate. They may have their origin both in the production process as well as in ingredients used by different producers.

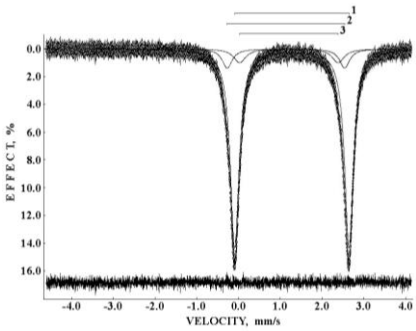


Fig. 1. Mössbauer spectrum of Sorbifer Durules ($FeSO_4$) fitted with three subspectra (1–3). T=295 K.

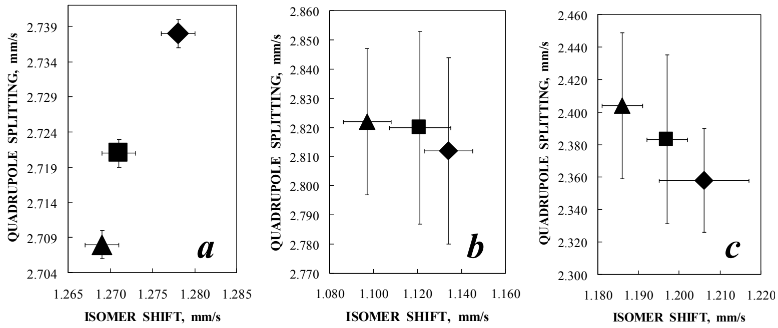


Fig. 2. Hyperfine parameters of (***a***) main component 1, (***b***) minor component 2 and (***c***) minor component 3 as found for $FeSO_4$–containing Sorbifer Durules (◆), Hemofer→ (■) and Falvit→ (▲).

References

[1] Oshtrakh M.I., Semionkin V.A., Grokhovsky V.I., Milder O.B., Novikov E.G. *J. Radioanal. Nucl. Chem.* **279**, 833 (2009).
[2] Oshtrakh M.I., Semionkin V.A., Milder O.B., Novikov E.G. *J. Mol. Struct.* **924–926**, 20 (2009).
[3] Oshtrakh M.I., Semionkin V.A., Milder O.B., Novikov E.G. *J. Radioanal. Nucl. Chem.* **281**, 63 (2009).
[4] Semionkin V.A., Oshtrakh M.I., Milder O.B., Novikov E.G. *Bull. Rus. Acad. Sci.: Phys.* **74**, 416 (2010).

PS3-3-58

Measurements in DNA molecules using Perturbed Angular Correlation Spectroscopy

Andréia dos Santos Silva, **Antonio Acleto Amaral, André Luis Lapolli, Rajendra Narain Saxena, and Artur Wilson Carbonari**

Instituto de Pesquisas Energéticas e Nucleares, IPEN-CNEN/SP, São Paulo, Brazil

The perturbed angular correlations (PAC) spectroscopy has been used to study the DNA, using ^{111}In(^{111}Cd) probe nucleus. The biological molecules studied were DNA of different mice lineages (A/J, C57BL/6, B6AF1, BXA1 and BXA2) infected by the strain of *T. cruzi*. This parasite may cause the Chagas disease when transmitted to humans. One of the advantages of applying PAC technique to biological molecules is that the experiments can be carried out on molecules in aqueous solution, approaching the function of molecules under conditions that are close to in vivo conditions. The samples were measured at the room temperature and at 77 K in each case. The samples measured at room temperature showed dynamic interaction with fast relaxation of the quadrupolar interaction A/J (λ = 7.6372 MHz); C57BL/6 (λ = 8.7097 MHz); B6AF1 (λ = 8.8570 MHz); BXA1 (λ = 18.0240 MHz) and BXA2 (λ = 15.9304 MHz), resulting in an exponential decay of the PAC spectra. The samples measured at the liquid nitrogen temperature on the other hand showed quite slow relaxation ($\lambda \sim 0$) of the quadrupolar interaction or only static interactions as expected at low temperatures: A/J ($\nu_{Q =}$ 141.975 MHz); C57BL/6 ($\nu_{Q =}$ 147.694 MHz); B6AF1 ($\nu_{Q =}$ 147.681 MHz); BXA1 ($\nu_{Q =}$ 217.346 MHz) and BXA2 ($\nu_{Q =}$ 221.828 MHz). The results showed, qualitatively, the existence of dynamic interactions between biomolecules and the probe nuclei. A systematic variation of the rotational diffusion parameter was observed that depends on the type of molecule and the sample temperature, showing that probe nuclei were in fact bound to the biomolecules.

PS3-4-80

^{57}Fe Quadrupole Splitting and Isomer Shift in Various Oxyhemoglobins: Study Using Mössbauer Spectroscopy

M.I. Oshtrakh[1], **A.L. Berkovsky**[2], **A. Kumar**[3], **S. Kundu**[3], **A.V. Vinogradov**[4],
T.S. Konstantinova[4], **V.A. Semionkin**[1,5]

[1] *Faculty of Physical Techniques and Devices for Quality Control, Ural State Technical University – UPI, Ekaterinburg, 620002, Russian Federation,*
e-mail: oshtrakh@mail.utnet.ru
[2] *Hematological Scientific Center of the Russian Academy of Sciences, Moscow, 125167, Russian Federation*
[3] *Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi - 110021, India*
[4] *Faculty of Internal Diseases Propedeutics, Ural State Medical Academy, Repin str., 3, Ekaterinburg, 620028, Russian Federation*
[5] *Faculty of Experimental Physics, Ural State Technical University – UPI, Ekaterinburg, 620002, Russian Federation*

Comparison of the heme iron electronic structure in various hemoglobins is very important in order to analyze structure-function relationship of oxygen carriers. It is well known that small stereochemical differences exist in the heme iron in different hemoglobins as well as in non-identical subunits in tetramer. Mössbauer spectroscopy is the most sensitive technique to study iron electronic structure in various species including iron-containing proteins. It was shown earlier that Mössbauer spectroscopy with a high velocity resolution increased possibilities of technique in accuracy of hyperfine parameters evaluation and revealing its small variations [1]. Mössbauer spectra of oxyhemoglobin samples from pig, rabbit, normal human and patients with blood system malignant diseases were measured using spectrometric complex with a high velocity resolution [2] at 90 K in 4096 channels. Then Mössbauer spectra were presented for analysis in 1024 channels by consequent summation of 4 neighboring channels. Mössbauer spectra were fitted in two ways using one quadrupole doublet (model of equivalent iron electronic structure in α– and β–subunits of hemoglobins) and superposition of two quadrupole doublets (model of non-equivalent iron electronic structure in α– and β–subunits of hemoglobins). Small variations of hyperfine parameters obtained within the first model are shown in Fig. 1. Hyperfine parameters obtained using both models were compared with structural and functional properties of hemoglobins.

This work was supported in part by the Russian Foundation for Basic Research (grant # 09-02-00055-a).

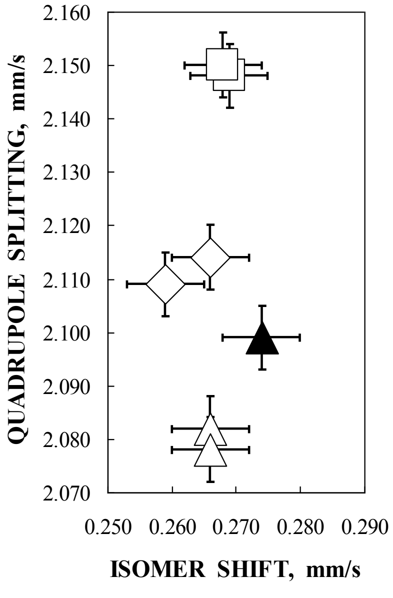


Fig. 1. Quadrupole splitting versus isomer shift for various oxyhemoglobins obtained using the first model fit: □ – pig, ◇ – rabbit, △ – normal human, ▲ – patient with multiple myeloma.

References

[1] Oshtrakh M.I., Semionkin V.A., Milder O.B., Novikov E.G. *J. Mol. Struct.* **924–926**, 20 (2009).
[2] Semionkin V.A., Oshtrakh M.I., Milder O.B., Novikov E.G. *Bull. Rus. Acad. Sci.: Phys.* **74**, 416 (2010).

PS3-5-91

Quantitative determination of phase transformations of the Tridymite-like $FePO_4$ catalyst pre and post oxidative dehydrogenation reactions to form Alkyl Methacrylates

Faiza B. Khan,[1] **Holger B. Friedrich**[1], **Krish Bharuth-Ram**[2]

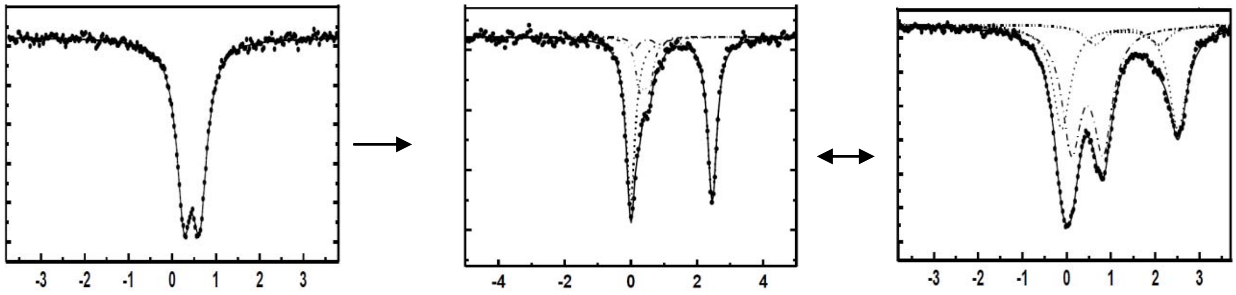
[1] *University of KwaZulu-Natal, School of Chemistry, Westville Campus, Durban, 4000,*
South Africa, e-mail:201295464@ukzn.ac.za

[2] *University of KwaZulu-Natal, School of Physics, Westville Campus, Durban, 4000,*
South Africa, e-mail:kbr@tlabs.ac.za

Alkyl methacrylates are of significant importance in the chemical industry. For example, free radical polymers, which contain the methacrylate backbone, are more rigid than acrylate polymers [1].
The aim of this project is focused on modification of the iron phosphate catalyst and optimizing conditions necessary for the formation of higher alkyl methacrylates.

The fresh and spent catalyst were characterised using Attenuated Total Reflection Infrared Spectroscopy (ATR-IR), Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES), Room temperature X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Mössbauer Spectroscopy, and BET surface area and Pore volume measurements. Additional techniques employed for the fresh catalyst included In-situ X-Ray Diffraction (XRD), Temperature Programmed Reduction and Oxidation (TPR, TPO), Temperature Programmed Desorption (TPD), Thermogravimetric and Differential Thermal Analysis (TGA-DTA/DSC).

The results obtained from certain techniques above were compared to the Mössbauer data and shall be discussed. Catalytic activation of the catalyst under certain reaction conditions had shown the formation of the active alpha phase, α-$Fe_3(P_2O_7)_2$, which is a mixed ferric and ferrous phosphate, and has been reported to be very active under catalytic conditions [2].



Initial uncalcined catalyst in Fe^{3+} $Fe_2P_2O_7$ – reduced catalyst α-$Fe_3(P_2O_7)_2$ – spent

Fig. 1. Phase transformations of the iron phosphate.

References

[1] R. Wilczynski, J.J. Juliette, Rohm and Haas Company, Methacrylic acid and Derivatives, Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 16, John Wiley & Sons, p. 227-270.
[2] J.M.M. Millet, *Catal. Rev.-Sci. Eng* **40 (1&2)**, 1-38 (1998).

PS3-6-113

Chemical states of ^{57}Fe in rock salt type crystals arising from ^{57}Mn

M. K. Kubo[1], T. Nagatomo[1,2], Y. Kobayashi[2], Y. Yamada[3], W. Sato[4], M. Mihara[5], J. Miyazaki[6], S. Sato[7], A. Kitagawa[7]

[1] International Christian University, Mitaka, Tokyo 181-8585, Japan, e-mail: kkubo@icu.ac.jp; [2] Advanced Meson Science Lab., Nishina Center for Accelerator-Based Science, RIKEN, Wako, Saitama 351-0198, Japan; [3] Dept. of Chemistry, Tokyo University of Science, Shijuku, Tokyo 1628601, Japan; [4] Grad. School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan; [5] Dept. of Chemistry, Kanazawa University, Kanazawa, Ishikawa 920-1192, Japan; [6] College of Industrial Technology, Nihon University, Narashino, Chiba 275-8575, Japan; [7] National Institute of Radiological Sciences (NIRS), Inage, Chiba 263-8555, Japan.

A study of ^{57}Fe in-beam Mössbauer spectroscopy using ^{57}Mn provides direct information on state of nuclear probes and on electronic properties of the materials around the probes. We have previously reported the studies on ^{57}Mn implanted into KMnO4 [1] and O2 solids [2]. Recently, our detection system was successfully improved to obtain in-beam Mössbauer spectra with large S/N ratio using HIMAC (Heavy Ion Medical Accelerator in Chiba). Here, we demonstrate the validity of this technique applied to the samples having rock-salt type crystal structure, NaF, NaCl and MgO.

The ^{57}Mn beam was produced as a nuclear projectile fragment of the ^{58}Fe beam, and implanted into a sample after passing through Pb/Al/acrylic plate degrader. A sample with 5mm in thickness was used. The ^{57}Fe Mössbauer spectrum of ^{57}Mn implanted into NaF measured at room temperature was relatively simple, which was fitted into the combination of a singlet (IS = −1.28 mm/s) and a doublet (IS = −1.17 mm/s, QS = 1.52 mm/s). The singlet peak is assigned to high-spin Fe^{2+} surrounded by six F^{-} ions, which substitute Na^{+} in NaF crystal. Whereas the assignment of the doublet is difficult; it might be an Fe atom with vacancy of F^{-} ions in neighbor, or an Fe atom in interstitial position of NaF lattice. NaCl showed a similar spectrum consisting of a singlet (IS = −1.12 mm/s) and a doublet (IS = −1.11 mm/s, QS = 1.41 mm/s). The singlet corresponded to the substitutional site and the doublet to a defect or interstitial site. The spectrum of MgO was analyzed as the sum of a singlet and doublets. Density functional calculations using ADF program set [3] applying cluster model were performed to estimate the electronic structure of the Fe atom in NaF lattice in various environment in order to make an assignment of the doublet peaks.

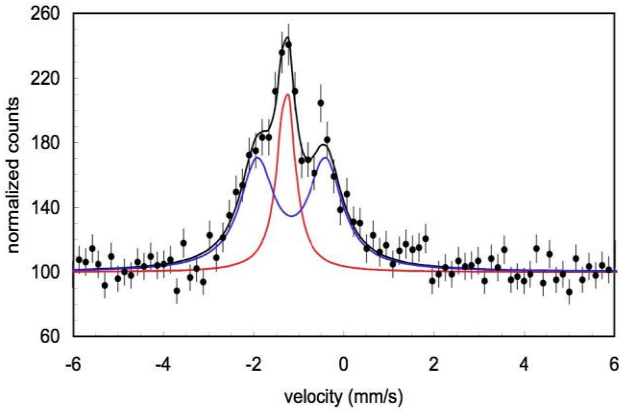


Figure 3 57Fe / 57Mn Mössbauer spectrum of NaF at RT.

References

[1] Y. Kobayashi, M. K. Kubo, Y. Yamada, T. Saito, H. Ueno, H. Ogawa, W. Sato, K. Yoneda, H. Watanabe, N. Imai, H. Miyoshi, K. Asahi, *J. Radioanal. Nucl. Chem.,* **255**, 403– 406(2003).

[2] Y. Kobayashi, H. Nonaka, J. Miyazaki, M. K. Kubo, H. Ueno, A. Yoshimi, H. Miyoshi, D. Kameda, K. Shimada, D. Nagae, K. Asahi, Y. Yamada, *Hyperfine Interact.,* **166**, 357–361(2006).

[3] ADF2008.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com

PS3-7-120

Reduction of Amorphous Fe(III)-hydroxide by the Binary Microbial Culture, Mössbauer Study

<u>N.I. Chistyakova</u>[1], V.S. Rusakov[1], A.A. Shapkin[1],
T N Zhilina[2], D.G. Zavarzina[2]

[1] *M.V.Lomonosov Moscow State University, Faculty of Physics, Leninskie gory, 119991 Moscow, Russia, e-mail:nchistyakova@yandex.ru*
[2] *Winogradsky Institute of Microbiology, Russian Academy of Sciences, 7/2, Prospekt 60-letiya Oktyabrya, 117312 Moscow, Russia*

The possibility of Fe (III)-reduction in alkaline environments has been subject to doubt due to the low mobility of Fe(III) under these conditions. However, this ability has been observed for *Geoalkalibacter ferrihydriticus* [1, 2]. Anaerobic alkaliphilic dissimilatory iron-reducing bacterium *G. ferrihydriticus* (strain Z-0531) and anaerobic alkaliphilic bacterium *Anaerobacillus alkalilacustre* (strain Z-0521) were isolated from sample of bottom sediments from low-mineralized soda lake Khadyn, Tuva (Russia) [3, 4]. *A. alkalilacustre* utilized mannitol as preferred substrate, producing formate, lactate and acetate as the main products. It did not reduce amorphous Fe(III)-hydroxide (AFH). *G. ferrihydriticus* used AFH as an electron acceptor and acetate as an electron donor and was not able to utilize mannitol.

The aim of our work was to study the process of iron mineral transformation in binary culture of these two bacteria, where mannitol was added as the only one substrate. ^{57}Fe Mössbauer spectroscopy at room and low temperatures was used as the main method of iron mineral determination. The concentration $n_{\mathrm{Fe(III)}}$ of initial AFH was varied. Mössbauer spectra of the sample obtained in iron-reduction process for $n_{\mathrm{Fe(III)}}$ =100 mM and measured at different temperatures are shown in Fig.1. The comparison of the room and low temperature spectra of this sample is indicative of superparamagnetic relaxation. The formation of siderite $FeCO_3$ and magnetically ordered phase (magnetite) were observed. The formation of magnetite was not observed for $n_{\mathrm{Fe(III)}}$ =10 mM, only siderite and the phase which spectrum parameters were close to the parameters of siderite were formed. It was also found when comparing some control probes and samples the joint growth of bacteria lead to a more intensive reduction of amorphous Fe(III)-hydroxide.

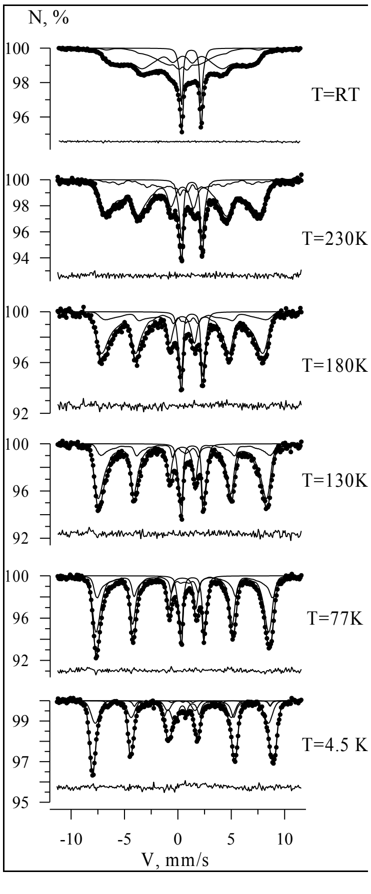


Fig. 1. Mössbauer spectra of samples measured at different temperatures ($n_{\mathrm{Fe(III)}}$ = 100 mM).

References

[1] N.I. Chystyakova, V.S. Rusakov, K.A. Nazarova, Yu.A. Koksharov, D.G. Zavarzina and J.–M. Greneche, *Hyperfine Interact.* **182** 55 – 63 (2008).

[2] N.I. Chystyakova, V.S. Rusakov, K.A. Nazarova, A.A. Shapkin, T.N. Zhilina, D.G. Zavarzina., *Izvestiya Rossiiskoi Akademii Nauk. Seriya Fizicheskaya* **74**, 433–437 (2010).

[3] D. G. Zavarzina, T. V. Kolganova, E. S. Boulygina, N. A. Kostrikina, T. P. Tourova and G. A. Zavarzin, *Microbiology* **75** 673–682 (2006).

[4] D. G. Zavarzina, T. P. Tourova, T. V. Kolganova, E. S. Boulygina, and T.N. Zhilina, *Microbiology* **78** 723–731 (2009).

PS3-8-127

Electric Field Gradient and Electronic Properties of Crown Thioether Compounds

Rafael Rodrigues do Nascimento,[1] **F. C. D. A. Lima**,[1] **M. B. Gonçalves**, [1] **H. M. Petrilli** [1]

[1]*Universidade de São Paulo, Instituto de Física, Departamento de Física*
dos Materiais e Mecânica, Grupo Nanomol,P-66318, São Paulo, Brazil, email:
rafaelr@if.usp.br

Crown thioethers are organic molecules that can act as molecular, metal and radioisotope carriers, ion-sensitive electrodes, phase transfer reagents and etc [1]. When these lock and key compounds are functionalized with radioisotopes, they present promising possibilities to be applied in drug design to treat and diagnose diseases. The Time Differential Perturbed Angular Correlation (TDPAC) technique has been suggested in the literature, in connection with different radioactive probes, to aid in this study [2,3]. An important issue to be addressed in the case of biomedical applications is the structural stability of the Crown thioethers, under different conditions, what can be done through state of the art *ab initio* electronic structure calculations. Here we study the electronic, structural and electrical hyperfine properties of some Crown thioethers complexed with Ag or Cd. We try to reproduce the different situations faced when there is a β decay of ^{111}Ag to ^{111}Cd as seen in a TDPAC experiment. We use the CP-PAW code, which is an all electron *ab initio* method in the Kohn-Sham scheme of the DFT [4] combining the Car-Parrinello quantum molecular dynamics [5] and the Projector Augmented Wave basis (PAW) set [6]. Our Electric Field Gradient (EFG) results are in a very good agreement with measurements [7] when the Cd+ atom is used to mimic the experimental situation. We also discuss the similarity in the electronic structures before and after the decay. We demonstrate in this issue the importance to evaluate the correct charge state in the *ab initio* analysis.

References

[1] Schubiger P. A., Alberto R. and Smith A., *Bioconjug. Chem.*, **7**, 165 (1996).
[2] Ctortecka B., PhD Thesis, Faculty of Physics and Earth Science, Universität Leipzig, 1999.
[3] Tröger W., *Hyperfine Interactions*, **120/121**, 117-128 (1999).
[4] Kohn W. and Sham L. J., *Phys. Rev. B.*, **140**, 1133 (1965).
[5] Car R. and Parrinello M., *Phys. Rev. Lett.*, **55**, 2493 (1985).
[6] Blöch P., *Phys. Rev. B*, **50**, 17953 (1994).
[7] Heinrich F., Ctortecka B. and Troger W., *Hyperfine Interactions*, **158**, 79-88 (2004).

PS3-9-131

Beta-NMR as a novel technique using radioactive beams for biophysical studies

M. Stachura[1], M.L. Bissell[2], G. Georgiev[3], A. Gottberg[4] , K. Johnston[5], M. Kowalska[6], K. Kreim[6], M. Luczkowski[7], G. Neyens[2], M. De Rydt[2], D.T. Yordanov[5], W.D. Zeitz[8], L. Hemmingsen[1]

[1] *University of Copenhagen, Department of Basic Sciences and Environment, Thorvaldsensvej 40, 1871 Frederiksberg C, Denmark, msta@life.ku.dk*
[2] *Katholieke Universiteit Leuven, Nuclear and Radiation Physics Section, Belgium*
[3] *CSNSM, Orsay, France*
[4] *Free University of Berlin, Institute of Experimental Physics, Germany*
[5] *PH-Department, ISOLDE, CERN*
[6] *Max Planck Institute for Nuclear Physics, Heidelberg, Germany*
[7] *University of Wroclaw, Faculty of Chemistry, Poland*
[8] *Helmholtz Institute, Berlin, Germany*

Beta-NMR is a technique where NMR resonances are observed as changes in beta-decay anisotropy. It has already been successfully applied in solid state physics and the technique holds great potential for successful applications in biology as well, although, it has never been applied to that field before.

Currently we are focused on setting up a new instrument at the ISOLDE/CERN which will allow to carry out the first measurements ever performed on biological samples. The combination of the ISOLDE facility and both optical pumping and tilted-foils opens up a wide spectrum of isotopes which are interesting from the biological point of view. With the use of beta-NMR one will gain the access to these properties of metalloproteins which are silent in most other spectroscopies.

The underlying physics of beta-NMR is basically the same as for classical NMR using stable isotopes what is a considerable advantage since the large expertise gained within the last decades of using this method in the field of biophysics and chemistry can be easily projected to future beta-NMR experiments. Moreover, this technique offers many advantages over NMR spectroscopy. Most notably, it is extremely sensitive, several orders of magnitude in comparison with standard NMR, and it may be applied for elements which are otherwise difficult to explore spectroscopically for certain biologically highly important oxidation states, such as Zn(II) or Cu(I).

We strongly believe that beta-NMR will contribute to studies of many important biological problems, such as structure and dynamics of molecules in solution, and therefore it would have a considerable impact in biological chemistry.

PS3-10-136

Ab-initio study of copper complexes

<u>Marcos Goncalves,</u>[1] Giovanni Caramori[2], Ana Ferreira[1], Helena Petrilli[1]

[1] *University of Sao PauloBrazil*
e-mail: browngon@if.usp.br
[2] *Federal University of Santa Catarina*

Schiff bases are compounds with two imine groups that form very stable transition metal complexes. Schiff base–copper complexes have been intensively studied as mimics of copper proteins [1], potential metallodrugs [2] and self assembled materials to be applied as biosensor [3]. These copper complexes show diversity of geometric configurations, electronic structures and very good catalytic activity in reactions involving molecular oxygen. These characteristics are related to differences in the ligand that need to reorganize to accommodate the ion. Coordination geometry, ligand type atoms, hydration energy and redox potential are some of characteristics that can influence the experimental response. Here we study a series of Schiff base–copper complexes using electronic structure calculations in the framework of the Density Functional Theory (DFT) using two computational codes: CP-PAW [4] and Gaussian 03 [5]. Our theoretical results for structural, electronic and hyperfine properties are compared with experimental data.

PS3-11-147

First Principles Electronic Structure Investigation of Order of Singlet and Triplet States of Oxyhemoglobin and ^{57m}Fe Nuclear Quadrupole Interactions

S.R. Badu[1], Archana Dubey[2], R.H. Scheicher[3], R.H. Pink[1], Lee Chow[2], K. Nagamine[4], N.Sahoo[5] and T.P. Das[1].

[1] Department of Physics, State University of New York at Albany, Albany, NY 12222, USA.
tpd56@albany.edu, shyambadu@albany.edu
[2] Departments of Physics, University of Central Florida, Orlando, Florida, USA
[3] Department of Physics, Condensed Matter Theory Group, Uppsala University, Uppsala, Sweden
[4] Department of Physics, University of California, Riverside.
[5] Department of Radiation Physics, UT MD Anderson Cancer Center, Houston, TX 77030

Interest in the possibility of magnetic character for oxyhemoglobin (OxyHb) has been recently stimulated by the observations of muon spin-lattice relaxation effects studied [1] with the muon-spin rotation (μSR) technique. In view of this, we have carried out first-principles electronic structure investigations involving Hartree-Fock theory combined with many body perturbation effects for the singlet and triplet states of OxyHb. Our results indicate that using two recent x-ray structural data [2, 3] for OxyHb, for only Hartree-Fock theory without many-body effects included, the singlet state lies above the triplet state by energies of about 0.08 and 0.13 a.u. for the two structures in Refs [2] and [3]. Incorporation of many-body effects by the perturbation method reverses the order, with the triplet state located 0.18 and 0.14 a.u. above the singlet state for the structures in Refs [2] and [3]. Physical reasons for these relative orderings of the singlet and triplet states will be discussed.

It is clear that OxyHb by itself would be in a singlet state at room temperature or below, since from our calculation, the triplet state lies about KT above the singlet state with T having the value of 44098 K and 56449 K for the two structural data in Refs [2] and [3]. Our calculated Mössbaubar nuclear quadrupole frequency in the singlet state is in good agreement with the experimental results, supporting the ordering of the singlet and triplet states.

As regards the muon spin lattice relaxation effects obtained by recent μSR measurements [1] at room temperature, the sensitive dependence of the singlet-triplet separation on many-body effects in our investigation suggests that it is possible that the singlet–triplet separation could be reversed or reduced significantly when a muon is trapped near an oxygen atom of the oxygen molecule, allowing the triplet to be occupied at room temperature and lead to significant muon spin–lattice relaxation. Muon spin-lattice relaxation could also be produced by the trapping of muonium in the singlet state making the OxyHb with trapped muonium system paramagnetic.

References

[1] K. Nagamine et al. Proc. Acad.Ser.B 83, 120 (2007).
[2] Massimo Paoli et al. J.Mol. Biol. 256, 775 (1996).
[3] Sam-Yong Park et al. J.Mol. Biol. 360, 690 (2006)

PS3-12-159

Study of hafnium sodium salts of DTPA using PAC Spectroscopy

Chain, C.Y.,[1] **Pasquevich, A. F.** [1,2]

[1]*Departamento de Física, IFLP, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, 1900 La Plata, Argentina, e-mail: yamil@fisica.unlp.edu.ar*
[2]*Comisión de Investigaciones Científicas- Provincia de Buenos Aires (CICPBA), Argentina*

The applications of PAC spectroscopy to biochemical subjects have progressed at a constant sustained rate in the last years. The principal limitations that face this type of systems concern the sample requirements: it is necessary to bind a suitable PAC isotope to the molecule of interest in stoichiomteric o substoichiometric amounts. In the biomedical field, the technique has been used to investigate organic compounds, lipid vesicles and macromolecules [1].

DTPA (diethylene triamine pentaacetic acid) is a polyamino carboxylic acid consisting of a diethylenetriamine backbone with five carboxymethyl groups. The molecule can be viewed as an expanded version of EDTA and it is used to treat the internal contamination with radioactive metals and as a “bridge” between isotopes and macromolecules in the radiopharmaceutical industry. Thus, the elucidation of the structure and dynamical behavior of metal-DTPA systems is of interest in both fields.

In this communication, PAC spectroscopy has been used to obtain the hyperfine parameters of hafnium sodium salts of DTPA at pH 4, 8, 9 and 10 using radioactive ^{181}Hf as probe nucleus. The samples were prepared by mixing proper amounts of solid DTPA, ^{181}Hf-HfF_4 in fluorhidric acid and sodium hydroxide 2M. Once the salts decanted, the supernatant was removed and the wet salts were measured at room temperature.

All the samples showed both dynamic and static interactions. The obtained hyperfine parameters, quadrupole frequency, asymmetry and the relaxation parameter are presented. Different behaviors were observed for the sample at pH 4 and the alkaline ones, indicating the possibility of ^{181}Hf being bonded to different ligands depending on the pH. Among the samples at alkaline pHs can be observed a variation tendency in the hyperfine parameters, corresponding to slight changes in the DTPA molecule as the pH varies.

References

[1] Hemmingsen et al., *Chemical Reviews* **104**, 4027 (2004) and references therein.

PS3-13-34

Negative thermal expansion and pressure induced amorphization in Zirconium tungstate as studied by ^{181}Ta TDPAC

R. Govindaraj, C. S. Sundar and A. K. Arora
Materials Science Group, Indira Gandhi centre for Atomic Research, Kalpakkam – 603102

Zirconium tungstate _ZrW_2O_8 is a cubic compound with three dimensional network of corner-linked ZrO_6 octahedra and WO_4 tetrahedra. Each WO_4 has one nonbridging W-O bond. ZrO_6 occupy face centered positions in the unit cell. This system exhibits negative thermal expansion isotropically over the temperature range 4–1050 K. Results of ^{181}Ta TDPAC study in zirconium tungstate imply the occurrence of four distinct Zr sites. It is interpreted that one site represents regular ZrO_6 and the other three sites are associated with contracted and distorted ZrO_6. Effective decrease in Zr-O bond length is understood to be due to an increase in the fractions of ZrO_6 octahedra which undergo contraction with temperature, thus explaining negative thermal expansion of the system [1]. Evolution of structures of ZrO_6 octahedra with isochronal annealing treatment has also been studied in zirconium tungstate amorphized by the application of a pressure of 5 GPa aiming at understanding pressure induced amorphization in the system [2].

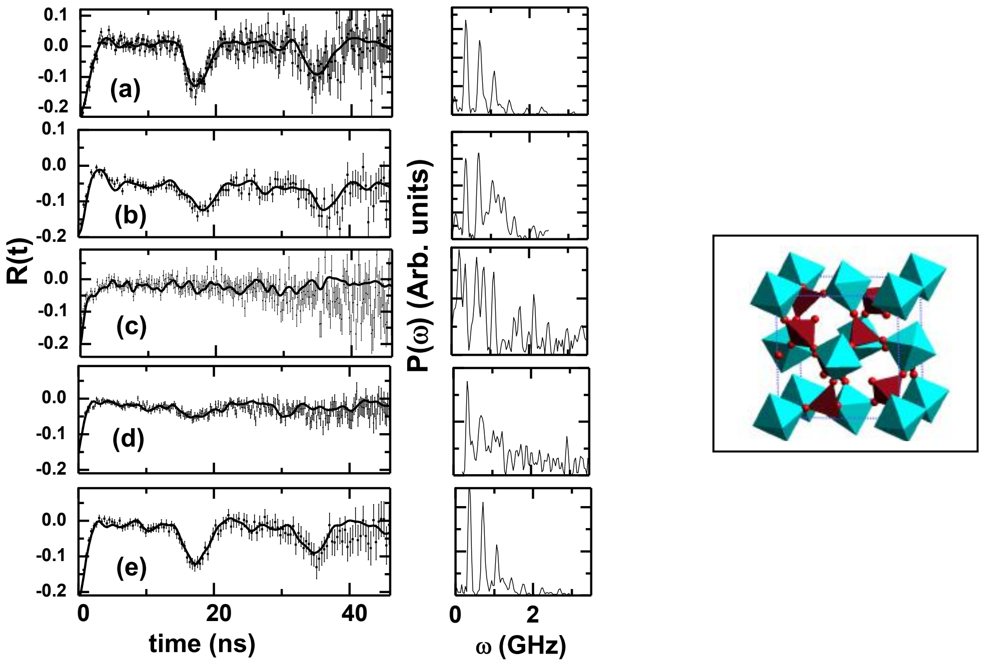


Figure 1. (a) and (b) correspond to Time dependent anisotropy spectra obtained in untreated reference Zirconium tungstate sample at 300 K and 433 K respectively, while Figs (c), (d) and (e) refer to time dependent anisotropy spectra obtained in as pressure amorphized and subsequent to annealing at 875 and 975 K respectively. Shown on the right hand side is the crystal structure of zirconium tungstate with ZrO_6 tetrahedal and WO_4 octahedral units.

References:

[1] Atomic scale study of negative thermal expansion in zirconium tungstate R. Govindaraj ,C. S. Sundar and A. K. Arora, *Phys. Rev*. B76, 012104 (2007)
[2] Studies of local structure at Zr sites in pressure amorphized zirconium tungstate R Govindaraj, C S Sundar and A K Arora, *J. Phys.: Condens. Matter* **21** (2009) 235402

PS3-14-87

Structural Phase Transitions in a [Chloranilic Acid]-[2-Pyrrolidone] (1:2) Molecular Complex with Hydrogen-Bond Networks

<u>Shota Morikawa</u>[1], **Teppei Yamada**[1], **Ryuichi Ikeda**[1], **Hiroyuki Ishida**[2], **Hiroshi Kitagawa**[1,3]

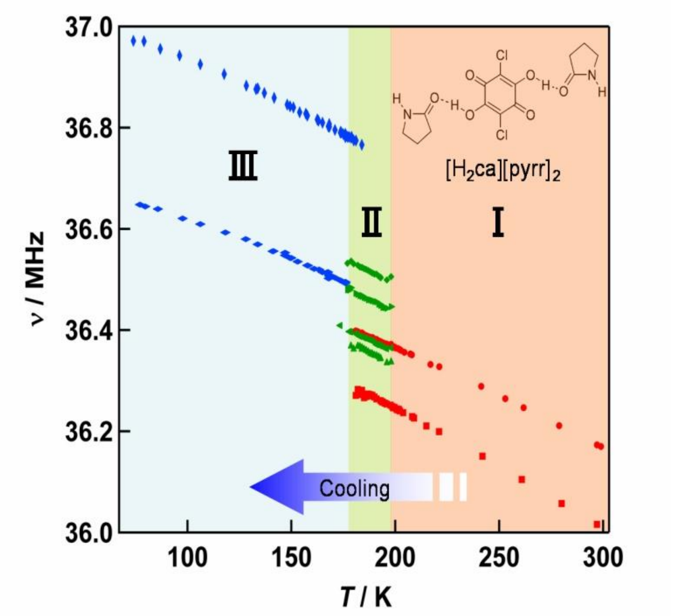
[1] *Kyoto Univ. Kitashirakawa Oiwake-cho, Sakyo-ku, Kyoto 606-8502, Japan, e-mail: morin@kuchem.kyoto-u.ac.jp,* [2] *Okayama Univ., 3-1-1, Tsushima-Naka, Kita-ku, Okayama 700-8530, Japan* [3] *JST CREST, Sanbancho 5, Chiyoda-ku,Tokyo 102-0075, Japan, e-mail: kitagawa@kuchem.kyotou.ac.jp*

Chloranilic acid has been widely studied as a proton donor forming hydrogen-bonds with various proton acceptors. Obtained complexes have been shown to have marked properties such as dynamic proton transfers, ferroelectricity, and so on.

In the present study, we prepared a new chloranilic acid complex with 2-pyrrolidone in search for new solid properties by measurements of single crystal X-ray diffraction (SCXRD), ^{35}Cl NQR, ^{1}H NMR, and differential scanning calorimetry (DSC). Crystals of [chloranilic acid]-[2-pyrrolidone] (1:2) complex were obtained by slow cooling of an acetonitrile solution containing 2-pyrrolidone (pyrr) and chloranilic acid (H2ca). The crystals were identified by elemental analysis and SCXRD. In the structure, it was found that pyrr and H2ca molecules are connected by hydrogen–bonds and make up a one-dimensional chain structure with hydrogen-bond networks. The one-dimensional chains are stacked by π -π interactions in the crystals.

On [H2ca][pyrr]2 crystals, we measured a temperature dependent ^{35}Cl NQR lines and spin-lattice relaxation times by using a Bruker BioSpin AVANCEII system. Two ^{35}Cl resonance lines were observed at room temperature (*Phase I*) in agreement with the SCXRD results. New four broad lines appear below 200 K (*Phase II*), where room-temperature two lines still persist with a gradually decrease of intensities upon cooling down to 175 K. Below 175 K (*Phase III*), another two lines with equal intensities appeared in the high frequency side. When heated from 77 K, these two peaks were repeated up to ca. 200 K where only the low-frequency peak disappeared. The high frequency peak survived with no anomaly at 200 K up to room temperature (*Phase Ia*), where the structure was shown to be different from the original one. It is expected that *Phase Ia* is stable and *Phase I* is a metastable phase. We believe this transition is due to an incommensurate structure.

Fig 1 Temperature dependence of ^{35}Cl NQR frequencies (ν) upon cooling



PS3-15-135

Mössbauer characterisation of Copper ferrite as a model system for the Fischer-Tropsch synthesis

Zandile Chonco[1], Eric van Steen[1], Michael Claeys[1] and Krish Bharuth-Ram[2]

[1]*Centre for Catalysis Research, Department of Chemical Engineering, University of Cape Town,*

Private Bag X3, Rondebosch, 7701, South Africa

Corresponding author: Tel: +27 21 650 5524, Fax: +27 21 650 4051, E-mail:

[2] *iThemba LABS, P.O.Box 722, Sommerset West 7129, South Africa*

zandile.chonco@uct.ac.za

The role of copper promotion as a promoter for iron-based Fischer-Tropsch catalysts has been extensively studied [1]. It has been observed that copper acts as a reduction promoter when activation is done in H_2 [2]. Wachs et al. [3] studied the effect of copper and silver as promoters on iron-based Fischer-Tropsch catalysts (activated in H_2) and observed that copper and silver did not show any effects on the performance of the iron-based Fischer-Tropsch catalyst, while others did observe an effect of copper in iron-based Fischer-Tropsch synthesis [4]. Wachs et al. attributed their findings to the absence of the intimate contact between the copper and silver with iron in their studies. However, little is known on how copper affects the iron-based Fischer-Tropsch catalyst when activated in CO or H_2/CO. During Fischer-Tropsch synthesis when using iron-based Fischer-Tropsch catalysts a change in crystallite sizes and also various iron phases are observed. These observed variables are reported to influence the performance of the iron-based catalysts. Therefore, highly sensitive characterization techniques are necessary for thorough study of these changes. Herein, reported is our investigation directed towards the study of the copper promotional effect on iron-based Fischer-Tropsch catalysts using copper ferrite ($CuFe_2O_4$) as a model system. The $CuFe_2O_4$ was prepared using a precipitation method, thereafter, characterised by the Mössbauer technique to determine the crystal structure of the $CuFe_2O_4$. Mössbauer spectroscopy was also used to the determine iron phases present in the copper ferrite system of the fresh copper ferrite, the material reduced in different atmospheres (H_2, CO , H_2/CO) and the material after use in the Fischer-Tropsch synthesis, in an attempt to understand the influence of the copper promotional effect.

References

[1]. M. Luo, R. O'Brien, B. H. Davis, *Catal. Lett.* **98***,* 17 (2004).

[2]. M. E. Dry in J.R. Anderson, M. Boudart (eds.), *Catalysis Science and Technology, vol 1,* Springer, New York, 159 (1981).

[3]. I. E. Wachs, D. J. Dwyer, E. Iglesia, *Appl. Catal.* **12**, 201 (1984).

[4]. D. B. Bukur, D. Mukesh, S. A. Patel, *Ind. Eng. Chem. Res.* **29**, 194, (1990).

PS3-16-74

^{57}Fe Hyperfine Interactions in M1 and M2 Sites of Olivine from Omolon Meteorite: Study Using Mössbauer Spectroscopy

D.G. Patrusheva[1], M.I. Oshtrakh[1], E.V. Petrova[1], V.I. Grokhovsky[1], V.A. Semionkin[1,2]

[1] Faculty of Physical Techniques and Devices for Quality Control and [2] Faculty of Experimental Physics, Ural State Technical University – UPI, Ekaterinburg, 620002, Russian Federation,
e-mail: patrushevadg@gmail.com, oshtrakh@mail.utnet.ru

Olivine (Fe, Mg)$_2$SiO$_4$ is a mineral with two crystallographically non-equivalent six-fold octahedral sites for Fe^{2+} and Mg^{2+} denoted as M1 and M2. These sites in olivine are occupied by Fe^{2+} and Mg^{2+} ions in different ways. The Fe–Mg distribution between two sites is of interest for mineral cooling history determination. Recently we demonstrated new possibilities in the study of ordinary chondrites and other meteorites using Mössbauer spectroscopy with a high velocity resolution [1–3]. In particular, in these works differences of hyperfine parameters for the M1 and M2 sites of olivine in bulk ordinary chondrites were revealed for the first time. In the present study olivine extracted from pallasite Omolon was investigated using Mössbauer spectroscopy with a high velocity resolution. Mössbauer spectra of olivine were measured using a spectrometric complex described in details elsewhere [4, 5] in 4096 channels at 295 and 90 K. Mössbauer spectrum of olivine at 295 K is shown in Fig. 1. This spectrum was fitted using superposition of two main doublets (1 and 2) and one minor doublet 3. Mössbauer hyperfine parameters for the minor doublet characterized ferric compound while those for the main doublets were correspondent to ferrous compounds with different values of isomer shift and quadrupole splitting. The 1st and the 2nd doublets were related to the ^{57}Fe nuclei in the M1 and M2 sites, respectively. Mössbauer spectrum of olivine measured at 90 K was fitted using two main doublets related to the ^{57}Fe nuclei in the M1 and M2 sites. It was found that quadrupole splitting values for the M1 and M2 sites simultaneously increased with temperature decrease while isomer shift values increased with temperature decrease in different way (Fig. 2). This fact may indicate differences in the second order Doppler shift and Debye temperature for the ^{57}Fe nuclei in the M1 and M2 sites of olivine.

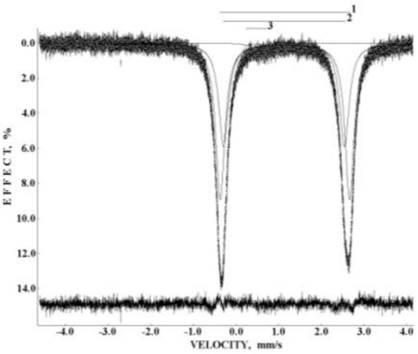


Fig. 1. Mössbauer spectrum of olivine from Omolon meteorite. T=295 K.

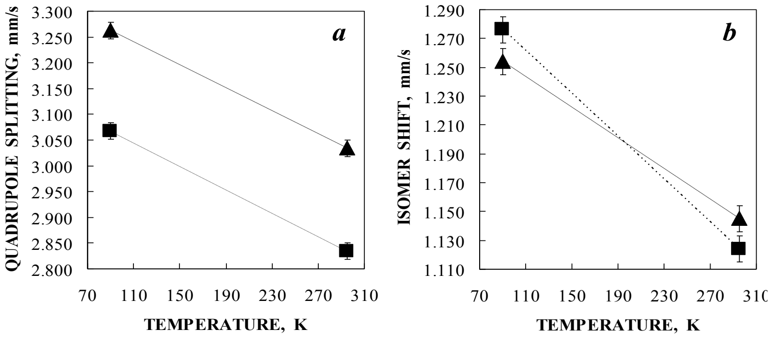


Fig. 2. Mössbauer hyperfine parameters for ^{57}Fe in the M1 sites (▲) and M2 sites (■) of olivine from Omolon meteorite: quadrupole splitting (***a***) and isomer shift (***b***) vs. temperature.

References

[1] Oshtrakh M.I., Petrova E.V., Grokhovsky V.I., Semionkin V.A. *Meteoritics & Planetary Sci*. **43**, 941 (2008).
[2] Oshtrakh M.I., Petrova E.V., Grokhovsky V.I., Semionkin V.A. *Hyperfine Interact*. **186**, 61 (2008).
[3] Grokhovsky V.I., Oshtrakh M.I., Petrova E.V., Larionov M.Yu., Uymina K.A., Semionkin V.A. *Eur. J. Mineral.* **21**, 51 (2009).
[4] Oshtrakh M.I., Semionkin V.A., Milder O.B., Novikov E.G. *J. Radioanal. Nucl. Chem*. **281**, 63 (2009).
[5] Semionkin V.A., Oshtrakh M.I., Milder O.B., Novikov E.G. *Bull. Rus. Acad. Sci.: Phys*. **74**, 416 (2010).

PS3-17-85

^{14}N NQR study of selected 1,4-benzoquinonedioximes

N. Singh and **D. Stephenson**

Chemistry Dept., University of the West Indies, St. Augustine, Trinidad and Tobago.
e-mail: nadia.singh@sta.uwi.edu or david.stephenson@sta.uwi.edu

1,4-benzoquinonedioximes are known for their use in industry and other applications[1]. They are effective non-sulfur vulcanizing agents for natural and synthetic elastomers. Additionally, their metal complexes have generated significant industrial and theoretical interest. This study examines the ^{14}N NQR data for a series of 1,4-benzoquinone-dioximes: unsubstituted, mono-, di- and tri-methyl substituted. The results show that as more methyl substituents are added to the ring a shift in the NQR values are observed. Comparison of unsubstituted and tri-substituted benzoquinonedioximes (Table 1) shows that the quadrupole coupling constant (χ) increases by about 1000 kHz and the asymmetry parameter (η) decreases from $\approx$ 0.7 to 0.3. Ab-initio calculations show that for the unsubstituted compound hydrogen bonding between oxime groups and pi-ring stacking is possible which cannot be accommodated for in heavily methyl substituted dioximes and this is responsible for the differences in the NQR parameters.

Table 1: ^{14}N NQR data for the 1,4-benzoquinonedioximes

Compound	ν_0 (kHz)	ν_- (kHz)	ν_+ (kHz)	χ (kHz)	η
1,4-benzoquinone dioxime	1654 1654	2673 2712	4360 4360	4689 4715	0.706 0.702
trimethyl-1,4-benzoquinonedioxime	950	3750	4700	5633	0.337

Double resonance cross relaxation [2] was used to record the ^{14}N NQR data. The ab-initio calculations were performed using GAMESS [3].

References

[1] http://chemicalland21.com/specialtychem/perchem/p-QUINONE%20DIOXIME.htm (last accessed 04-28-10)
[2] D. Stephenson and J. A. S. Smith, *Proc R Soc Lond A* **416**, 149 (1988).
[3] M. W. Schmidt et al., *J. Comput. Chem.* **14**, 1347 (1993).

PS3-18-11

Spectroscopic and Mineral Magnetic Studies on some Ancient Pottery Samples

R.Venkatachalapathy[1], **C.Manoharan**[2], **N.Basavaiah**[3], **S.Vasanthi**[4], **K.Veeramuthu**[2]

[1]*Center of Advanced Study in Marine Biology, Annamalai University, Parangipettai -608 502, India. Email: venkatr5@rediffmail.com*
[2]*Department of Physics, Annamalai University, Annamalainagar- 608 002, India.*
[3]*Indian Institute of Geomagnetism, New Panvel, Navi Mumbai- 410 218, India.*
[4]*State Archaeological Department, Tamilnadu, India*

^{57}Fe Mössbauer absorption spectra and FTIR spectra were recorded for archaeological pottery samples obtained from the excavated site of Nedungur [Lat.10° 57'N; Long.77°51'E]. The physical and chemical state of iron (Fe^{2+}/Fe^{3+}) and iron oxide phases obtained using Mössbauer spectra were used to establish the temperature and atmosphere of firing and also to correlate the color of the sample. The clay mineral type and its structural deformation due to firing were established using Fourier Transform Infrared spectra. The mineral types and domain states of the constituent magnetic fine particles were elucidated using variation of susceptibility at various frequency and temperature under low field. An attempt has also been made to correlate the magnetic parameters from the percentage of Fe^{2+}/Fe^{3+} and iron oxides. The information obtained paves a way for a better understanding of the technological development that took place in the ancient past and also the suitability of the samples for determination of reliable ancient geomagnetic field intensity values.

Keywords: FTIR, XRD, Mössbauer, Magnetic properties, Pottery shreds.

PS3-19-49

Mössbauer Spectroscopic and Mineral Magnetic studies on Archaeological Potteries from Tamilnadu, India

R.Venkatachalapathy[1], R. Ilango[2], C. Manoharan[3], T.Radhakrishna[4]

[1]*Center of Advanced Study in Marine Biology, Annamalai University, Parangipettai -608 502, India. Email: venkatr5@rediffmail.com*
[2]*Department of Physics, Government Arts College (Men), Krishnagiri-635 001,India*
[3]*Department of Physics, Annamalai University, Annamalainagar- 608 002, India.*
[4]Center for Earth Science Studies,Akkulam, Trivandrum . 695 031, India.

Mössbauer Spectroscopy is extremely sensitive to minute changes in the chemical environment and provides a means of investigating the chemical states in which atoms reside with incredible resolution. Since iron is common in virtually all clays, Mössbauer spectroscopy provides a method to analyse many of the chemical states within ceramics. This technique has become an increasingly useful tool to archaeologists and also questions related to the provenance and manufacture of ancient pottery. For the present study, the archaeological pottery samples from Modur (Lat 12º 13'N; Lon 78º 10'E) and Andipatti (Lat 12º 13'N; Lon 78º 44'E), Tamilnadu, India, have been subjected to Mössbauer spectroscopic and mineral magnetic measurements. A knowledge of the state of the iron in fired potteries, under which conditions, it was fired, like the firing temperature, the oxidizing or reducing character of the kiln atmosphere and colouring mechanism has been well established. Rock magnetic measurements have also been carried out in order to identify the magnetic minerals present, which are responsible for the record of ancient geomagnetic field intensity. From the suitable samples the paleointensity values are estimated.

Keywords: Mössbauer, Magnetic properties, Pottery shreds

PS3-20-10

Application of Mössbauer spectroscopy in investigation of wall rock alteration at uranium deposit

Jun LIN,[1] **Ya-xin YANG**[2]**, Yuan-fu Hsia**[3]

[1] *Key Laboratory of Nuclear Analysis Techniques, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China, e-mail: jlin1978@gmail.com*
[2] *East China Institute of Technology, Fuzhou 344000, China, e-mail: yxyang63@hotmail.com*
[3] *Department of Physics, Nanjing University, Nanjing 210093, e-mail: hsia@nju.edu.cn*

Pitchblende as the micro/cryptocrystalline uraninite, normally UO_{2+x}, is common U^{4+} mineral species, and is the main ore mineral in the hydrothermal U deposits. Pitchblende always contains certain amount U^{6+} in the formula of UO_{2+x}, where x reaches the maximum value as 0.25. The investigation shows that the mineral composition varies as the lodes formed at different stages and changes outwards from the center of the lode. It also indicates that sulfur/H_2S and the ferrous minerals may play an important role as a reducer in the deposition of the pitchblende from uraniferrous solution where the uranium migrates mainly in the form of various U^{6+} compounds. So, the pitchblende deposition is considered to be a reduction – oxidation process between U^{6+}-bearing solution and the rock as diabase is enriched in ferrous minerals.

In general, the iron-bearing minerals with different valence charge could be distinguished macroscopically by their colors. However, it is quite difficult when the iron-bearing minerals are in small amount and highly dispersed, such as the wall rock alteration. In such a circumstance, Mossbauer spectroscopy is of great advantages compared to other methods because of its sensitivity for distinguish the valence of iron.

Samples were collected from different zones (the pitchblende lode, the chloritized alteration zone and the weakly altered diabase) at a uranium deposit (Fig. 1). Fig. 2 shows the Mossbauer spectra of these samples, where a ~ f corresponding to the sites labeled in Fig 1. Based on the Mossbauer spectra, the main iron mineral in the lode is pyrite, and in the altered zone there is less pyrite relative to that in the lode. There are more original minerals in weakly altered diabase zone. The difference among these three zones originates from the difference of rock alteration. The alteration decreases according to the increase of distance to the center of the lode, from pyritization to chloritzation gradually. The ratio of pyrite decreases with increasing distance to the lode center, while altered ripidolite is most abundant in the altered zone of chloritization.

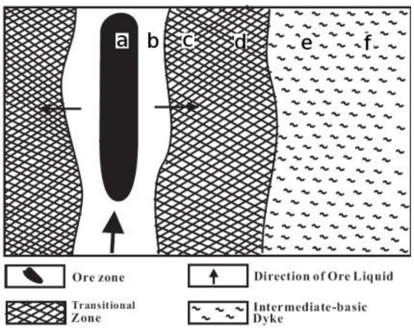


Fig. 1. Sketch of sampling sites.

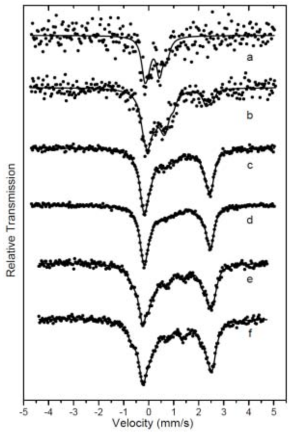


Fig 2. Mossbauer spectra of samples from various sites.

PS3-21-14

Debye temperature in σ-phase Fe-V alloys

Jakub Cieslak[1], Michael Reissner[2], Stanisław M. Dubiel[1], Benilde F. O. Costa[3] and Walter Steiner[2]

[1]*Faculty of Physics and Computer Science, AGH University of Science and Technology,*
30-059 Krakow, Poland, e-mail: dubiel@novell.ftj.agh.edu.pl
[2]*Institute of Solid State Physics, Vienna University of Technology, 1040 Wien, Austria*
[3]*CEMDRX Department of Physics, University of Coimbra, 3000-516 Coimbra, Portugal*

Among about 50 examples of a σ-phase (tetragonal unit cell - structure type D^{14}_{4h} $P4_2/mnm$) known to exist in binary alloy systems the one in FeV is of particular importance due to a wide composition-temperature range in which σ can be formed as well as to the strongest magnetism it shows [1]. The former offers favourable conditions for investigation of compositional dependence of various physical properties as well as testing various theoretical models.

This contribution reports on Debye temperatures, Θ_D, determined from a temperature dependence of the average centre shift, based on the Debye model, for a series of the σ-phase $Fe_{100-x}V_x$ samples with $34.4 \leq x \leq 59.0$. As displayed in Fig. 1, $\Theta_D(x)$ dependence is not monotonous, but two minima – one at $x \approx 40$ and the other at $x \approx 48$ – and a maximum at $x \approx 43$ are observed. Such behaviour and the fact that the amplitude of a change in Θ_D reaches ~40% is unexpected and it is quite puzzling. The behaviour will be discussed in a context of influence of composition of other physical properties characteristic of the samples such as Curie temperature, average isomer shift and average magnetic moment per Fe atom.

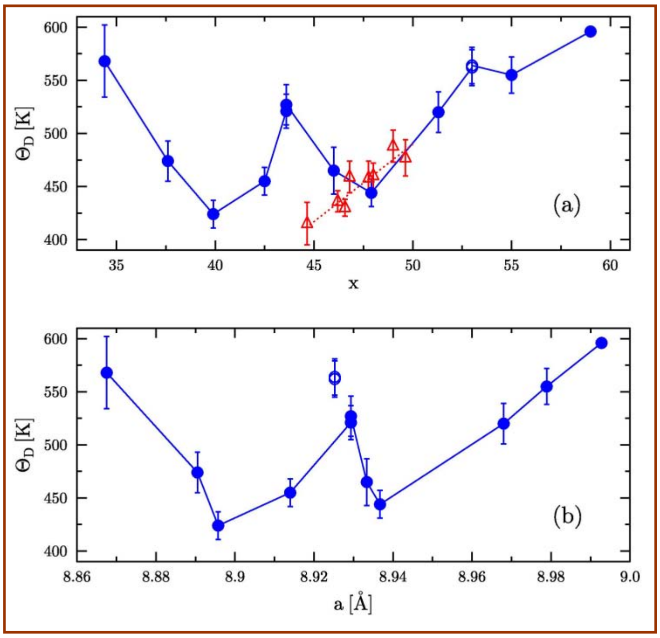


Fig. 1 (a) Dependence of the Debye temperature, θ_D, on vanadium concentration, *x*, and (b) on the lattice constant, *a*. Open symbols stand for policrystalline and open ones for nanocrystalline samples. Triangles in (a) represent θ_D for σ-FeCr alloys.

References

[1] J. Cieślak, B. F. O. Costa, S. M. Dubiel, M. Reissner , W. Steiner, *J. Magn. Magn. Mater.* **321** (2009) 2160

PS3-22-48

Lattice Location and Diffusion of Interstitial Fe in MgO

T. E. Mølholt[1], **R. Mantovan**[2], **H. P. Gunnlaugsson**[3], **K. Bharuth-Ram**[4], **M. Fanciulli**[2,5], **K. Johnston**[6], **Y. Kobayashi**[7], **G. Langouche**[8], **H. Masenda**[9], **D. Naidoo**[9], **S. Ólafsson**[1], **R. Sielemann**[10], **A. Svane**[3], **G. Weyer**[3], **H. P. Gíslason**[1]

[1]*Science Institute, University of Iceland, Reykjavík, Iceland, e-mail: tem4@hi.is;* [2]*Laboratorio MDM-IMM-CNR, Milano, Italy;* [3]*Department of Physics and Astronomy, Aarhus University, Denmark;* [4]*School of Physics, University of KwaZulu-Natal, South Africa;* [5]*Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy;* [6]*PH Dept, ISOLDE/CERN, 1211 Geneva 23, Switzerland;* [7]*The Institute of Physical and Chemical Research, Wako, Japan;* [8]*Instituut voor Kern-en Stralingsfysika, University of Leuven, Belgium;* [9]*School of Physics, University of the Witwatersrand, South Africa;* [10]*Helmholtz Zentrum, Berlin, Germany.*

3d-metal doped MgO has been suggested as a model system for dilute magnetic semi-conductors [1]. However, the physics of 3d-metal impurities is poorly understood [2,3]. We present an ^{57}Fe emission Mössbauer study on dilute Fe impurities in single-crystalline MgO (77 – 649 K) following implantation of radioactive ^{57}Mn$^+$ ($T_{½}$ = 85.4 s) at the ISOLDE facility at CERN. Due to the recoil imparted on the daughter ^{57*}Fe atoms in the β^--decay ($\langle E_R \rangle = 40$ keV) interstitial ^{57m}Fe atoms are created. Figure 1 shows the central part of the measured Mössbauer spectra at different temperatures (see [3] for details). At low temperatures the central part is dominated by an asymmetric quadrupole doublet (red) assigned to Fe in heavily damaged/amorphous regions caused by the implantation. At high temperatures the spectra are dominated by a single line (pink) assigned to Fe^{2+} on substitutional Mg sites. During the fitting procedure a single line had to be introduced, the line of interest her, which is attributed to interstitial Fe (blue). The wings of the spectra show a magnetic sextet structure assigned slowly relaxating Fe^{3+} (green); more details of this component are described elsewhere [4]. The interstitial line exhibits a broadening at elevated temperatures which can be associated with diffusional jumps of interstitial Fe on the time-scale of the decay lifetime of the Mössbauer state (140 ns). A diffusion coefficient of $D = 1.4(3)\times10^{-9}$ cm^2/s at 300 K is thus obtained. This value is orders of magnitude higher than suggested for vacancy-assisted Fe diffusion in MgO [5]. However, there is experimental evidence for a fast diffusion of 3d-metal impurities in MgO [2,3]. The Mössbauer parameters of the interstitial Fe are in good agreement with theoretical calculations for interstitial Fe atoms is located at the face of the rock salt fcc MgO crystal structure.

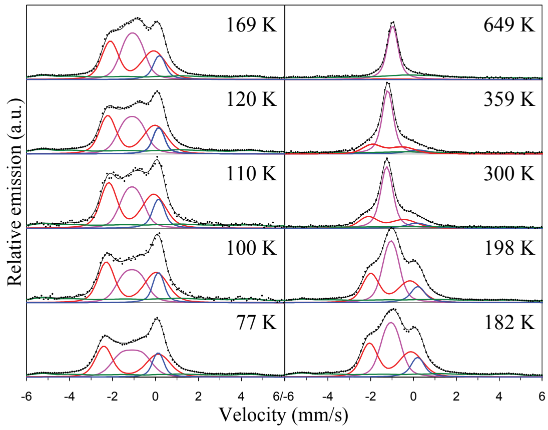


Fig. 1. Central part of the measured Mössbauer spectra at the temperatures indicated.

References

[1] J. Narayan, N. Sudhakar, D. K. Pandya, D. K. Avasthi, A. I. Smirnov, *Appl. Phys. Lett.*, **93**, 082507 (2008).
[2] M. Lu, C. Lupu, J. W. Rabalais, *Appl. Phys. Lett.*, **81**, 5033 (2002).
[3] R. A. Weeks, J Gastineau, E. Sonder, *Phys. Status Solidi (a)* **61**, 265.
[4] T. E. Mølholt et al. (2010) this conference.
[5] M. J. L. Sangster, A. M. Stoneham, *J. Phys.*, *C*, **17**, 6093 (1984).

PS3-23-72

Lattice sites of Fe in Al_2O_3 following implantation of ^{57}Mn

H. P. Gunnlaugsson[1], R. Mantovan[2], T. E. Mølholt[3], D. Naidoo[4], K. Johnston[5], K. Bharuth-Ram[6], G. Langouche[7], S. Ólafsson[2], R. Sielemann[8], G. Weyer[1], and the ISOLDE collaboration[5]

[1] *Department of Physics and Astronomy, Aarhus University, DK-8000 Århus C, Denmark,*
e-mail: hpg@phys.au.dk.
[2] *Laboratorio MDM, IMM-CNR, Via Olivetti 2, 20041 Agrate Brianza (MB), Italy.*
[3] *Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavík, Iceland.*
[4] *School of Physics, University of the Witwatersrand, WITS 2050, South Africa.*
[5] *PH Dept, ISOLDE/CERN, 1211 Geneva 23, Switzerland.*
[6] *School of Physics, University of KwaZulu-Natal, Durban 4001, South Africa.*
[7] *Instituut voor Kern-en Stralings fysika, University of Leuven, B-3001 Leuven, Belgium.*
[8] *Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany.*

Radioactive ^{57}Mn ($T_{\frac{1}{2}}$ = 1.5 min) has been implanted into Al_2O_3 single crystals held at 110 – 666 K at the ISOLDE facility at CERN. Mössbauer emission spectra were measured on the 14.4 keV γ-rays of the daughter ^{57*}Fe nucleis. The analysis of the obtained Mössbauer spectra reveals four spectral components listed below (see Fig. 1) assigned as follows:

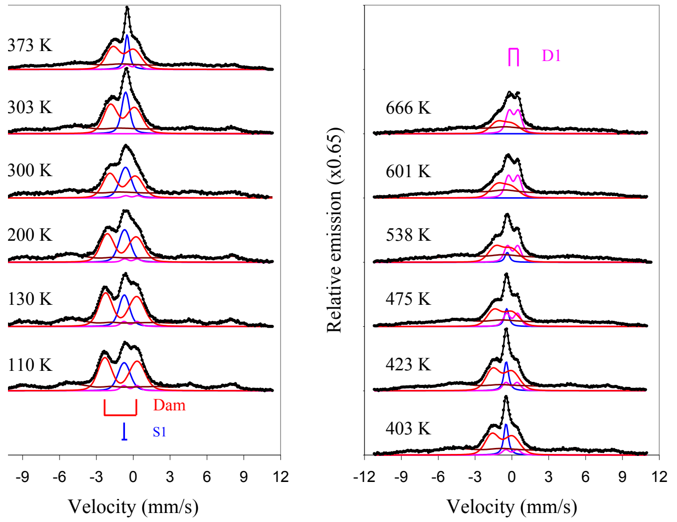


Fig. 1. ^{57}Fe Mössbauer spectra recorded after implantation of ^{57}Mn into Al_2O_3 single crystals held at the temperatures indicated.

Dam: A quadrupole-split component assigned to Fe^{2+} in heavily damaged, possibly amorphous local environment created in the implantation process. S1: A single line due to Fe in cubic environment. The properties of this line are inconsistent with interstitial Fe; it is suggested to originate from Fe in nano-precipitates of η-Al_2O_3. D1: A quadrupole-split component, which, on the basis of the hyperfine parameters and temperature dependence, is suggested to be due to Fe^{4+}. Sex: A Fe^{3+} magnetically-split sextet component showing slow paramagnetic relaxation. Analysis of the line broadening of this sextet component with the method described in [1] shows it to be compatible with (slow) spin-lattice relaxations. In-depth argumentation for the assignments of components will be presented and discussed together with comparison to supportive data obtained previously from stable ^{57}Fe [2] and radioactive ^{57}Co implantations [3].

References

[1] T. E. Mølholt *et al.*, (2010) this conference.
[2] C. J. McHargue *et al.*, *Nucl. Instr. Meth. B* **19/20** (1987) 813-821
[3] I. Dézsi *et al.*, *J. Phys.: Condens. Matter* **12** (2000) 2291–2296

PS3-24-96

Mössbauer study of ^{57}Fe in GaAs and GaP following ^{57}Mn^{+} implantation

H. Masenda[1], D. Naidoo[1], K. Bharuth-Ram[2,3], H. P. Gunnlaugsson[4], G. Weyer[4], W. B. Dlamini[2], R. Mantovan[5], R. Sielemann[6], M. Fanciulli[5,7], T. E. Mølholt[8], S. Ólafsson[8], G. Langouche[9], K. Johnston[10] and the ISOLDE Collaboration[10].

[1]School of Physics, University of the Witwatersrand, WITS 2050, South Africa, Email: hilary.masenda@physics.org, [2]School of Physics, University of KwaZulu-Natal, Durban 4001, South Africa, [3]iThemba LABS, P.O. Box 722, Somerset West 7129, South Africa, [4]Department of Physics and Astronomy, Aarhus University, Ny Munkegade 120, DK-8000 Århus C, Denmark, [5] Laboratorio MDM, IMM-CNR, Via Olivetti 2, 20041 Agrate Brianza (MB), Italy, [6]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany, [7]Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy, [8]Science Institute, University of Iceland, Dunhaga 3, 107 Reykjavik, Iceland, [9]Instituut voor Kern en Stralingsfysika, University of Leuven, 3001 Leuven, Belgium, [10]EP Division, CERN, CH-1211 Geneva 23, Switzerland.

Ion implantation provides a precise method of incorporating dopant atoms in semiconductors, provided lattice damage due to the implantation process can be annealed. We have undertaken ^{57}Fe Mössbauer spectroscopy measurements on GaAs and GaP single crystal samples implanted with radioactive ^{57}Mn^{+} ions ($T_{½}$ = 1.5 min) at the ISOLDE facility, CERN. The samples were held at temperatures between 77 – 700 K in an implantation chamber and implanted with fluences up to 10^{12} ion/cm^{2}. Mössbauer spectra were recorded with a resonance detector equipped with stainless steel electrodes enriched in ^{57}Fe and mounted on a conventional velocity drive system outside the chamber. The fitting of the measured Mössbauer spectra required four components (Fig. 1): (i) an asymmetric doublet (D1) attributed to Fe atoms in distorted environments due to implantation damage, two single lines: (ii) S1 assigned to Fe on substitutional Ga sites, (iii) the other (S2) to Fe in interstitial sites, and (iv) a low intensity symmetric doublet (D2) assigned to impurity-vacancy complexes.

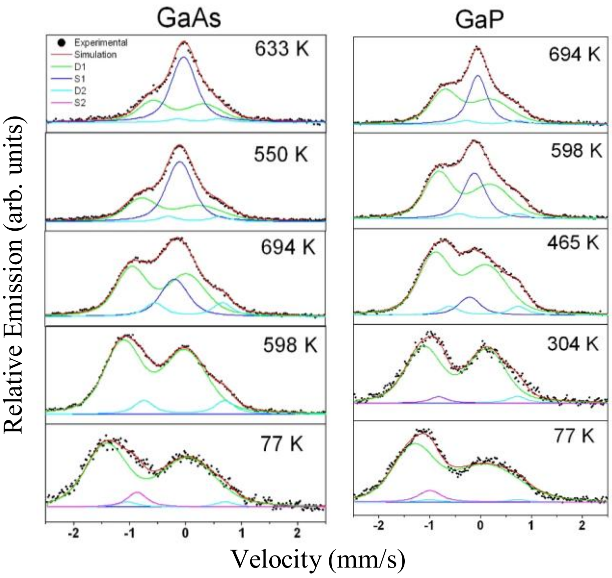


Fig. 1. Mössbauer spectra obtained after implantation of ^{57}Mn* in GaAs and GaP, at temperatures indicated. The solid lines show the different fitting components and their sum.

At temperatures above 400 K, the extracted hyperfine parameters of the damage site for both materials show pronounced variation, evidencing changes in the immediate environment of the Mössbauer probe nucleus and also possibly to the Fe-defect bonding mechanism. Fig. 2 shows the variation in site fractions with temperature. The annealing of the radiation damage is more pronounced in GaAs as compared to GaP and more will be discussed in detail during the presentation.

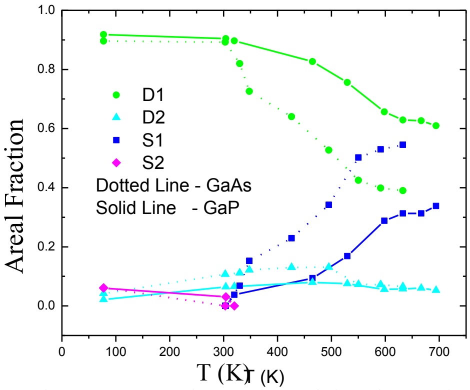


Fig. 2. Comparison of areal fractions of the different spectral components as a function of temperature in GaP and GaAs.

PS3-25-22

Study of Nanosized Magnetic Materials by SEDM Technique

V.G.Semenov,[1] **V.V.Panchuk**[1], **S.M.Irkaev**[2]

[1] *Dept. Chemistry, St.Petersburg State University Universitetskii pr.26, 198504 St.Petersburg, Russia Presenting author: val_sem@mail.ru*
[2] *Institute for Analytical Instrumentation RAS, Rishgski pr.26 190103 St.Petersburg, Russia, e-mail:sobir_irkaev@mail.ru*

Magnetic properties of nanostructure materials show the high variety and considerably differ from a massive one [1]. Before 40 years ago the main techniques for studying dynamics processes involved in interaction of nucleus with electron shell have been nuclear magnetic (NMR) and electron spin resonance (ESR). The Mössbauer spectroscopy technique, owing to its high sensitivity to hyperfine interaction between the nucleus and its environment, has greatly extended the range of substances that can be investigated, and in certain cases has become a unique method for studying these phenomena. Most of experiments that used Mössbauer spectroscopy to study various dynamic processes (e.g., diffusion, paramagnetic, spin-spin, spin-lattice relaxation, etc.) were done in the conventional transmission geometry. This technique is simple enough, but, in some applications it leads to difficulties in resolving the contributions from dynamic processes to the total spectrum. For example, in the case of slow relaxation the transmission spectrum is characterized by line broadening only. However, the broadening may be caused also by multiphase effects, unresolved hyperfine electric and magnetic interactions that lead to an ambiguity in spectrum interpretation. These problems may be solved through application of selective excitation double Mössbauer effect (SEDM) technique [2]. The Mössbauer spectrum measured in this case bears information on solid-state processes that occur during the nucleus lifetime: if within this time the nucleus manages to exchange energy with its environment, the energy of the re-emitted gamma-quantum will differ from that of the gamma-quantum exciting the nucleus. The SEDM technique, by its potential possibilities, can be powerful method of investigation of relaxation processes in solids. The method gives the unique possibility to obtain direct evidence for occurrence of relaxation and also to determine qualitative and quantitative characteristics of the processes even in situation where Mössbauer spectra are essentially broadened by other physical reasons.

Capabilities of SEDM technique in the investigation of magnetic properties of small particles are illustrated by the analysis of magnetite nanoparticles (Fe_3O_4) and aluminosubstituted goethite system $Fe_{(1-x)}Al_xOOH$.

References

I.P.Suzdalev .Nanotehnologija: fiziko-chemistry nanoclusters, nanostructures and nanomaterials (In Russian). M: the Com.Book, 2006, 320.

V.G. Semenov, S.M.Irkaev, Yu.N. Malsev. Highly sensitive Mössbauer spectrometer for SEDM and RSMR investigations. NIM **B** 95, (1995) 253-259

PS3-26-37

Size effects on local magnetism of single Fe impurity in nano-crystalline noble metals: A TDPAD investigation.

S.N. Mishra, and P. Ayyub

Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai-400005, India, email: mishra@tifr.res.in

We have employed the in-beam time differential perturbed angular distribution (TDPAD) technique to study the effects of finite lattice size on local magnetism and Kondo interaction of single Fe impurity in metallic hosts. In this direction, we have measured local susceptibility and 3d spin relaxation rate of recoil implanted ^{54}Fe nuclei, produced by the fusion evaporation reaction ^{12}C(^{45}Sc,p2n)^{54}Fe, in bulk and nano-crystalline Cu and Ag hosts. The nanocrystalline were prepared by DC-magnetron sputtering technique [1] and were characterized by X-ray diffraction and electron microscopy measurements. The TDPAD measurements were carried out the 14-MV tandem accelerator at TIFR, Mumbai. The 10^+ isomeric state in ^{54}Fe with $T_{1/2}$=360 ns, g_N = 0.728 was used as nuclear probe for the detection of static and dynamic magnetic response of Fe in the hosts under investigation. Fig. 1 displays the local susceptibility of Fe defined as β-1 = ($\hbar\omega_L/g_N\mu_N B_{ext}$) -1 measured as a function temperature. Here, ω_L is the Larmor frequency and Bext is the external magnetic field applied. The measured β(T), in all the hosts studied; show Curie-Weiss temperature dependence from which the Fe magnetic moment and T_K could be extracted. A comparison of the β(T) results for the nanocrystalline hosts visa vie their bulk counterparts, clearly indicate a strong influence of lattice size on Fe magnetism, especially the Kondo temperature T_K. While, size reduction for Cu increases the Fe moment with a concomitant reduction of T_K, the effect is opposite in nanocrystalline Ag hosts.

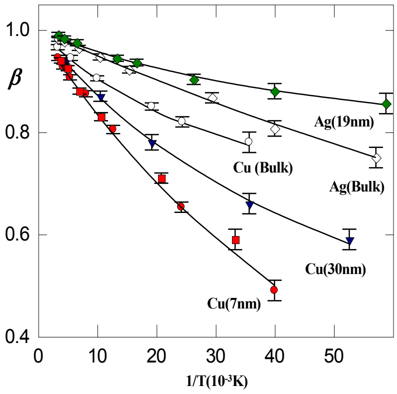


Fig 1: Local susceptibility of Fe in bulk and nanocrystalline Cu and Ag hosts.

References

[1] S.N. Mishra, S. Bose, P. Vasa and P. Ayyub, Phys. Rev. B 71, 094429 (2005)

PS3-27-38

Zr/Hf/Zr nanostructures studied by perturbed angular correlations

A.M.L. Lopes[1], M.R. Gomes[1], L.M. Redondo[1,2], M.R. Silva[1,2] and J.C. Soares[1]

[1] *Centro de Física Nuclear da Universidade de Lisboa, Av. Prof. Gama Pinto, 2, 1649-003, Lisboa, Portugal, e-mail:Armandina.lima.lopes@cern.ch* [2] *Instituto Superior de Engenharia de Lisboa, Rua Conselheiro Emídio Navarro, 1, 1959-007, Lisboa, Portugal*

The current technological necessities are compelling some fields of research to provide/study new nanostructure architectures that in the near future will fulfill the low cost, high performance and environmentally friendly paradigm. In fact, the research in metal-metal or metal-oxide nanostructures, in particular in Hf and Zr metals and their oxides, is being pushed by the prospect of application in several areas ranging from energy conversion and storage, catalysis to microelectronics [1-3]. One of the most prominent examples is observed in microelectronics where metal/HfO_2 structures are being studied as poly-Si/SiO_2 junction replacers in metal–oxide–semiconductor field-effect transistors [2]. Insight in metal/metal and metal/oxide interdiffusion/oxidation, upon annealing treatments, is of major importance for the mentioned technological applications [3]. Those insights can be obtained by local probe techniques such as perturbed angular correlations (PAC) that can provide detailed information at a nanoscopic level. In this work the PAC technique is used to locally monitor the oxidation or possible interdiffusion processes in a Zr/Hf/Zr nano-heterostructure. This trilayer was prepared by the electron gun thermal evaporation method on a SiO_2 substrate. In order to perform PAC measurements with the ^{181}Hf probe the system was neutron irradiated. The measurements were performed for different annealing times and temperatures, up to 780 K. The changes on the Hf local environment arising from the oxidation or interdiffusion processes were followed by the evolution of the EFG parameters of the Hf-metal, HfO_2 and oxygen deficient HfO_{2-x} regions (see fig 1). It was observed that the Hf layer is oxygen free for temperature below 619 K. The measurements also indicate that at 619 K first a thin layer of HfO_{2-x} emerges at the Hf surface and then a nanostructured HfO_2 layer continually grows at the expense of the Hf metal-component. Moreover up to 780 K no Hf (or Zr) interlayer diffusion was observed.

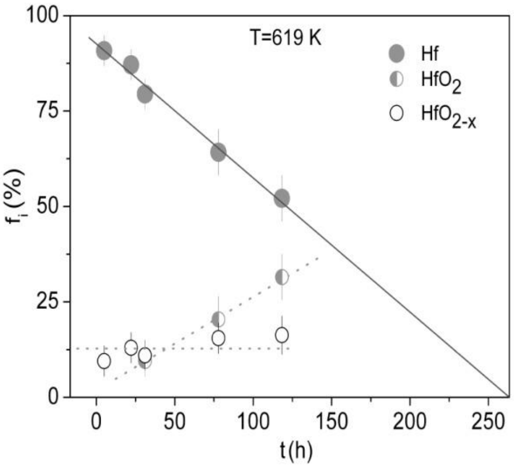


Figure 4 Time dependence of the fraction of the probes interacting with the different local environments at 619 K.

References

[1] J. Baxter, Z. Bian, et. al, Energy Environ. Sci., 2, 551 (2009)
[2] Robert F. Service, Science, **323**, 1000 (2009)
[3] R. Chau, B. Doyle, S. Datta, J. kavalieros and kevin Zhang, Nature materials **6**, 810 (2007)

PS3-28-39

Characterization of nanostructured HfO_2 films using Perturbed Angular Correlation (PAC) technique

Fabio Henrique de Moraes Cavalcante[1], Maria Ribeiro Gomes[1], Artur Wilson Carbonari[2], Luciano Fabrício Dias Pereira[2], Daniel de Abreu Rosseto[2], Luís Manuel Redondo[1], José Mestkik-Filho[2], Rajendra Narain Saxena[2], and José Carvalho Soares[1]

[1]Centro de Física Nuclear da Universidade de Lisboa (CFNUL), Lisboa, Portugal
fabiohmc@cii.fc.ul.pt
[2] Instituto de Pesquisas Energéticas e Nucleares (IPEN-CNEN/SP), São Paulo, Brasil

After three decades mainly SiO_2 was used as a gate dielectric in the silicon based CMOS (complementary-metalOxide-semiconductors) technology, and since integrated circuits are getting continuously smaller, the use of SiO_2 is facing its technological limits. High-k materials substituting the SiO_2 are currently under intense R&D to face the down-scaling process including the present CMOS technology. The basic idea is to find a material with a higher dielectric constant than that of SiO_2, which is compatible with the present Si technology. Hafnium dioxide (HfO_2) is an excellent candidate for gate dielectric in silicon transistors due to its high chemical stability, excellent dielectric properties ($k \approx 23$) and mechanical hardness. Even though significant efforts have been dedicated to the investigation of Hf based gate dielectric material systems, key issues like bulk and interface oxygen diffusion, charge trapping, still lack a complete understanding when the target is a long-term operation of HfO_2 based devices. Those studies are not focuses only in potential applications but are concerned also with fundamental physics problems. Crucial insight in the physics of these systems can be achieved only by atomic scale studies with direct measurements on the local structure and electronic environment. This work will report the investigation on HfO_2 nano-films using Perturbed Angular Correlation (PAC) technique, where the presence of hafnium in the film assures the possibility of using ^{181}Ta as probe. The HfO_2 nano-films with different thicknesses were deposited on Si substrates using an electron beam evaporation process. The results will be discussed in terms of the physics underlying the local environment on the scale of a few atomic lengths monitoring microscopic regions.

PS3-29-65

Temperature dependent studies of Zinc nanoferrite synthesized by spray pyrolysis

Jacob Mathew M ,[1] **Jess jacob**[1], **Vinod V**[2]

[1] *Dept. of Physics, S.B.College, Changanacherry, Kottayam-686103,India, e-mail: jacob.chrisdale@gmail.com*
[2] *S.B. College of Engineering, Pathanamthitta ,Kerala ,India, e-mail: vvinodteacher@yahoo.com2*

Spinel ferrites –both in bulk and nanoform-have wide applications in modern world. Wide range of methods has been used to synthesis nanostructure spinel ferrites. We herein report the synthesize and Mossbauer study of unagglomerated, nanosized zinc ferrite prepared at moderately low temperature using spray technique. The process involves preparation of polymer precursor by taking high purity zinc nitrate (Merck), ferric nitrate (Loba) and Polyvinayl Alcohol (PVA), all in aqueous form, as starting materials [1]. The Zn:Fe molar ratio was kept at 1:2. The resulting viscous mixture of PVA metal nitrates is spray dried around 130 ^{o}C to obtain a fluffy powder. The fluffy black powders were subsequently heat treated at temperatures 250^{o}C, 350^{o}C, 450^{o}C and 550^{o}C for 20 minutes. The as-synthesized nanoparticles of $ZnFe_2O_4$ were characterized by X-ray (λ =1.5406Å), Transmission electron microscope (TEM), EDAX, Vibrating Sample Magnetometer (VSM) and Mossbauer spectrometer. The grain size of the nanoferrite is determined using Scherrer's formula. To understand the effect of temperature on particle size , we have sintered samples at different temperatures. The particle sizes and Mossbauer parameters are shown in table. The average particle size varies from 13 to 35 nm as the sintering temperature increases from 250^{o}C to 550^{o}C.The lattice parameters are almost constant at a value of ~8.44nm.The Mossbauer spectra of all the sintered samples show a single doublet. The doublets are attributed to the presence of superparamagnetism in the sample.

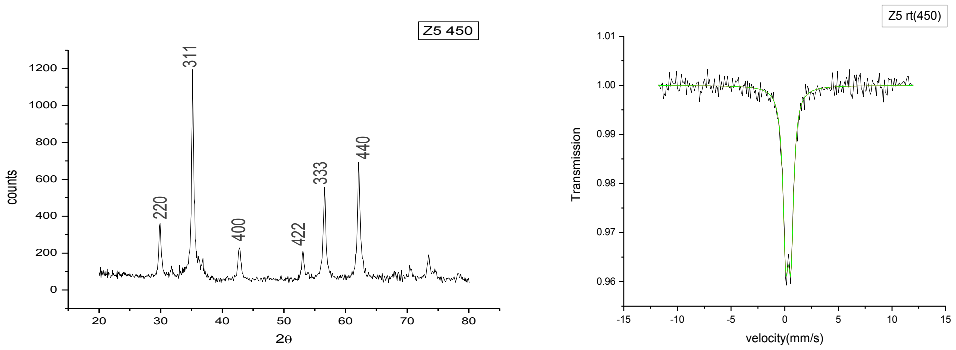


Fig.1 Representative XRD and Mossbauer patterns of the $ZnFe_2O_4$ samples

Samples at different temperature	IS(mm/s)	QS(mm/s)	Particle Size(nm)
Z5-250	0.3522	0.5706	13.1309
Z5-350	0.3454	0.5472	10.9908
Z5-450	0.3352	0.4864	20.7246
Z5-550	0.3555	0.4269	35.5877

[1] P Pramanik, Chemical synthesis of nanosized oxides. Bull. Mater. Sci.,**19**,957(1996).

PS3-30-75

Electric field gradients in nanoparticles of $HfAl_2$ and $HfAl_3$ intermetallic compounds

Agnieszka Kulińska, **Paweł Wodniecki**

Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, e mail: Agnieszka.Kulinska@ifj.edu.pl

Perturbed angular correlation (PAC) method was applied to study the electric field gradients in nanopowders of the $HfAl_2$, $HfAl_3$ and Hf_2Al_3 intermetallic compounds, obtained via mechanical alloying or after ball milling of the thermally alloyed compound. The influence of the ball milling procedure on the experimentally obtained hyperfine interaction parameters was determined. A strong dependence of the PAC pattern on the milling time was evidenced and attributed to the structural disorder. The thickness of the outer damaged part of the grains depends on the crystallographic structure of the milled material. In $HfAl_3$ sample, we observed the influence of the milling procedure on the phase transformation. The mechanical alloying process causes serious and stable damage in the powder particle of $HfAl_2$ sample, these defects cannot be removed by annealing up to 900°C. In the Hf_2Al_3 sample after 60 minutes of milling and subsequent annealing at 700°C, the decomposition of Hf_2Al_3 into two phases HfAl and $HfAl_2$ was observed. The quadrupole frequency distribution δ increased with decreasing grain size (see Fig. 1.).

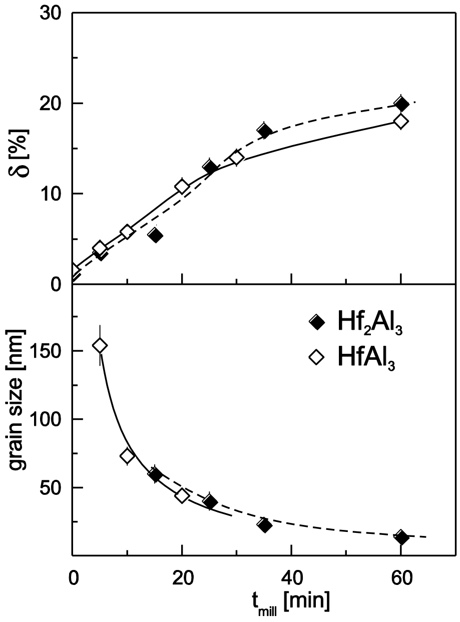


Fig. 1. The milling time dependence of the grain size and δ distribution for $HfAl_3$ and Hf_2Al_3 samples.

PS3-31-89

Laser Deposition of Iron on Graphite Substrates

Yasuhiro Yamada,[1] **Hiromi Yoshida**[1]**, Yoshio Kobayashi**[2]

[1] *Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan,*
e-mail: yyasu@rs.kagu.tus.ac.jp
[2] *RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

Laser deposition is a very useful technique to produce films, which is applied in many fields. We have previously reported the study on iron carbide films produced by laser deposition of iron in a C_2H_2 atmosphere. Iron carbide films with various Fe/C composition ratios were produced by varying the pressure of a C_2H_2 atmosphere and the substrate temperatures during deposition [1]. Here, we report the laser deposition of iron onto amorphous graphite substrates in order to produce Fe/C species with excess amount of C atoms. The Fe/C products were studied using Mössbauer spectroscopy, X-ray diffraction (XRD), and scanning electron micro spectroscopy SEM.

Laser light from a YAG laser (532 nm) was focused by a convex lens onto the target ^{57}Fe metal block. Laser-evaporated Fe atoms were deposited on a graphite substrate. The temperature of the substrate was maintained at the desired temperature (300–600 K range) using a resistive heater. One pulse of laser ablation produces 4 x 10^{-9} mol of Fe atoms, and the amount of the laser-deposited Fe was controlled by varying the number of laser pulses. Mössbauer spectra of the Fe/C on the graphite substrates were measured at room temperature in a transmission geometry using a ^{57}Co/Rh source.

Laser depositions of Fe were performed while the temperature of the graphite substrates was kept at 570 K, and their Mössbauer spectra are shown in Fig. 1. The amounts of Fe deposited on the graphite substrates are indicated as equivalent thickness of α-Fe. Laser evaporated Fe atoms have high translational energy (several hundreds eV) and reacts with graphite to form Fe/C compounds. The Mössbauer spectrum of the sample with a small amount of Fe (10 nm) was fitted into a combination of two sets of sextets and a doublet. The sextets were assigned to cementite Fe_3C and α-Fe, and the doublet (δ = 0.3 mm/s, ΔE_Q = 1.1 mm/s) was assigned to amorphous iron carbide. The intensity ratio of the sextet absorption of Fe_3C was approximately 3:4:1:1:4:3, which indicates that the nuclear spin orientation of Fe_3C is parallel to the substrate surface. Increasing the amount of Fe (25 nm), the yields of α-Fe increased as it may produced on the top of Fe/C surface. Similar experiments were performed at lower temperature at 300 K, and the yield of amorphous Fe/C was enhanced, while Fe_3C decreased.

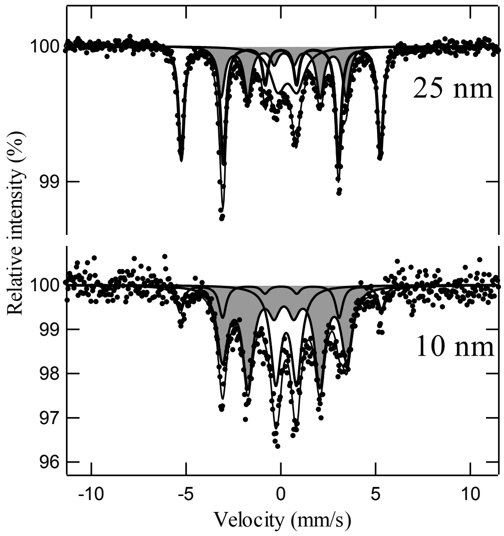


Fig. 1. Room-temperature Mössbauer spectra of the Fe/C produced by laser-deposition of Fe onto amorphous graphite substrates at 570 K. The amounts of Fe are indicated in the figure as equivalent thickness of α-Fe.

References

[1] Y. Yamada et al., *Abstract book and proceedings of ICAME2009* (2009).

PS3-32-134

Investigation of hyperfine interaction in the nanostructured HfO_2 by PAC spectroscopy

D. A. Rossetto[1], L. F. D. Pereira[1], F. H. M. Cavalcante[2], G. A. Cabrera-Pasca[1], J. Mestnik-Filho[1], A. W. Carbonari[1], R. N. Saxena[1].

[1] *Instituto de Pesquisas Energéticas e Nucleares IPEN-CNEN/SP, Av. Lineu Prestes 2242, São Paulo CEP:05508-000, Brazil, e-mail: danielross@usp.br*
[2] *Centro de Física Nuclear da Universidade de Lisboa (CFNUL), Av. Prof. Gama Pinto 2, 1649-003, Lisbon, Portugal*

Hafnium oxide is one of the new dielectric materials that is likely to replace silicon dioxide in semiconductor industry because of its excellent physical and chemical properties. Obtaining detailed information about this material, such as defects in the crystal lattice is quite important because they can alter its macroscopic characteristics thus changing it from a dielectric in to a semiconductor material with magnetic properties. In the present study we have used PAC technique to measure the hyperfine interactions in nanostructured samples of HfO_2 using ^{181}Hf-^{181}Ta nuclear probe. Samples of HfO_2 were prepared by the well known sol-gel method to obtain nanostructured material. After gel formation, samples were calcined at 320ºC in air. The samples were characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS), where the crystal structure, morphology and grain size were determined. The results showed a unique phase with monoclinic structure of HfO_2. The particle diameter was found to be in the range 30-40 nm. The samples were irradiated at the IEA-R1 reactor at IPEN with thermal neutron flux $\Phi = 5x10^{13}$ n.cm^{-2}.s^{-1} during 10 hours to produce ^{181}Hf through (n, γ) reaction on ^{180}Hf. After neutron irradiation the samples were annealed at temperatures which varied between 400°C and 900°C in vacuum, in air and in nitrogen atmosphere. PAC measurements were performed at room temperature after each annealing procedure. The results show the presence of two different electric quadrupole interactions. One of these interactions, with a well-defined frequency $\nu_q \sim 780$ MHz and $\eta \sim 0.4$ was assigned to the probe nuclei substituting regular Hf sites in the HfO_2 structure. The other interaction with highly distributed frequency $\nu_q \sim 1000$ MHz and a smaller fraction, which varied with the annealing temperature, was associated with the probe nuclei occupying sites with structural defects near the surface of the nanoparticles.

PS3-33-154

Study of nanoconfigurations in Zircon-Mullite composites using Perturbed Angular Correlations

Cecilia Y. Chain[1], **Alberto F. Pasquevich**[1], **Patricia C. Rivas**[2], **Jorge A. Martínez**[1], **María C. Caracoche**[1], **Nicolás M. Rendtorff**[3], **Maria S. Conconi**[3], **Esteban F. Aglietti**[3]

[1]*Departamento de Física, IFLP, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CICPBA, 1900 La Plata, Argentina, e-mail: yamil@fisica.unlp.edu.ar*
[2]*Facultad de Ciencias Agrarias y Forestales, Universidad Nacional de La Plata, IFLP,CONICET, 1900 La Plata, Argentina.*
[3]*Centro de Tecnología de Recursos Minerales y Cerámica, CONICET-CIC, 1897 M. B. Gonnet, Argentina*

It has been recently published [1] that some commercial zircons exhibit, at nanoscopic scale, hyperfine interactions without associated x-ray diffraction signals which have been assigned to aperiodic regions within the crystalline lattice.

It is known that zircon is a material often used in the ceramic industry due to its good refractory properties. Within this research field, zircon-mullite $ZrSiO_4$-($3Al_2O_3.2SiO_2$) composites of different compositions have been studied from the mechanical point of view [2].

In this work the Perturbed Angular Correlations technique has been applied to investigate the nanoconfigurations content in $(ZrSiO_4)_{(1-x)}$-$(3Al_2O_3.2SiO_2)_x$ composites being x=15, 25, 35 and 45% wt. Preliminary results indicate an important discrepancy between Rietveld analyses and PAC relative fractions determined in the studied composites (see figure 1).

The aim is to enlighten ceramic designers about the existence of nondiffractant portions in the material that could play some relevant role in the refractory performance.

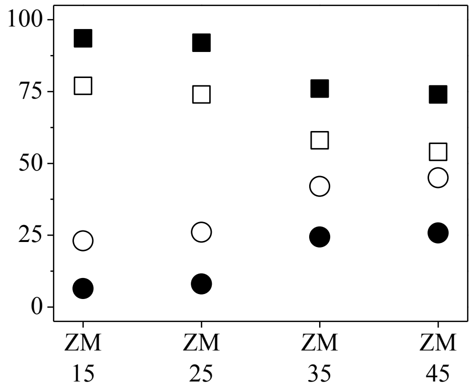


Figure 1: Relative fractions determined by XRD (full symbols) and PAC (open symbols) for the different composites. Squares represent Zircon and circles stand for ZrO_2.

References

[1] Rendtorff, N. M., Conconi, M. S., Aglietti, E. F., Chain, C. Y., Pasquevich, A. F., Rivas, P. C., Martínez, J. A., Caracoche, M. C.: Phase quantification of mullite-zirconia and zircon commercial powders using PAC and XRD techniques. To be published in Hyperfine Interactions, DOI: 10.1007/s10751-010-0177-4, (2010)

[2] Rendtorff, N. M., Conconi, M. S., Aglietti, E. F.: Mechanical and fracture properties of zircon–mullite composites obtained by direct sintering. Ceramics International 35, 2907–2913 (2009)

PS3-34-158

Synthesis and characterization of nanoparticles of cobalt and nickel ferrites dispersed in mesoporous silicon oxide

Tiago Braga,[1] B. M. C. Sales[1], A.N. Pinheiro[1], W. Herrera[1], I. Dinola[2], Y. Xing[2], E. Baggio-Saitovich[2], A. Valentini[1]

[1] *Universidade Federal do Ceará, Brazil, e-mail: icdinola@if.uff.br*
[2] *Centro Brasileiro de Pesquisas Físicas, Brazil*

Cobalt and nickel ferrites containing nanoparticles dispersed in silicon (Si) oxides were prepared via a polymeric precursor derived from the Pechini method [1]. The samples were characterized by X-ray diffraction (XDR), Mössbauer spectroscopy (MS), vibrating sample magnetometry (VSM) and N2 adsorption/desorption isotherms (BET). Therefore, investigations using XRD revealed that the spinel structure of $CoFe_2O_4$ (JCPDS 02-1045) and $NiFe_2O_4$ (JCPDS 44-1485) phases were formed and the crystallite sizes of the samples were calculated from the XRD patterns using the Debye–Scherrer formula and the calculated results indicate that the resultants are the nanometer-sized crystalline powders. Nevertheless, Mössbauer spectra revealed that the spinel structure of nickel and cobalt ferrite besides the presence of γ-Fe_2O_3. On other hand, Mossbauer spectroscopy measurements at 300 K show that nanoparticles are in the superparamagnetic regime being completely blocked at 4.2 K. The superparamagnetic relaxation due to maghemite and ferrites particles was also observed from magnetization measurement at 300 and 50 K.

Furthermore, Brunauer–Emmett–Teller analysis shows that the ferrites has a high surface area between 439 and 346 m^2g^{-1} and Barrett–Joyner–Halenda method exhibit a narrow pore size distribution, with the majority of the porous diameter located in the range of 16 to 238 Å characteristic of mesoporous materials.

References

[1] A. Valentini et al. Micropo. Mesopor. Mater. 68 (2004) 151.

PS3-35-163

Mössbauer Spectroscopy and neutron diffraction study of the mechanosynthesis of nanocrystalline $MgFe_2O_4$

V. Šepelák[1], I. Bergmann[2], A. Feldhoff[3], F. J. Litterst[4], K. D. Becker[5], J. M. Cadogan[6], M. Hofmann[7], M Hoelzel[7], J. L. Wang[8,9], M. Avdeev[9], S. J. Campbell[8]

[1] Institute of Nanotechnology, Karlsruhe Institute of Technology,
D-76344 Eggenstein-Leopoldshafen, Germany
[2] Volkswagen AG, D-38436 Wolfsburg, Germany
[3] Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover,
D-30167 Hannover, Germany
[4] Institute of Condensed Matter Physics, Braunschweig University of Technology,
D-38106 Braunschweig, Germany
[5] Institute of Physical and Theoretical Chemistry, Braunschweig University of Technology,
D-38106 Braunschweig, Germany
[6] Department of Physics and Astronomy, University of Manitoba, Winnipeg, MB, R3T 2N2, Canada, e-mail: cadogan@physics.umanitoba.ca
[7] Technische Universität München, ZWE, FRM-II, D-85747 Garching, Germany
[8] School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Australian Defence Force Academy, Canberra ACT 2600, Australia
[9] The Bragg Institute, ANSTO, Lucas Heights, NSW 2234 Australia

Nanosized spinel-type ferrites are key materials for advancements in electronics, magnetic storage and ferrofluid technologies as well as bio-inspired applications. Magnesium ferrite, $MgFe_2O_4$, is an important member of the spinel family: apart from its extensive magnetic and electronic applications, it is used in heterogeneous catalysis and adsorption, and sensor technology. Mechanosynthesis is a powerful method for the production of novel, high-performance, and low-cost nanomaterials [1].

The evolution of nanocrystalline $MgFe_2O_4$ by high-energy milling a mixture of MgO and α-Fe_2O_3 has been investigated by Mössbauer spectroscopy and X-ray powder diffraction [2]. High resolution TEM has confirmed the ordered nature of the inner core of nanoparticles surrounded by a disordered surface shell/interface region as concluded from analyses of zero and applied field spectra [2]. Neutron diffraction measurements have been carried out (SPODI, FRM-II) on a series of 7 samples of MgO and α-Fe_2O_3 milled for periods of 0.25 h to 12 h. This has enabled details of the transformation of the initial crystalline MgO and Fe_2O_3 phases via intermediate states to the final nanocrystalline mechanosynthesised $MgFe_2O_4$ product to be investigated. A comparison of the findings from the complementary Mössbauer effect and neutron diffraction studies will be presented.

References

[1] V. V. Boldyrev, *Russ. Chem. Rev.* **75,** 177 (2006).
[2] V. Šepelák, A. Feldhoff, P. Heitjans, F. Krumeich, D. Menzel, F. J. Litterst, I. Bergmann, K. D. Becker, *Chem. Mater.*, **18,** 3057 (2006)

PS3-36-110

Room temperature ferromagnetism in MWCNTs synthesized by chemical vapor deposition technique

S. Gautam[1,3], **K.H. Chae**[1], **J.H. Song**[1], **S. Augustine**[2], **J.K. Kang**[2] , **J.Y. Kim**[3], **and K. Asokan**[4]

[1]*Nano Analysis Center, Korea Institute of Science and Technology, Seoul 136-791, S. Korea, e-mail:sgautam71@kist.re.kr*
[2]*Material Science and Engineering, KAIST, Daejeon 305-701, S. Korea*
[3]*Pohang Accelerator Lab, Pohang University of Science and Technology, 791-784, S. Korea*
[4]*Inter-University Accelerator Center, New Delhi -India*

Carbon nanotubes (CNTs) possess unique mechanical and electronic properties suitable for fabricating the nano-scale building blocks of nanodevices. Such nanoscale magnetic materials may be used in spin-dependant electronic devices and magnetic data storage. Because small particles depend strongly on the size [1], the control of their size and shape is indispensable for advance applications. In this study, MWCNTs synthesized by chemical vapor deposition (CVD) technique are investigated with synchrotron radiations at Pohang Light Source (PLS), Korea. Near edge x-ray absorption spectroscopy (NEXAFS) measurement at C K, Co $L_{3,2}$ and Fe $L_{3,2}$–edges, and x-ray magnetic circular dichroism (XMCD) at Co and Fe L3,2 –edges have been carried at 7B1 XAS KIST and 2A MS beamline respectively to understand the electronic structure and responsible magnetic interactions at room temperature. X-ray absorption spectroscopy (XAS) at C K-edge shows significant p-bonding and Co and Fe L-edges proves the presence of Co^{2+} and Fe^{2+} in octahedral symmetry. Fe and Co doped MWCNTS shows good XMCD spectra at 300K. The effect on the magnetism is also studied through soft heavy ion (SHI) radiations and magnetism is found enhanced [Fig.1] and change in the electronic structure in Co-CNTs is investigated.

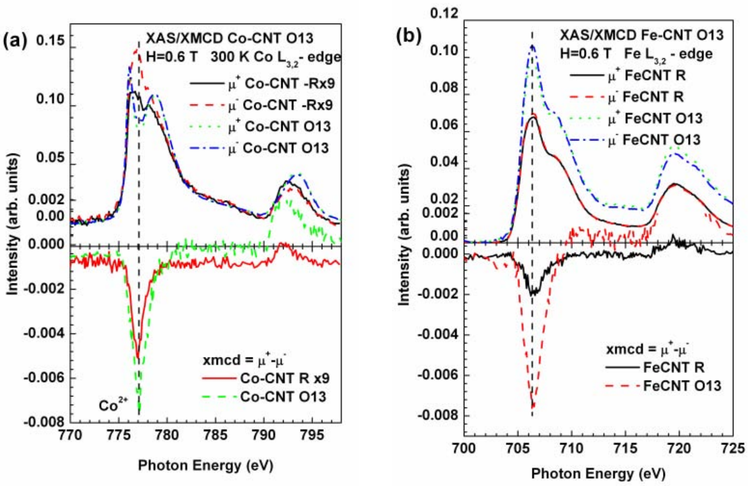


Fig. 1: Showing XMCD spectra for MWCNTs at room temperature. (a) Co $L_{3,2}$ -edge for un-SHI and SHI (O 1e13 ions/cms^2). SHI spectra intensity is multiplied 9 times for comparison. (b) Fe L3,2 –edge spectra for un-SHI and SHI (O 1e13 ions/cms^2).

References

[1] E. Wohlfarth, in: G. Rado, H. Suhl (Eds.), Magnetism, Vol. 3 (Academic Press, New York, 1963).

PS3-37-145

Test of Variational Methods for Studying Hyperfine Interactions of Molecular and Solid State Systems by Application to Atomic Systems

R.H. Pink[1], S.R. Badu[1], Archana Dubey[2], R.H. Scheicher[3], K. Raghunathan[4], L. Chow, and T.P. Das[1.2]

[1]Department of Physics, State University of New York at Albany, Albany, NY 12222, USA
tpd56@albany.edu, rpink77@gmail.com

[2]Departments of Physics, University of Central Florida, Orlando, Florida, USA

[3]Department of Physics, Condensed Matter Theory Group, Uppsala University, Uppsala, Sweden

[4]Theoretical Physics Department, University of Madras, Chennai, Tamilnadu , India.

The Many-Body Perturbation Theory (HFMBPT) procedure using Hartree-Fock Hamiltonian as zero order, and handling its difference from the actual Hamiltonian for atomic systems as a perturbation, has been extensively applied in the latter part of the last century to an extensive number of atoms, using non-relativistic theory for light atoms and fully relativistic Dirac theory for heavier atoms to study hyperfine interactions and a number of other properties with excellent agreement with experiment.

Unfortunately due to the multicenter nature of molecular and solid state systems, the wave-functions for the ground and excited states needed to carry out many-body perturbation theory investigations cannot be obtained by solving one dimensional radial equations in Hartree-Fock theory in atoms and so variational methods have to be adopted. We have tested two current methods, namely the variational Hartree-Fock many-body perturbation theory (VHFMBPT) method which is the logical successor to HFMBPT for atomic systems and the variational density functional theory (VDFT), which uses a chosen exchange-correlation interaction potential between the electrons in the Hamiltonian for the system.

We have, made applications of the VHFMBPT and VDFT methods to study the magnetic hyperfine constant A in the spin Hamiltonian A $\mathbf{I}\cdot\mathbf{S}$, where **I** and **S** are the nuclear and electronic spins in the atom, in phosphorous and lithium and made comparisons with experiment and the results from the accurate HFMBPT procedure. For phosphorous, the HFMBPT procedure leads to direct (D), exchange core polarization (ECP), and many body(MB) contributions to A of 0.0, -62.4 and 112.3 MHz, totaling 49.8 MHz as compared to 55.055 MHz from experiment, the difference having been ascribed to relativistic effects which are currently under investigation. The VHFMBPT results for (D+ECP) and MB are -37.4 and 72.6 MHz totaling 35.2 MHz, the trends among the various contributions being the same as in HFMBPT. For the VDFT approach using the (B3LYP) procedure, only the total value of A of -11.2 MHz is obtained from the currently available program, differing from experiment and the other two theoretical results in sign and with substantially lower magnitude. For lithium, the HFMBPT and VHFMBPT contributions have similar trends and the total agrees with experiment very well for HFMBPT and is somewhat smaller in size for VHFMBPT. For VDFT the total result is substantially larger than experiment. Suggestions will be made for improvements in the VHFMBPT and VDFT results.

References

[1] N.C. Dutta, et al. *Phys. Rev.* Lett. 21 1139 (1968) and references there in.
[2] E. S. Chang, et al. *Phys. Rev.* 174,1 (1968) and references there in..
[3] Alfred Owusu et al. Phys. Rev. A56, 305 (1997) and references there in.

PS3-38-5

Low Frequency Spin Echo in Multiple Pulse NQR Spin Locking

Gregory Kibrik,[1] **Gregory Furman**[2]

[1] *Perm State University, Russia*
e-mail: gkibrik@mail.ru
[2] Physics Department, Ben Gurion University, P.O.B. 653, Beer Sheva, 84105, *Israel*

Multiple-pulse method is one of the most effective and promising high-resolution nuclear quadrupole resonance (NQR) techniques for the study of solids. This method is very effective in the study of the spin lattice relaxation processes due to a slow atomic motion. Usually the theoretical description of multiple-pulse experiments both in NMR [1] and NQR [2] is based on the construction of the cyclicity effective time independent Hamiltonian by using the conditions for periodicity and cyclicity of the pulsed action. Then the dynamics of a spin system subjected by pulsed RF fields is presented in an equivalent form as the motion of nuclear spins in a constant effective field [3]. The magnitude and direction of this effective field are determined by parameters of the multiple-pulse sequence. An experimental measurement of the value of the effective field is important for the confirmation of this theoretical model. It is reasonable to suggest that an additional field with a low frequency close to resonance one in the effective field should cause resonance absorption of energy.

Indeed, we have observed multi-frequency resonances in polycrystalline $KClO_3$ irradiated simultaneously by a multiple-pulse radiofrequency sequence and a low frequency field swept in the range 0 - 80 kHz [4].

In the present paper we studied experimentally resonance transitions in the nuclear spin system of polycrystalline $KClO_3$ subjected by a simultaneous action of a multiple-pulse RF sequence and an additional pulse low frequency (LF) field. As result we observed the spin echo signal with unusual envelope shape.

References

[1] Ivanov Y. N., Provotorov B. N. and Fel'dman E. B., Pis'ma v Z. Eksp. Teor. Fiz. 27, 164 (1978) ; Sov. Phys. JETP 24, 135 (1978).
[2] Ainbinder N. E. and Furman G. B., Z. Eksp. Teor. Fiz. 85, 988 (1983); Sov. Phys. JETP 58, 575 (1983),
[3] Maricq M. M., Phys. Rev. Lett. 56, 1433 (1986).
[4] Furman G. B., Kibrik G.E., and A.Yu. Polyakov, Hyperfine Interactions 159,157 (2004).

PS3-39-6

Phase Transition and Proton Exchange in 1,3-Diazinium Hydrogen Chloranilate Monohydrate

T. Asaji[1], **M. Hoshino**[1], **H. Ishida**[2], **A. Konnai**[3], **Y. Shinoda**[4], **J. Seliger**[5,6], **and V. Ţagar**[6]

[1] *Department of Chemistry, College of Humanities and Sciences, Nihon University, Tokyo 156-8550, Japan, e-mail: asaji@chs.nihon-u.ac.jp;* [2] *Okayama University, Japan;*
[3] *National Maritime Research Institute, Japan;* [4] *Bruker AXS K. K., Japan;*
[5] *University of Ljubljana, Slovenia;* [6] *»Jozef Stefan« Institute, Slovenia*

In the hydrate crystal of 1:1 salt with 1,3-diazine and chloranilic acid (H_2ca), (1,3-diazineH)·H_2O·Hca, an unique hydrogen-bonded molecular aggregate is formed. A single proton transfer from chloranilic acid to 1,3-diazine results in 1,3-diazinium cation, 1,3-diazineH^+, and hydrogen chloranilate anion, Hca^-, in the crystal. There exist hydrogen bonds between the 1,3-diazinium ion and the water (H_2O) of crystallization, and between the H_2O and the hydrogen chloranilate ion. X-ray crystal analysis [1] revealed proton disorder in the N-H…O hydrogen bond at 225 K (Fig. 1). In order to reveal dynamic aspect of this disorder, ^{35}Cl NQR measurements were conducted. Fig. 2 shows temperature dependence of the NQR frequencies. Two resonance lines observed at 35.973 and 35.449 MHz at 321 K split into four lines below T_c = 198 K clearly showing occurrence of a solid-solid phase transition; 36.565, 36.357, 36.011, 35.974 MHz at 77 K. Temperature dependence of spin-lattice relaxation time T_1 in high-temperature phase was observed to obey an Arrhenius-type relation with the activation energy of 8.5 kJ mol^{-1}. This result leads to the conclusion that proton exchange in the N-H…O hydrogen bond takes place in the high-temperature phase. Below T_c the symmetry related N-H…O hydrogen bonds shown in Fig. 1 become non-equivalent and one of them falls in the ordered state [1]. Specific heat measurements by DSC resulted in the transition entropy ΔS = 1.3 J K^{-1} per 1 mole [(1,3-diazineH)·H_2O·Hca]$_2$ which is far less than $2R$ ln2 = 11.5 J K^{-1} mol^{-1}. It may be expected that proton ordering is not complete even in LTP and proton exchange in the two hydrogen bonds does not occur independently but concertedly in the high-temperature phase.

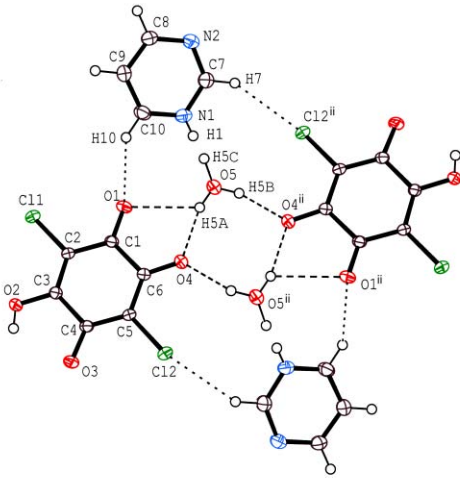


Fig. 1 Hydrogen-bonded

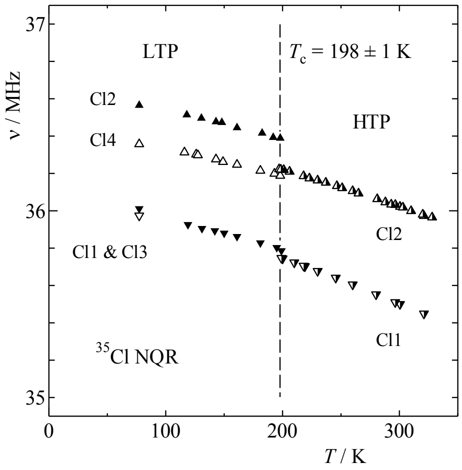


Fig. 2 Temperature dependence of

References

[1] K. Gotoh, T. Asaji, and H. Ishida, *Acta Cryst.* **C66** (2010) o114.

PS3-40-50

^{127}I NQR and ^{1}H NMR Studies of 4-Aminopyridinium Tetraiodoantimonate(III); Molecular Motion and Phase Transition

Hiromitsu Terao[1], **Yoshihiko Kai**[1], **Kazuyo Kita**[1], **Yoshihiro Furukawa**[2]

[1] *Faculty of Integrated Arts and Sciences, Tokushima University, Tokushima 770-8502, Japan,*
e-mail: htterao@yahoo.co.jp
[2] *Faculty of School Education, Hiroshima University, Higashi-Hiroshima 739-8524, Japan*

The DTA measurements of the title compound 4-$NH_2PyHSbI_4$ (Py = C_5H_4N) have revealed that the compound can exist in two modifications of β- and α-phases at room temperatures as shown in Fig. 1. The stable β-phase transformed to the meta-stable α-phase by heating above ca. 362 K and successive cooling. The α-phase further underwent a first-order phase transition of α(I)-phase ↔ α(II)-phase at ca. 272 K (on heating). Corresponding discontinuities were observed on the ^{1}H NMR T_1 curves at these temperatures.

Though the crystal structures have not yet been clarified for these phases, the observed resonance lines due to ^{127}I NQR ($m = \pm 1/2 \leftrightarrow \pm 3/2$) may be assigned to the terminal and the bridging I atoms by considering their frequencies, indicating an existence of one dimensional infinitive anion chain structures formed of SbI_6 octahedra. The β-phase was characterized by two higher-frequency lines of the terminal I atoms around ca. 136 MHz and two lower-frequency ones of the bridging I atoms around ca. 114 MHz throughout the measured temperatures (Fig. 2). Meanwhile no NQR signals were observed in the α(I)-phase, but two signals, assignable to the terminal and the bridging I atoms respectively, were observed in the α(II)-phase between 77 K and ca. 240 K, above which the disappearance of the signals occurred (Fig. 2).

The second moment M_2 values of ^{1}H NMR spectra at 290 K showed that the 4-NH_2PyH^+ cations resided in the rigid lattice with 8 G^2 in the β-phase but in the α(I)-phase the M_2 value largely reduced to 2 G^2, suggesting that the cations rotate about an axis more symmetric than pseudo 3-fold axis. On the other hand, the cations in the α(II)-phase may reside in the rigid lattice as judged from the T_2* values. The activation energy of 21 kJ mol^{-1} was estimated for the reorientational motion in the α(I)-phase from the ^{1}H NMR T_1 measurements (Fig. 3).

The results of ^{127}I NQR as well as of ^{1}H NMR indicate a similarity on the structures of the β-phase and the α(II)-phase to those of the low-temperature phase and the room temperature phase of 4-$NH_2PyHSbBr_4$ [1,2], respectively.

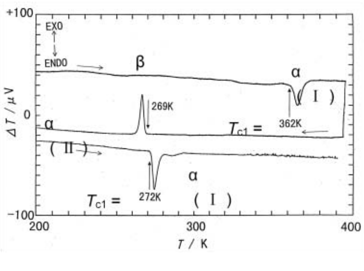
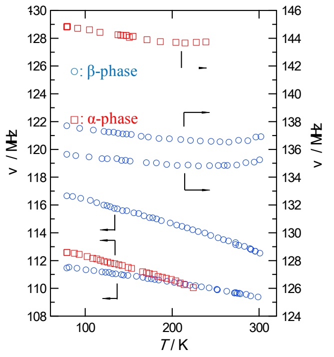


Fig. 1. DTA curves.



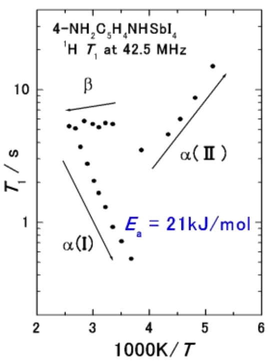


Fig. 3. ^{1}H NMR T_1.

References

[1] M. Hashimoto et al., *Z. Naturforsch.* A **55**, 167 (2000).
[2] M. Hashimoto et al., *Bull. Chem. Soc. Jpn.* **76**,749 (2003).

PS3-41-83

Two and three frequency multipulse sequence for NQR of N-14 nuclei.

G.V.Mozzhukhin[1], B.Z.Rameev[2,3], N.Dogan[3], R.Khusnutdinov[4]
[1] *Kazan State Power Engineering University, 420066 Kazan/Russian State university of Im.Kant, Kaliningrad, Russian Federation,*
e-mail:mgeorge@yandex.ru
[2] *Kazan Physical-Technical Institute, 420029 Kazan, Russian Federation,*
e-mail:rameev@superonline.com
[3] *Gebze Institute of Technology, 41400 Gebze-Kocaeli, Turkey*
[4] *Kazan State Power Engineering University, 420066 Kazan, Russian Federation*

Nuclear Quadrupole resonance has an application for the detection of the explosives and drugs in the passengers baggage in airports and landmine detection [5]. The NQR frequency range of the nitrogen compounds lays between 0.4 and 5.2 MHz. The requirements for detection of the explosives in passengers baggage include the detection of the small quantities of the explosives (15-20 grams) in big volume (near 160 litres[6]). Thus the problem of the sensitivity for NQR scanners is very actual. The decreasing of the threshold of low quantity of the samples inside the big volume is very important for security applications. The physical methods for the improvement of the sensitivity of the NQR of the N-14 nuclei are following: multipulse NQR methods[7] , double NMR-NQR[8], double cross-level method[9, 10, 11], multifrequency NQR[12, 13].

However the application of theses methods are depends on the parameters of the samples. For instance the application of cross-polarization methods produces the gain of the signal to noise ratio in the case of the direct bond between proton and nitrogen nuclei and suitable relaxation parameters. The double NQR-NMR and double cross-level methods were successfully investigated for trinitrotoluene $C_6H_2(NO_2)_3CH_3$ (TNT) and $C_5H_8N_4O_{12}$ (PETN)[4-7]. In other side HMX ($C_4H_8N_8O_8$) and RDX ($C_3H_6N_6O_6$) are not suitable for double NQR-NMR experiments. We propose the two and three frequency method in three levels energy NQR system for the increase of the signal to noise ratio for the explosives detection of the nitrogen compounds without H-N bond.

Our methods include following properties: i) the gain of the NQR signal in comparison of one frequency case up to 1.5 in two frequency excitation; ii)the absence of the problem of long transition process after power radiofrequency pulses in three frequency multipulse sequence; iii)the generation of two and three frequency multipulse sequences with quasistationery NQR states. The experiments were carried out on RDX at room temperature.

References

---

[5] J.B.Miller, G.A.Barrall. American scientist, Vol. 93 (1), 2005, 50-57.

[6] G.V.Mozzhukhin, S.V.Molchanov, G.S.Kupriyanova, A.V.Bodnya, V.V.Fedotov, Hao Guoxin, Jin Yanbo, Ren Tianliang, Zhang Guojin. In:Explosives Detection using Magnetic and Nuclear Resonance Techniques. Series: NATO Science for Peace and Security Series. Subseries: NATO Science for Peace and Security Series B: Physics and Biophysics. Fraissard, Jacques; Lapina, Olga (Eds.) Springer 2009, 295 p., 231-244.

[7] R.A. Marino, S.M. Klainer. J. Chem. Phys. 67, 3388-3389 (1977).

[8] R. Blinc, T. Apih, and J. Seliger, Appl. Magn. Reson. 25, 523-534 ,(2004)

[9] T.N. Rudakov, P.A. Hayes, Journal of Magnetic Resonance 183, 96–101(2006)

[10] Thurber, K.R., Sauer, K.L., Buess, M.L., Klug, C.A.,Miller, J.B. Journal of Magnetic Resonance, 177 (1), p.118-128, Nov 2005

[11] J.Luţnik, J.Pirnat, V.Jazbinšek, T.Apih, A.Gregorovič, R.Blinc, J.Seliger, Z.Trontelj. Applied Physics Letters, Sep 2006

[12] G.V. Mozzhukhin, B.Z. Rameev, N. Doğan, B. Aktaş. In: Explosives Detection using Magnetic and Nuclear Resonance Techniques. Series: NATO Science for Peace and Security Series. Subseries: NATO Science for Peace and Security Series B: Physics and Biophysics. Fraissard, Jacques; Lapina, Olga (Eds.) Springer, 2009, 205-230

[13] K.L.Sauer, B.H.Suits, A.N.Garroway, J.B.Miller.. J. Chem. Phys. 118, 5071-5081 (2003).

PS3-42-102

^{35}Cl NQR in glassy crystal, 2,5-dichlorothiophene

S. Minoshima, S. Hagiwara, H. Fujimori, and T. Asaji

Graduate School of Integrated Basic Sciences, Nihon University
Sakurajosui, Setagaya-ku, Tokyo 156-8550, Japan.
e-mail: fujimori@chs.nihon-u.ac.jp

A glass transition is a freezing phenomenon of a molecular configurational motion. It is observed not only in liquid state but also in crystalline state. In the previous case the whole positional and orientational disorders remain, but in the latter case the positions of the center of molecules are fixed and only the partial orientational disorder remains. The glass transitions in the stable crystalline states were found in thiophene [1], 2-chlorothiophene [2, 3], 3-chlorothiophene [4,5], 2,5-dichlorothiophene [6], and so on.

2,5-Dichlorothiophene, which has the melting point of 232.72 K, has three crystalline phases, the most stable one and the two meta-stable ones [6,7]. In the most stable crystalline phase a glass transition was observed at 138 K. The activation energy for the molecular reorientational motion, which freezes out at the glass transition temperature, can be estimated to be about 45 kJ mol^{-1} [6]. The NQR experiments for 2,5-dichlorothiophene were carried out in the three crystalline phases to get more detailed information about molecular motion related to the glass transition.

^{35}Cl NQR signals were observed by use of a spin-echo method. Broad NQR signals, which had the full width of about 80 kHz at half maximum, were observed in the most stable crystalline phase. The resonance frequency was 35.40 MHz and 34.90 MHz at 77 K and 209 K, respectively. There observed no anomaly at the glass transition point in the temperature dependence of the frequency. Sharp NQR signals, which had the full width of about 8 kHz at half maximum, were observed in the two meta-stable crystalline phases.

The temperature dependence of the spin-lattice relaxation times, T_1, in the most stable crystalline phase was interpreted by the contributions of the lattice vibrations and the molecular rotations. The activation energy of the molecular rotations was estimated to be about 40 kJ mol^{-1} by the least-squares fitting.

References

[1] P. Figuiere, H. Szwarc, M. Oguni, and H. Suga, *J. Chem. Thermodyn.* **17,** 949 (1985).
[2] H. Fujimori and M. Oguni, *J. Phys. Chem. Solids* **54,** 607 (1993).
[3] H. Fujimori and T. Asaji, *Z. Naturforsch* **55a**, 183 (2000).
[4] H. Fujimori, A. Todoroki, T. Asaji, and M. Oguni, *Slow Dynamics in Complex Systems* 685 (AIP, New York, 2004).
[5] H. Fujimori, T. Kaneko, T. Asaji, *Hyperfine Interact* **181**, 87 (2008).
[6] H. Fujimori, K. Matsuda, A. Todoroki, T. Asaji, and M. Oguni, *J. Non-Cryst. Solids* **352**, 4790 (2006).
[7] N. Tanimoto and H. Fujimori (unpublished).

PS3-43-111

^{7}Li Quadrupole-Perturbed NMR Observation of Biased Li-ion Ordering in the Paraelectric Phase of Weakly Substitutionally Disordered $K_{1-x}Li_xTaO_3$

Boštjan Zalar,[1] **Andrija Lebar,**[1] **David C. Ailion,**[2] **R. O. Kuzian,**[3]
I. V. Kondakova,[3] **and V. V. Laguta**[3,4]

[1] *J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia, e-mail: bostjan.zalar@ijs.si*
[2] *Department of Physics, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA*
[3] *Institute for Problems of Materials Sciences, Krzhizhanovskogo 3, 03180 Kiev, Ukraine*
[4] *Institute of Physics, AS CR, Cukrovarnicka 10, 16253 Prague, Czech Republic*

Substitution of K ions with Li ions in the $KTaO_3$ lattice is a textbook example of how to induce structural disorder, leading to a glass-like behavior [1]. Li impurities act like randomly interacting electric dipoles, with six discrete instantaneous orientations pointing along the cubic axes. For low Li concentrations x, dipolar glass state is established at low temperatures. At high temperatures, no behavior reminiscent of Li-Li pair interplay has been observed, apart from a two-timescale Li dynamics [2,3]. The absence of satellite transition features in the quadrupole-perturbed ^{7}Li ($I = 3/2$) NMR spectra [2,3] is somewhat surprising, since the statistical probability of Li-Li pairs is far from being negligible for Li-concentrations at which dipolar state is formed at low temperatures ($x \leq 0.04$).

We show that Li-pairs can indeed be detected via ^{7}Li quadrupole-perturbed NMR in the $K_{1-x}Li_xTaO_3$ single crystals with concentrations ranging from $x = 0.0035$ to $x = 0.12$, at temperatures far above the nominal glass transition temperature. The contributions from both isolated, cubic Li ions, and from Li-Li pairs, can clearly be resolved in the NMR spectrum. The “pairs” are detected as very low intensity, but well resolved, quadrupole satellites (Fig. 1). Their temperature-dependent splitting, equivalently the average quadrupole coupling constant, is indicative of energetic nonequivalence of various pair configurations. The dependence of integral intensities of the satellite lines on concentration x is in accordance with the above “pair” scenario. Our experimental observations are also supported by the results of local density approximation (LDA) calculations of electric field-gradient (EFG) tensor at the Li site.

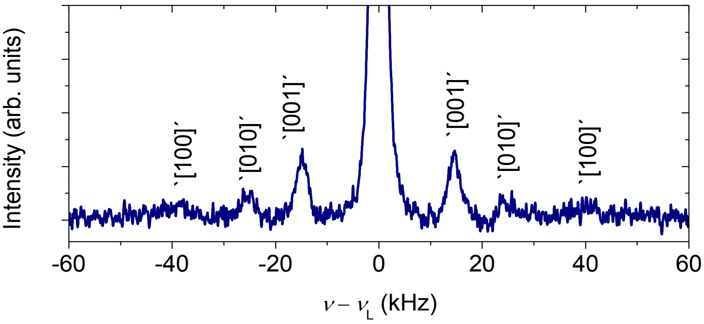


Fig. 1. Room temperature ^{7}Li quadrupole-perturbed NMR spectrum of $K_{0.88}Li_{0.12}TaO_3$ at a general orientation of the crystal with respect to the external magnetic field. Satellite transitions are marked according to the orientations of Li-Li pairs.

References

[1] U. T. Höchli et al., *Adv. Phys.* **51**, 589 (2002).
[2] J. J. van der Klink et al.,*Phys. Rev. B* **27**, 89 (1983).
[3] J. J. van der Klink et al., *Phys. Rev. B* **30**, 52 (1984).

PS3-44-149

The cross-correlation effects in relaxation of quadrupolar nuclei in the multipolar spin systems

Kupriyanova G.S.

Faculty of Physics, Immanuil Kant State University, ul.A.Nevskogo,14, 236041 Kaliningrad, Russia
e-mail: *galkupr@yandex.ru*

The relaxation theory of Bloch-Wangsness-Redfield [1] has been used widely for interpretation of the data in solid-state and high resolution NMR relaxation experiments. However, there are difficulties in extracting dynamic information on some systems in the presence of nuclear spins with I>1/2. These difficulties associated with tremendous calculator work for obtaining matrix representation of relaxation superoperator for multipolar spin systems and with the complexity of solving the relaxation equations for spin density matrix. The restriction of basis set for relaxation superoperator in mutlipolar spin system may lead to loss of the relevant physical observables induced by the relaxation . Such situation arises if the interference interactions give the contributions in the relaxation.

In the present paper a theoretical treatment of the longitudinal and transverse nuclear magnetic relaxation of quadrupolar nuclear of any spin in multipolar spin systems is proposed in the operator representation without preliminary selection of basis set in the presence of quadrupolar-chemical shift anisotropy interference, based on the second order time dependent perturbation theory [2]. The operator representations are particularly attractive since they permit us to avoid dealing with individual matrix elements.

The main equations for longitudinal and transverse relaxation of quadrupolar nuclear in multipolar spin system were derived if the relaxation is defined by chemical shift anisotropy, quadrupolar interactions and mixed fluctuations. The theory was applied to study of a relaxation and a line shape of quadrupolar nucler of spin S=1, 3/2, 3 in anisotropic molecular system in the presence of Q-CSA cross-correlation and in dipolar coupled spin system IS (I=1/2, 1). . The effects of high rank multipoles on lineshape and longitudinal relaxation of S=3 spin system were studied in the presence of Q-CSA cross-correlation. It was found that quadrupolar interaction induced magnetic multipolar the same evenness but Q-CSA inteference interaction course multipolar rank higher on one. The necessity of quantitative estimates of the values of Q-CSA cross-correlation contributions requires working out of new methods of exciting of particular types of coherence, and the methods for their registration. We also discuss the possibility of the application of traditional schemes for the excitation of multiquantum coherence for spin systems with quadrupolar nuclei.

References

[1] R.R. Ernst, G.Bodenhausen, A.Wokaun, Principles of Nuclear Magnetic Resonance in One and Two Dimentions, Clarendon Press, Oxford. 1987

[2] Kupriyanova G. S. *Appl. Magn. V.26, 283 (* 2004).

PS3-45-105

Br NQR relaxation and successive phase transitions of $CH_3NH_3HgBr_3$

H. Niki[1], K. Higa[1], Y. Okada[1], M. Oshiro[1], M. Yogi[1], and H. Terao[2]

[1] *Department of Physics, Faculty of Science, University of the Ryukyus, Nishihara, Okinawa 903-0213, Japan; e-mail: niki@sci.u-ryukyu.ac.jp*

[2] *Department of Chemistry, Faculty of Integrated Arts and Sciences, Tokushima University, Minamijosanjima-cho, Tokushima 770-8502, Japan*

The temperature dependence measurements of ^{81}Br NQR frequencies in $CH_3NH_3HgBr_3$ by using a super-regenerative type spectrometer have revealed that it undergoes three characteristic successive phase transitions between 77 K to ca. 300 K [1]. Each phase transition seems to be closely related to the motions of methyl ammonium cation as a partial or whole. In this work a pulse NQR method was applied to the sample crystals to get more precise information about the nature of the phase transitions; the results of the ^{81}Br NQR relaxation measurements as well as the frequency reinvestigations are reported.

The first-order nature of the phase transitions of IV↔III at 127 K and of III↔II at 187 K were confirmed by the observations of the hysteresis on the NQR frequencies in the process of heating and cooling in addition to the observation of frequency jumps in the temperature dependence curves (the numbering of the phases is the reverse order as used in Ref. [1]). On the other hand, the second-order type phase transition temperature of II↔I was determined as 239 K.

The $1/T_1$ vs. T curves of the ν_2 resonance line (88 MHz) for ^{81}Br NQR shows a larger increase of $1/T_1$ with temperatures in the phase IV than the other phases and an enhancement of $1/T_1$ for the second-order II↔I phase transition at 239 K (Fig.2). The enhancement of $1/T_1$ indicates the onset of the molecular motion of the cation as a whole on the II→I phase transition (The local environment is shown in Fig. 3). Meanwhile the IV↔III and the III↔II phase transitions may be related to the rotational motions of CH_3 and NH_3 groups, respectively.

References

[1] H. Terao and T. Okuda, *Z. Naturforsch.* **45**, 343 (1990).

[2] M. Körfer, H. Fuess, J. W. Bats, and G. Klebe, *Z. Anorg. Allg. Chem.* **525**, 23 (1985).

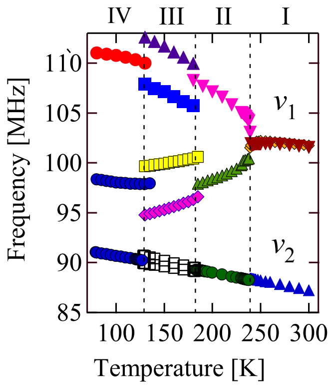


Fig. 1. Temperature dependence of ^{81}Br NQR frequency in $CH_3NH_3HgBr_3$.

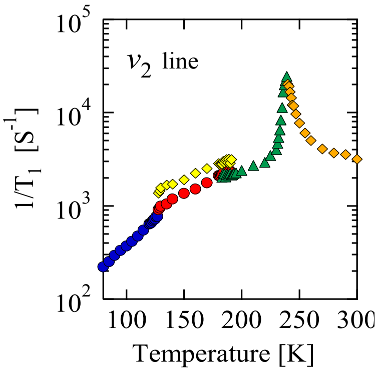


Fig. 2. Temperature dependence of $1/T_1$ for ν_2 line on ^{81}Br NQR in $CH_3NH_3HgBr_3$.

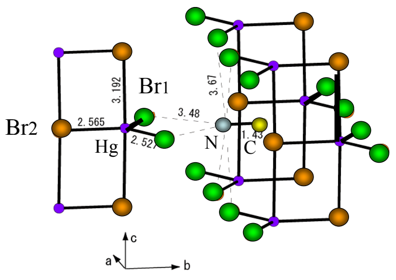


Fig. 3. The local environment of Br atoms in the phase I of $CH_3NH_3HgBr_3$ (from [2]).

PS3-46-103

Magnetic Moment of Isomeric States in ^{175}Ta

Vivek Kumar[1], P. Thakur[1], A.K. Bhati[1], R.P. Singh[2] and R.K. Bhowmik[2]

[1] *Department of Physics, Panjab University, Chandigarh-160014, India*
e-mail: v_chandel@hotmail.com
[2] *Inter University Accelerator Centre, New Delhi - 110 067, India*

The present measurements are the part of the systematic investigations of the static electromagnetic moments of $9^-/2$ and $21^-/2$ isomeric states in odd-A Ta nuclei. The lighter isotopes, ^{171}Ta and ^{173}Ta have been found to have decay properties different from those of heavier isotopes $^{175\text{-}181}$Ta, where the configuration assignments of the low-lying Nilsson proton intrinsic states have been firmly established. The $9^-/2$ (E=132 keV, $T_{1/2}$ = 222 ns) and $21^-/2$ (E=1565.9 keV, $T_{1/2}$=1950 ns) isomeric states are identified in ^{175}Ta [1] nucleus as single quasiproton and three quasiparticle states, respectively.

The isomeric states in ^{175}Ta have been populated through the nuclear reaction ^{160}Gd(^{19}F, 4nγ) ^{175}Ta using a 87 MeV pulsed ^{19}F beam with pulse width of 2 ns and repetition period of 1μs at 15 UD pelletron accelerator facility of Inter University Accelerator Centre, New Delhi. The target consisted of 632 μg/cm2 enriched ^{160}Gd evaporated on thick Ta backing (35 mg/cm2). The external magnetic field of 8.390(50) kG (measured by a Hall probe) perpendicular to the beam-detector plane was provided by a C-type electromagnet and calibrated with respect to the magnetic moment of the $5^+/2$ state (E=197 keV, $T_{1/2}$=89.3 ns) in ^{19}F nucleus [2]. From the analysis of the LSQ fitted values of the Larmor frequency $\omega_L = gH\mu_N/\hbar$ (H is the external applied magnetic field), we obtained g-factor for $9^-/2$ and $21^-/2$ as 0.631(9) & 0.542(21) respectively.

References

[1] F.G. Kondev et al., Nucl. Phys. A **601,** 195 (1996).
[2] R. Firestone, V. Shirley, C. Baglin, C. Franck, J. Ziplin: Table of isotope, Eighth edition, John Wiley and sons inc., New York.

PS3-47-106

The quadrupole moments of Zn and Cd isotopes – an update

H. Haas,[1] **J.G. Correia**[1]

[1] *Instituto Tecnológico e Nuclear, Estrada Nacional 10, P-2685 Sacavém, Portugal, and CERN/PH-IS, CH-1211 Geneve-23, Switzerland, e-mail: heinz.haas@cern.ch*

Precise nuclear quadrupole moments (Q) are a prerequisite for any quantitative analysis of measured quadrupole coupling constants. While historically good precision of calculated electric field gradient (EFG) values for normalization could only be achieved for atoms, the progress of calculations for molecules and solids in recent times has opened up a new possibility. Thus in many cases now values for Q have been obtained in this way [1].

Here we have used the full-potential linearized augmented plane waves (FLAPW) method to obtain updated values of Q for the Zn and Cd isotopes. The most reliable results come from the calculations in the hexagonal metals. Here accurate lattice constants at 4 K have been determined and precise values for the coupling constants are known. For error analysis numerous calculations were made using different density functionals and computational parameters. In particular a very dense mesh of k-points in the Brillouin zone was needed.

The final results (absolute values) are:

Q (^{67}Zn, g. st.) = 0.145 (3) b
Q (^{111*}Cd, 5/2+) = 0.764 (15) b

Calculations of the EFG in various other compounds, mostly halides, give results in agreements with these values, of less precision, however. To check the procedures employed the EFG in several simple gallium and indium halides was calculated. The resultant quadrupole moments agree within 1% with the precisely known values.

Using the experimentally determined ratios of Q, generally known with high accuracy, the moments of the other Zn and Cd isotopes can be obtained. In the case of Cd the trends of coupling constants from optical spectroscopy and perturbed angular distribution measurements must be considered for this purpose.

References

[1] P. Pyykkö, *Mol. Phys.* **106**, 1965 (2008) and references therein.

PS3-48-122

Magnetic Moment of the $3/2^+$ State in ^{165}Ho

M. Tanigaki,[1] **Y. Ohkubo**[1], **A. Taniguchi**[1], **S. Izumi**[2], **and T. Shinozuka**[3]

[1] *Research Reactor Institute, Kyoto University, Kumatori, Osaka 590-0494, Japan,*
e-mail: tanigaki@rri.kyoto-u.ac.jp
[2] *Graduate School of Science, Tohoku University, Aoba-ku, Sendai 980-8578, Japan*
[3] *Cyclotron and Radioisotope Center, Tohoku University, Aoba-ku, Sendai 980-8578, Japan*

Electromagnetic moments of nuclei are important physical quantities not only for nuclear structure studies, but also for investigation of the electromagnetic structures in materials. Reliable values of electromagnetic moments of radioactive nuclei are essential especially for probe nuclei of rare-earth elements in ferromagnetic materials through hyperfine interactions since it is difficult to apply the conventional NMR technique due to their very high resonance frequencies and shallow skin depths. One such example is Ho in Fe, which, as Torumba et al. have pointed out, is important for evaluating first principle calculations [1].

This time, we succeeded in observing the Larmor precession for the 362 keV state in ^{165}Ho($I^\pi = 3/2^+$, $T_{1/2} = 1.512$ μs) in Dy_2O_3 by use of the perturbed angular correlation technique, intending to determine the magnetic moment and apply it to the measurement of the hyperfine field at Ho in Fe.

The 362 keV state in ^{165}Ho was populated as a decay product of ^{165}Dy, which in turn was produced by the neutron activation of ^{164}Dy in natural Dy_2O_3 power. A static external magnetic field of 3 kG was applied to the sample at room temperature. The Larmor frequency for the 362 keV state in ^{165}Ho in Dy_2O_3 was determined to be –32.3 ± 0.6 MHz. The magnetic moment for this state was tentatively deduced to be +2~3 μ_N under the assumption that the paramagnetic correction factor for free Ho^{+3} ions [2] is applicable to the present case. Taking the uncertainty of the paramagnetic correction factor in Dy_2O_3 into account, the deduced magnetic moment would be consistent with a simple model calculation of the magnetic moment for rotational state nuclei. An accurate evaluation of the paramagnetic correction factor for Ho in Dy_2O_3 is now in progress to finalize the magnetic moment value.

References

[1] D. Torumba, V. Vanhoof, M. Rots, and S. Cottenier, Phys. Rev. B **74** (2006) 014409.

[2] C. Günther and I. Lindgren, in Perturbed Angular Correlations, eds. E. Karlsson, E. Matthias, and K. Siegbahn (North-Holland, Amsterdam, 1964) p. 355.

PS3-49-99

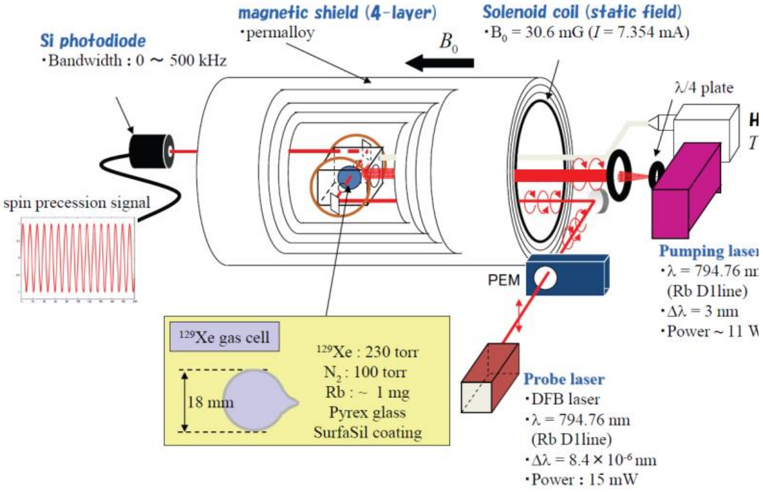
Electric dipole moment search in ^{129}Xe atom with an optical-coupling nuclear spin oscillator

__K. Asahi__,[1] T. Inoue,[1] A. Yoshimi,[2] T. Furukawa,[1] M. Tsuchiya,[1] H. Hayashi,[1]
T. Nanao,[1] K. Suzuki,[1] M. Uchida,[1] H. Ueno,[2] Y. Matsuo,[2] and T. Fukuyama[3]

[1] *Dept.Physics, Tokyo Inst. of Technology, 2-12-1 Oh-okayama, Meguro-ku, Tokyo 152-8551, Japan*
E-mail: asahi@phys.titech.ac.jp
[2] *Nishina Accelerator Research Center, RIKEN, 2-1 Horosawa, Wako-shi, Saitama 351-0198, Japan*
[3] *Global Innovation Research Organization, Ritsumeikan Univ., Kusatsu, Shiga 525-8577, Japan*

Nuclear spin in a diamagnetic atom, such as Xe, Hg, and Rn, constitutes an almost ideally isolated system that follows quantum mechanical laws. In fact the spin relaxation time for, *e.g.*, ^{129}Xe nucleus in an atom of Xe ranges upto several hundreds of seconds, and can serve as an exclusive testing ground for fundamental symmetries by means of intricate spin control.

We are developing a nuclear spin oscillator of a new type, which employs a feedback scheme based on an optical spin detection and succeeding spin control by a transverse field application [1,2]. This spin oscillator parallels the conventional spin maser in many points, but exhibits advantages and requirements that are different from those with the spin maser. By means of the optical-coupling nuclear spin oscillator, an experimental setup to search for an electric dipole moment (EDM) in a spin 1/2 diamagnetic atom ^{129}Xe is being developed. Until now, a frequency precision of 9 nHz has been attained which, with the application of an electric field of 10 kV/cm, would correspond to an EDM precision better than the current experimental limit of 4.0×10^{-27} e cm for ^{129}Xe atom [3] but still a step worse than that for ^{199}Hg [4].



References

[1] K. Asahi, M. Uchida, A. Yoshimi, T. Inoue and N. Hatakeyama, *AIP Conf. Proc.* **915**, 206 (2007).
[2] A. Yoshimi, K. Asahi, K. Sakai, M. Tsuda, K. Yogo, H. Ogawa, T. Suzuki, and M. Nagakura, *Phys. Lett.* A **304**, 13 (2002).
[3] M.A. Rosenberry and T.E. Chupp, *Phys. Rev. Lett.* **86**, 22 (2001).
[4] M. Romalis, W. C. Griffith, J. P. Jacobs and E. N. Fortson, *Phys. Rev. Lett.* **86**, 2505 (2001).

PS3-50-138

Polarization Creation in Proton-Rich ^{28}P via Charge Exchange Reactions and Measurement of Its Electric Quadrupole Moment

K. Matsuta,[1] M. Mihara[1], D.M. Zhou[2], Y.N. Zheng[2], D. Nishimura[1], T. Nagatomo[3],
D.Q. Yuan[2], S. Momota[4], T. Izumikawa[5], Y. Zuo[2], P. Fan[2], S.Y. Zhu[2], T. Ohtsubo[6],
M. Fukuda[1], Y. Namiki[6], M. Nagashima[6], T. Minamisono[7], D. Kameda[8],
T. Sumikama[9], A. Kitagawa[10], M. Kanazawa[10], M. Torikoshi[10], S. Sato[10],
R. Matsumiya[1], J. Komurasaki[1], D. Ishikawa[1], H. Hirano[6], S. Takahashi[6],
T. Kubo[6], R. Yamada[6], Y. Shimbara[6], Y. Nojiri[4], T. Suzuki[11],
X.Z. Zhang[2], J. R. Alonso[12], G.F. Krebs[12]and T.J.M. Symons[12]

[1] Dept. of Physics, Osaka Univ., Osaka 560-0043, Japan, matsuta@vg. phys.sci.osaka-u.ac.jp,
[2] CIAE, P.O. Box 275-50, Beijing 102413, P.R. China, [3]Int. Christian Univ., Tokyo 181-8585, Japan,
[4]Kochi Univ. of Tech., Kochi 782-8502, Japan, [5]RI Center, Niigata Univ., Niigata 951-8510, Japan,
[6]Niigata Univ., Niigata 951-2181, Japan, [7]Fukui Univ. of Thech., Fukui 910-8505, Japan,
[8]RIKEN, Saitama 351-0198, Japan, [9]Tokyo Univ. of Science, Chiba 278-0022, Japan,
[10]NIRS, Chiba 263-8555, Japan, [11]Nihon Univ., Tokyo 156-8550, Japan,
[12]Lawrence Berkeley Lab., CA 94720, USA

The degrees of polarization of proton rich nucleus ^{28}P produced in charge exchange reactions ^{28}Si + ^{9}Be -> ^{28}P + X, and ^{28}Si + ^{1}H -> ^{28}P + X have been observed at 100*A* MeV. Utilizing thus obtained polarized nuclei, β-nuclear quadrupole resonance (β-NQR) of ^{28}P implanted in Al_2O_3 have been observed for the first time. ^{28}P is of our present interest, since this nucleus may develop proton halo structure, which may be possible from the rather shallow proton separation energy of 2.065 MeV, and was suggested from the rather large reaction cross section compared with the neighboring nuclei [1]. In our previous study, the magnetic moment of ^{28}P was determined precisely [2], which showed at least the dominance of the configuration with the $s_{1/2}$ proton, which may develop proton halo. In the present work, we tried to measure the electric quadrupole moment of ^{28}P.

The experimental procedure is similar to the previous work [2], the proton-rich ^{28}P nuclei were produced and were polarized through charge exchange reactions ^{28}Si + ^{9}Be -> ^{28}P + X, and ^{28}Si + ^{1}H -> ^{28}P + X, at 100 *A* MeV, and were separated by a separator. They were then implanted in a Pt catcher cooled down to 15 K. The degree of polarization was measured by means of NMR utilizing β-ray asymmetric emission. Then the ^{28}P nuclei were implanted in a single crystal Al_2O_3 and the NQR were observed as shown in Fig. 1. The polarization mechanism in these reactions and the quadrupole moment of ^{28}P will be discussed at the meeting.

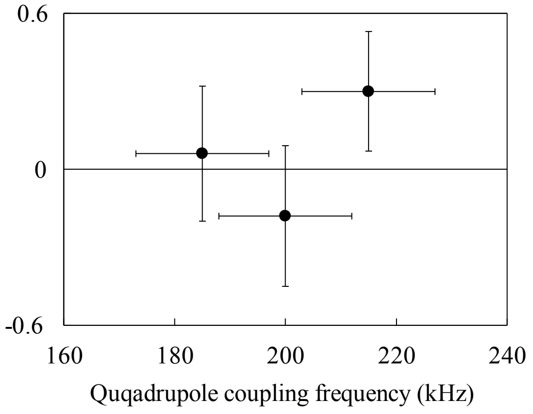


Fig. 1. Typical β-NQR spectrum of ^{28}P in Al_2O_3.

References

[1] Liu, Z.Z., Ruan, M., Zhao, Y.L., et al.: Phys. Rev., C 69, 034326 (2004).
[2] D.M. Zhou et al., Hyperfine Interact. 180, 37(2007); K. Matsuta et al., Nucl. Phys. A805, 359(2008).

PS3-51-88

Laser Deposition of Iron on Graphite Substrates

Yasuhiro Yamada,[1] **Hiromi Yoshida**[1]**, Yoshio Kobayashi**[2]

[1] *Tokyo University of Science, 1-3 Kagurazaka, Shinjuku, Tokyo 162-8601, Japan,*
e-mail: yyasu@rs.kagu.tus.ac.jp
[2] *RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

Laser deposition is a very useful technique to produce films, which is applied in many fields. We have previously reported the study on iron carbide films produced by laser deposition of iron in a C_2H_2 atmosphere. Iron carbide films with various Fe/C composition ratios were produced by varying the pressure of a C_2H_2 atmosphere and the substrate temperatures during deposition [1]. Here, we report the laser deposition of iron onto amorphous graphite substrates in order to produce Fe/C species with excess amount of C atoms. The Fe/C products were studied using Mössbauer spectroscopy, X-ray diffraction (XRD), and scanning electron micro spectroscopy SEM.

Laser light from a YAG laser (532 nm) was focused by a convex lens onto the target ^{57}Fe metal block. Laser-evaporated Fe atoms were deposited on a graphite substrate. The temperature of the substrate was maintained at the desired temperature (300–600 K range) using a resistive heater. One pulse of laser ablation produces 4×10^{-9} mol of Fe atoms, and the amount of the laser-deposited Fe was controlled by varying the number of laser pulses. Mössbauer spectra of the Fe/C on the graphite substrates were measured at room temperature in a transmission geometry using a ^{57}Co/Rh source.

Laser depositions of Fe were performed while the temperature of the graphite substrates was kept at 570 K, and their Mössbauer spectra are shown in Fig. 1. The amounts of Fe deposited on the graphite substrates are indicated as equivalent thickness of α-Fe. Laser evaporated Fe atoms have high translational energy (several hundreds eV) and reacts with graphite to form Fe/C compounds. The Mössbauer spectrum of the sample with a small amount of Fe (10 nm) was fitted into a combination of two sets of sextets and a doublet. The sextets were assigned to cementite Fe_3C and α-Fe, and the doublet (δ = 0.3 mm/s, ΔE_Q = 1.1 mm/s) was assigned to amorphous iron carbide. The intensity ratio of the sextet absorption of Fe_3C was approximately 3:4:1:1:4:3, which indicates that the nuclear spin orientation of Fe_3C is parallel to the substrate surface. Increasing the amount of Fe (25 nm), the yields of α-Fe increased as it may produced on the top of Fe/C surface. Similar experiments were performed at lower temperature at 300 K, and the yield of amorphous Fe/C was enhanced, while Fe_3C decreased.

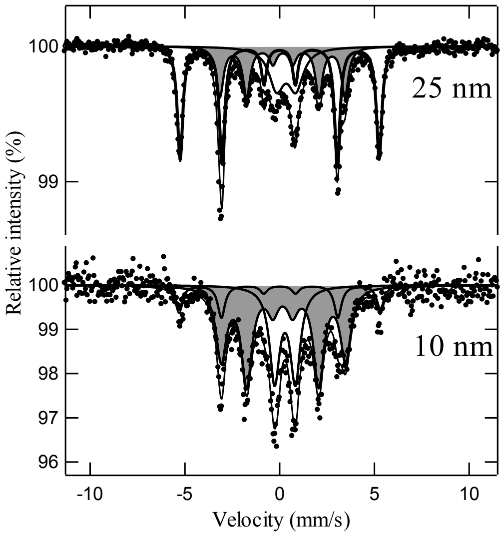


Fig. 1. Room-temperature Mössbauer spectra of the Fe/C produced by laser-deposition of Fe onto amorphous graphite substrates at 570 K. The amounts of Fe are indicated in the figure as equivalent thickness of α-Fe.

References

[1] Y. Yamada et al., *Abstract book and proceedings of ICAME2009* (2009).

PS3-52-177

^{7}Li Quadrupole-Perturbed NMR Observation of Biased Li-ion Ordering in the Paraelectric Phase of Weakly Substitutionally Disordered $K_{1-x}Li_xTaO_3$

Boštjan Zalar,[1] **Andrija Lebar,**[1] **David C. Ailion,**[2] **R. O. Kuzian,**[3]
I. V. Kondakova,[3] **and V. V. Laguta**[3,4]

[1] *J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia, e-mail: bostjan.zalar@ijs.si*
[2] *Department of Physics, University of Utah, 115 South 1400 East, Salt Lake City, Utah 84112, USA*
[3] *Institute for Problems of Materials Sciences, Krzhizhanovskogo 3, 03180 Kiev, Ukraine*
[4] *Institute of Physics, AS CR, Cukrovarnicka 10, 16253 Prague, Czech Republic*

Substitution of K ions with Li ions in the $KTaO_3$ lattice is a textbook example of how to induce structural disorder, leading to a glass-like behavior [1]. Li impurities act like randomly interacting electric dipoles, with six discrete instantaneous orientations pointing along the cubic axes. For low Li concentrations x, dipolar glass state is established at low temperatures. At high temperatures, no behavior reminiscent of Li-Li pair interplay has been observed, apart from a two-timescale Li dynamics [2,3]. The absence of satellite transition features in the quadrupole-perturbed ^{7}Li ($I = 3/2$) NMR spectra [2, 3] is somewhat surprising, since the statistical probability of Li-Li pairs is far from being negligible for Li-concentrations at which dipolar state is formed at low temperatures ($x \leq 0.04$).

We show that Li-pairs can indeed be detected via ^{7}Li quadrupole-perturbed NMR in the $K_{1-x}Li_xTaO_3$ single crystals with concentrations ranging from $x = 0.0035$ to $x = 0.12$, at temperatures far above the nominal glass transition temperature. The contributions from both isolated, cubic Li ions, and from Li-Li pairs, can clearly be resolved in the NMR spectrum. The "pairs" are detected as very low intensity, but well resolved, quadrupole satellites (Fig. 1). Their temperature-dependent splitting, equivalently the average quadrupole coupling constant, is indicative of energetic nonequivalence of various pair configurations. The dependence of integral intensities of the satellite lines on concentration x is in accordance with the above "pair" scenario. Our experimental observations are also supported by the results of local density approximation (LDA) calculations of electric field-gradient (EFG) tensor at the Li site.

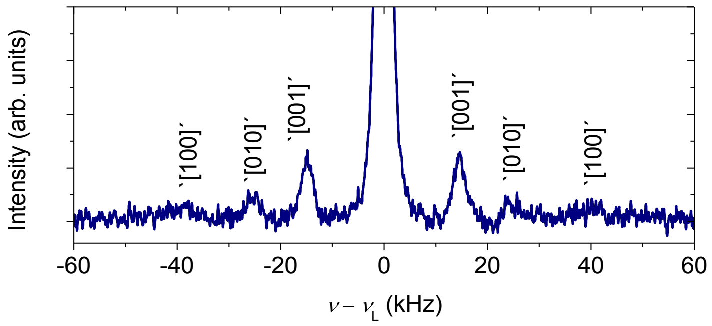


Fig. 1. Room temperature ^{7}Li quadrupole-perturbed NMR spectrum of $K_{0.88}Li_{0.12}TaO_3$ at a general orientation of the crystal with respect to the external magnetic field. Satellite transitions are marked according to the orientations of Li-Li pairs.

References

[1] U. T. Höchli et al., *Adv. Phys.* 51, 589 (2002).
[2] J. J. van der Klink et al.,*Phys. Rev. B* 27, 89 (1983).
[3] J. J. van der Klink et al., *Phys. Rev. B* 30, 52 (1984).

PS3-53-31

Electric-Field Gradient calculations with the full-potential code FPLO

Katrin Koch,[1] **Helge Rosner,**[1] **Klaus Koepernik**[2]

[1]MPI for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany,
e-mail: katrinkoch79@gmail.com, rosner@cpfs.mpg.de
[2] IFW Dresden, Institute for Solid State Research, P.O. Box 270116 01171 Dresden, Germany,
e-mail: k.koepernik@ifw-dresden.de

The ultimate goal of solid state physics is to explain the properties of solids, based on nothing more than the quantum interactions between their elementary building blocks: electrons and nuclei. The daily work of solid state experimentalists and theoreticians can be considered as making steps towards this goal. In this process, cross-links between theory and experiment are particularly useful. An example of a quantity that can both be calculated and measured with high accuracy, is the electric-field gradient (EFG). It contains valuable information about many aspects of solids, as for instance the electron density, the crystal structure, magnetism or chemical bonding.

An EFG module was recently implemented into the FPLO code [1]. The FPLO package (www.fplo.de) is a full-potential local-orbital minimum-basis code [2, 3] to solve the Kohn-Sham equations on a regular lattice using the local spin density approximation (LSDA). The situation of a chemically disordered structure is covered by a CPA solver [4], relativistic effects can be treated in a related 4-component code [5], and the LSDA+U formalism is implemented [6].

In this poster, we show several examples where the calculation and evaluation of the EFG helped to gain deeper insight into some fundamental properties of solids.

References

[1] K.Koch Koch *Dissertation TU Dresden* (2009).
[2] K. Koepernik and H. Eschrig, *Phys. Rev. B* **59**, 1743 (1999).
[3] I. Opahle, K. Koepernik, and H. Eschrig, *Phys. Rev. B* **60**, 14035 (1999).
[4] K. Koepernik, B. Velicky, R. Hayn, and H. Eschrig*, Phys. Rev. B* **55**, 5717 (1997).
[5] H. Eschrig, M. Richter, I. Opahle*, Relativistic Solid State Calculations, in: Relativistic Electronic Structure Theory,* Part 2. Applications Theoretical and Computational Chemistry, vol.13, pp.723 - 776, Elsevier, (2004)
[6] H. Eschrig, K. Koepernik, and I. Chaplygin*, J. Solid State Chemistry* 176, 482 (2003).

PS3-54-181

First Principles Cluster Study of Electronic Structures, Locations and Hyperfine Interactions of Isolated Atoms and Ions in Silicon

R.H. Pink,[1] S.R. Badu[1], R.H. Scheicher[2], L. Chow[3], M.B. Huang[4], T.P. Das[1,3]

[1] *Dept. of Physics, State University of New York at Albany, Albany, New York, 12222, USA,* tpd56@albany.edu
[2] *Dept. of Physics, Condensed Matter Theory, Uppsala University, Uppsala, Sweden.*
[3] *Dept. of Physics, University of Central Florida, Orlando, Florida, 32816, USA*
[4] *College of Nanoscale Science and Engineering, State University of New York at Albany, Albany, New York, 12222, USA*

The electronic structures of very dilute transition metal (TM) atom and ion (Mn^0, V^{2+}, Cr^+, and Mn^{2+}) complexes in silicon hosts have been studied using the Hartree-Fock procedure[1,2] combined with many-body perturbation theory with the aim to study the locations of TM atoms and ions and their hyperfine interactions. The clusters studied involved the TM atom and ions at the hexagonal interstitial (H_i), tetrahedral interstitial (T_i) and substitutional (S) locations, with the TM atoms and ions occupying a preexisting vacancy for the substitutional case. The nearest and next nearest neighbors of the TM atom and ions were included in the clusters for all of the sites studied. The energies of the centers were also studied for small variations in positions of the TM atom and ions along the <111> axis, and perpendicular to this direction. From the results of these studies, it is concluded that the binding energy and the total energy curves with respect to displacements of the TM systems around the H_i, T_i and S positions support the S and T_i sites as the possible binding sites for all the systems, the magnitudes of the binding energies favoring the S center. Channeling studies however suggest that both T_i and S sites are the likely locations of Mn TM systems. We have therefore investigated the hyperfine interaction constants (A) at both of these sites for Mn^0 and M^{2+} including many-body effects which are rather important because the unpaired electrons are in d-like orbitals and have no direct contributions. Our results for A for Mn^0 and Mn^{2+} when compared with experimental results[3] from Electron Paramagnetic Resonance (EPR) measurements show that the latter data can be explained with only the Mn^{2+} ion at the T_i sites, with the value for A from the Mn^0 results too small to explain the EPR results. This investigation illustrates the importance of the hyperfine interactions of the TM system, together with results from channeling measurements, in deciding on the charge states and locations of the TM systems in the silicon hosts, which in turn are important for a first-principles understanding of the ferromagnetic behavior of TM systems in Silicon.

References

[1] T.P. Das, Chapter 1 Pages 1-28 in T.A. Kaplan and S.D. Mahanti, *Electronic Properties of Solids Using Cluster Methods*, Chapter 1, Plenum Press, New York (1995).
[2] R.H. Pink, S.R. Badu, A. Dubey, R.H. Scheicher, J. Jeong, S.R. Byahut, L.Chow, M.B. Huang and T.P. Das *International Conference on Magnetic Materials (ICMM-2007) Proceedings*, pgs. 235-244, American Institute of Physics (2008).
[3] H.H. Woodbury and G.W. Ludwig, *Phys. Rev* **177**, 102 (1960).

PS3-55-180

First Principles Study of Nuclear Quadrupole Interactions in Single and Double Chain DNA and Solid Nucleobases

S.R. Badu[1], R.H. Pink[1], Archana Dubey[2], R.H. Scheicher[3], H.P. Saha[2], Lee Chow[2], M.B. Huang[1], N.Sahoo[4] and T.P. Das[1].

[1] *Department of Physics, State University of New York at Albany, Albany, NY 12222, USA.* tpd56@albany.edu, shyambadu@albany.edu [2] *Departments of Physics, University of Central Florida, Orlando, Florida, USA* [3] *Department of Physics, Condensed Matter Theory Group, Uppsala University, Uppsala, Sweden* [4] *Department of Radiation Physics, UT MD Anderson Cancer Center, Houston, TX 77030*

We have studied the Nuclear Quadrupole Interactions (NQI) of ^{17}O, ^{14}N and ^{2}H nuclei for free nucleobases and nucleobases in single strand (sDNA), double strand DNA (dsDNA) and in solid state. Our first principles investigation was carried out using the Gaussian 2009 set of programs to implement the Hartree-Fock procedure combined with many-body effects included using many-body perturbation theory. The positions of the atoms were taken from structural data for DNA systems [1], for solid nucleobases from x-ray data [2-5] and by geometry optimization based on the total energy for the free nucleobases. As expected for NQI in general, many-body effects are found to be small. Results will be presented for the nuclear quadrupole coupling constants (e^2qQ) and asymmetry parameters (η) for the nucleobases in the various systems, and trends in e^2qQ and η in the different systems will be discussed. Our results show that there are substantial changes in the NQI parameters e^2qQ and η, at the positions of the nuclei, on going from free nucleobases to the nucleobases attached to single strand DNA (sDNA), between the latter and the nucleobases in double strand DNA (dsDNA) and between free nucleobases and solid nucleobases. Our results for the ^{17}O NQI parameters in the solid nucleobases agree well with experimental results [6] obtained by the magic angle spinning nuclear magnetic resonance technique. Comparison with the results of an earlier theoretical investigation [6] on the solid nucleobases with our theoretical results will be presented and discussed.

It is hoped that the results of experimental measurements of NQI parameters for ^{17}O nuclei in these nucleobases for single strand and double strand DNA and for other nuclei (^{14}N and ^{2}H) will be available in the future to compare with our theoretical predictions.

References

[l] Tjandra N. et al, J. Am. Chem. Soc. 122, 6190 (2000).
[2] McClure R.J. et al, Acta Cryst. B29, 1234 (1973).
[3] Ozeki K. et al, Acta Cryst. B25,1038 (1969).
[4] Kistenmacher Thomas J. and Rossi Miriam, Acta Cryst. B33, 253 (1977).
[5] Thewalt Ulf et al, Acta Cryst. B27, 2358 (1971).
[6] Wu Gang et al, J. Am. Chem. Soc. 124, 1768 (2002).

PS3-56-182

First Principles Study of Muonium Trapping and Associated Magnetic Hyperfine Interactions in Nucleobases in Single and Double Chain DNA and Solid Nucleobases

S.R. Badu[1], R.H. Pink[1], Archana Dubey[2], R.H. Scheicher[3], Lee Chow[2], M.B. Huang[2] and T.P. Das[1].

[1]Department of Physics, State University of New York at Albany, Albany, NY 12222, USA. tpd56@albany.edu, *[2] Departments of Physics, University of Central Florida, Orlando, Florida, USA [3] Department of Physics, Condensed Matter Theory, Uppsala University, Uppsala, Sweden [4]College of Nanoscale Science and Engineering, State University of New York at Albany, Albany, New York, 12222, USA*

DNA is the most important molecule for biology in particular and for life in general. Owing to its great importance for life processes, any unchecked damage in DNA molecules can have dramatic consequences for the affected organism. For understanding the origin of the damage at an electronic level, it is important to have a detailed knowledge of the electronic structure of DNA and related systems

We have presented our systematic study of the Nuclear Quadrupole Interaction (NQI) in another Abstract at this conference. Here we present the results of our investigations on the trapping of muonium (Mu) in the free nucleobases, nucleobases in single and double chain DNA and in solid nucleobases. The study of Mu trapping and the associated muon hyperfine interaction complements the (NQI) study in the diamagnetic DNA systems by providing magnetic information dependent on the electronic structure of the systems associated with the unpaired spin electron provided by the trapped Mu. It also provides insights into the nature of the trapping process and associated hyperfine properties for impurities in general and the procedure for studying them.

For our investigation, we have used the first-principles procedure of Hartree-Fock theory combined with many-body perturbation theory (MBPT) to include many-body electron correlation effects. These latter effects are very important because they influence both the stabilities of the Mu trapping sites and the associated hyperfine interaction properties. It was also important to introduce relaxation effects in the positions of the nearest neighbors of the trapped Mu impurity. These effects were found to be sizable and influenced the strengths of the trapping of Mu at the sites found, however they are not sensitive to many-body correlation effects, an important result for the future in making careful trapping studies more practicable.

Results obtained for muonium hyperfine interaction at the trapped muonium sites will be presented. The main contributor to the hyperfine interaction properties is found to be the Fermi Contact isotropic term. However electron-nuclear dipole-dipole hyperfine interaction also makes significant contributions. The predicted hyperfine constants for the Muonium and the nearest neighbor nuclei are utilized to obtain theoretical values of the level crossing frequencies in the presence of applied magnetic fields and compared with available experimental data [2].

References

[1] R.H. Pink et al., Hyp. Int. **176**, 39(2007)
[2] Penny L Hubbard et al., J. Phys. Chem. A108, 9302 (2004).

HFI/NQI 2010

List of participants

Name	Email	Institution	Country
ALEKSEEV, Igor	iea-1960@yandex.ru	St. Petersburg State University	RUSSIA
ALEXANDER, Kamzin	kamzin@mail.ioffe.ru	Loffe Physical-Technical Institute	RUSSIA
ALEXANDROVNA, Polina	polina.agzamova@usu.ru	Ural State University	RUSSIA
ALP, Esen Ercan	alp@anl.gov	Argonne National Laboratory	UNITED STATES OF AMERICA
ASAJI, Tetsuo	asaji@chs.nihon-u.ac.jp	Nihon University	JAPAN
BAGGIO SAITOVITCH, Elisa	elisa@cbpf.br	Centro Brasileiro de Pesquisas Fisicas	BRAZIL
BANERJEE, Debashis	dbanerjee@vecc.gov.in	Bhabha Atomic Research Centre	INDIA
BARBOSA, Marcelo	marcelo.barbosa@cern.ch	Instituto Tecnológico e Nuclear	PORTUGAL
BHARUTH-RAM, Krish	kbr@tlabs.ac.za	University of KwaZulu-Natal	SOUTH AFRICA
BLAHA, Peter	pblaha@theochem.tuwien.ac.at	TU Vienna	AUSTRIA
BLUMENFELD, Yorick	yorick.blumenfeld@cern.ch	CERN	SWITZERLAND
BUTZ, Tilman	butz@physik.uni-leipzig.de	University of Leipzig	GERMANY
CADOGAN, Sean	cadogan@physics.umanitoba.ca	University of Manitoba	CANADA
CARBONARI, Artur	carbonar@ipen.br	IPEN-CNEN/SP	BRAZIL
CAVALCANTE, Fabio	fhmcavalcante@cii.fc.ul.pt	Universidade de Lisboa	PORTUGAL
CHAIN, Cecilia Y.	pasquevi@gmail.com	Instituto de Física La Plata (IFLP)	ARGENTINA
CHISTYAKOVA, Nataliya	nchistyakova@yandex.ru	M.V.Lomonosov Moscow State University	RUSSIA
CHOH, Sung-Ho	springchoh@hanmail.net	Korea University	REPUBLIC OF KOREA
CIESLAK, Jakub	cieslak@novell.ftj.agh.edu.pl	AGH The University	POLAND
CONNELL, Simon	Simon.connell@cern.ch	University of Johannesburg	SOUTH AFRICA
COSTA, Messias	messias@if.usp.br	IPEN	BRAZIL
COTTENIER, Stefaan	stefaan.cottenier@ugent.be	Universiteit Gent	BELGIUM
DALMAS DE REOTIER, Pierre	pierre.dalmas-de-reotier@cea.fr	CEA/INAC	FRANCE
DAMONTE, Laura C.	damonte@fisica.unlp.edu.ar	Instituto de Física La Plata (IFLP)	ARGENTINA
DARRIBA, Germán	darriba@fisica.unlp.edu.ar	Universidad Nacional de La Plata	ARGENTINA
DAS, Satyendra Kumar	satyen@vecc.gov.in	Bhabha Atomic Research Centre	INDIA
DAS, Tara Prasad	tarapdas@gmail.com	University at Albany	UNITED STATES OF AMERICA

DE PINHO OLIVEIRA, Goncalo	goncalo.nuno.de.pinho.oliveira@cern.ch	Universidade de Lisboa-CFNUL	PORTUGAL
DEICHER, Manfred	manfred.deicher@tech-phys.uni-sb.de	Universität des Saarlandes	GERMANY
DIAS PEREIRA, Luciano Fabrício	lpereira@ipen.br	Instituto de Pesquisas Energéticas e Nucleares - Universidade de São Paulo	BRAZIL
DINóLA, Isabel Cristina	icdinola@if.uff.br	Centro Brasileiro de Pesquisas Físicas	BRAZIL
DLAMINI, Wendy Bonakele	dlaminiw@ukzn.ac.za	University of KwaZulu-Natal	SOUTH AFRICA
DOGRA, Rakesh	drdogra@yahoo.com	Department of Applied Physics	INDIA
DOLO, Jappie Jafta	dolojj@qwa.ufs.ac.za	University of the Free State	SOUTH AFRICA
ERRICO, Leonardo	errico@fisica.unlp.edu.ar	UNLP	ARGENTINA
EVENSON, Bill	bill@evenson.ch	Utah Valley University / Brigham Young University	UNITED STATES OF AMERICA
FUJIMORI, Hiroki	fujimori@chs.nihon-u.ac.jp	Nihon University	JAPAN
FURMAN, Gregory	gregoryf@bgu.ac.il	Ben Gurion University in the Negev	ISRAEL
GONçALVES, João	joaonsg@ua.pt	Universidade de Aveiro	PORTUGAL
GUNNLAUGSSON, Haraldur	hpg@phys.au.dk	Aarhus University	DENMARK
HAGIWARA, Shoko	shagi@chs.nihon-u.ac.jp	Graduate school of Nihon University	JAPAN
HALEVY, Itzhak	halevyi@caltech.edu	NRCN	ISRAEL
HASS, Heinz	Heinz.haas@cern.ch	Inst. Tecno. E Nuclear - CERN/EP-SC	PORTUGAL SWITZERLAND
HEMMINGSEN, Lars	lhe@life.ku.dk	University of Copenhagen	DENMARK
HOFSäSS, Hans	hans.hofsaess@phys.uni-goettingen.de	II. Physikalisches Institut	GERMANY
HONDA, Hisashi	hhonda@yokohama-cua.c.jp	Yokohama City University	JAPAN
HORTA BELO, João	joao.horta.belo@gmail.com	IFIMUP - Science Faculty at Porto University	PORTUGAL
HUTCHISON , Wayne	w.hutchison@adfa.edu.au	The University of New South Wales	AUSTRALIA
IKEDA, Ryuichi	raikeda@w6.dion.ne.jp	University of Tsukuba	JAPAN
IRKAEV, Sobir	sobir.irkaev@gmail.com	Institute for Analytical Instrumentation of RAS	
JOHNSTON, Karl	karl.johnston@cern.ch	ISOLDE/CERN	SWITZERLAND
JUERGENS, Daniel	djuerge@gwdg.de	II. Physikalisches Institut	GERMANY
KELLO, Vladimir	kelloe@fns.uniba.sk	Comenius University	SLOVAKIA
KESSLER, Patrick	patrick.kessler@cern.ch	Helmholz-Inst. f. Strahl.- u. Kernp-Univ. Bonn	GERMANY
KESSLER, Patrick	kessler@jimcasy.de	HISKP	GERMANY
KHAN, Faiza Bibi	201295464@ukzn.ac.za	University of KwaZulu-Natal	SOUTH AFRICA

KIBRIK, Gregory	lkibrik@mail.ru	Perm State University	RUSSIA
KLAUSS, Hans-Henning	h.klauss@physik.tu-dresden.de	University of Technology Dresden	GERMANY
KOBAYASHI, Yoshio	kyoshio@riken.jp	RIKEN	JAPAN
KOCH, Katrin	katrinkoch79@gmail.com	Katholieke Universiteit Leuven	GERMANY
KUBO, Kenya	kkubo@icu.ac.jp	International Christian University	JAPAN
KULI?SKA, Agnieszka	Agnieszka.Kulinska@ifj.edu.pl	Institute of Nuclear Physics Polish Academy of Sciences	POLAND
KUMAGAI, Ken-ichi	thanks@spa.att.ne.jp	Hokkaido?University	JAPAN
LANGOUCHE, Guido	guido.langouche@kuleuven.be	University of Leuven	BELGIUM
LIN, Jun	jlin1978@gmail.com	Shanghai Institute of Applied Physics	CHINA
LITTERST, Jochen	j.litterst@tu-bs.de	TU Braunschweig	GERMANY
MACFARLANE, Andrew	wam@chem.ubc.ca	University of British Columbia	CANADA
MARTINS CORREIA, Joao Guilherme	guilherme.correia@cern.ch	ITN (Instituto Tecnologico e Nuclear)	PORTUGAL
MASENDA, Hilary	hilary.masenda@physics.org	University of Witwatersrand	SOUTH AFRICA
MASLENNIKOV, Dmitry	dm.masl@gmail.com	Radium Khlopin Institute	RUSSIA
MATSUTA, Kensaku	matsuta@vg.phys.sci.osaka-u.ac.jp	Dept. of Physics	JAPAN
MELO MENDONCA, Tania	taniamel@mail.cern.ch	IFIMUP and IN - Institute of Nanosciences and Nanotechnologies	PORTUGAL
MIBU, Ko	k_mibu@nitech.ac.jp	Nagoya Institute of Technology	JAPAN
MIHARA, Mototsugu	mihara@vg.phys.sci.osaka-u.ac.jp	Osaka University	JAPAN
MISHRA, S.N.	mishra@tifr.res.in	Tata Institute of Fundamental Research	INDIA
MORIKAWA, Shota	morin@kuchem.kyoto-u.ac.jp	Kyoto University	JAPAN
MUTO, Suguru	suguru.muto@kek.jp	KEK	JAPAN
MUñOZ, Emiliano Luis	munoz@fisica.unlp.edu.ar	Departamento de Física e Instituto de Física La Plata (IFLP	ARGENTINA
MöLHOLT, Torben Esmann	tem4@hi.is	Science Institute	ICELAND
NAGATOMO, Takashi	nagatomo@riken.jp	International Christian University	JAPAN
NAIDOO, Deena	deena.naidoo@wits.ac.za	University of the Witwatersrand	SOUTH AFRICA
NAKAMURA, Shin	shin@koala.mse.teikyo-u.ac.jp	Teikyo University	JAPAN
NIKI, Haruo	niki@sci.u-ryukyu.ac.jp	University of the Ryukyus	JAPAN
NOERTERSHAEUSER, Wilfried	w.noertershaeuser@uni-mainz.de	Johannes Gutenberg-Universitaet Mainz	GERMANY
NOWIK, Israel	nowik@vhuji.ac.il	Racah Institute of Physics	ISRAEL
OHTSUBO, Takashi	tohtsubo@np.gs.niigata-u.ac.jp	Niigata University	JAPAN
OLIVEIRA SILVA,	tito@ifsc.usp.br	University of Sao Paulo	BRAZIL

Rodrigo			
ORLOV, Valery	orlov@mbslab.kiae.ru	Russian Research Center "Kurchatov Institute"	RUSSIA
OSHTRAKH, Michael	oshtrakh@mail.utnet.ru	Ural State Technical University - UPI	RUSSIA
PANICH, Alexander	pan@bgu.ac.il	Physics Department	ISRAEL
PATRUSHEVA, Daria	patrushevadg@gmail.com	Ural State Technical University - UPI	RUSSIA
PETERSEN, Philippe	petersen@if.usp.br	University of São Paulo	BRAZIL
PETRILLI, Helena Maria	hmpetril@if.usp.br	Universidade de São Paulo- Instituto de Fisica	BRAZIL
POLESHCHUK, Oleg	poleshch@tspu.edu.ru	Tomsk State Pedagogical University	RUSSIA
RAMOS, Juliana	emrjmr@superig.com.br	IPEN USP	BRAZIL
REISSNER, Michael	reissner@ifp.tuwien.ac.at	Vienna University of Technology	AUSTRIA
RENTERíA, Mario	renteria@fisica.unlp.edu.ar	Universidad Nacional de La Plata - IFLP (CONICET)	ARGENTINA
RICHARD, Diego	richard@fisica.unlp.edu.ar	UNLP-CONICET	ARGENTINA
ROSSETTO, Daniel	danielross@usp.br	IPEN/CNEN	BRAZIL
SALMAN, Zaher	zaher.salman@psi.ch	Paul Scherrer Institut	SWITZERLAND
SANTOS, Brianna	briannabs@yahoo.com.br	IPEN/CNEN	BRAZIL
SAXENA, Rajendra	rnsaxena@ipen.br	IPEN-CNEN/SP	BRAZIL
SCHEICHER, Ralph	ralph.scheicher@fysik.uu.se	Uppsala University	SWEDEN
SEDYKH, Vera	suvorov@dio.ru; sedykh@issp.ac.ru	Institute of Solid State Physics	RUSSIA
SELIGER, Janez	janez.seliger@fmf.uni-lj.si	"Jozef Sefan" Institute	SLOVENIA
SEMENOV, Valentin	val_sem@mail.ru	Department of Chemistry of St.Petersburg State University	RUSSIA
SERGEEV, Ilya	sergueev@esrf.fr	ESRF	FRANCE
SEVERIJNS, Nathal	nathal.severijns@fys.kuleuven.be	Kath. Univ. Leuven	BELGIUM
SHARMA, Mahavir Prasad	mps.phy@gmail.com	Department of Phsyics	
SIBANDA, Wisdom Nkosilathi	wnsibanda@hotmail.com	University of the Witwatersrand	SOUTH AFRICA
SIELEMANN, Rainer	sielemann@helmholtz-berlin.de	Helmholtz-Zentrum Berlin für Materialien und Energie	GERMANY
SILVA, Andréia	asilva@usp.br	IPEN	BRAZIL
SILVA, Renilson Adriano	ras@usp.br	Instituto de Pesquisas Energéticas e Nucleares (IPEN)	BRAZIL
SINGH, Nadia	nadiabeepath@hotmail.com	The University of the West Indies	WEST INDIES
STACHURA, Monika	msta@life.ku.dk	University of Copenhagen	DENMARK
STEFFENS, Michael	steffens@hiskp.uni-bonn.de	Helmholtz-Institut für Strahlen- und Kernphysik der	GERMANY

		Universität Bonn	
STONE, Jirina	j.stone@physics.ox.ac.uk	Oxford Physics	UNITED KINGDOM
STONE, Nicholas	n.stone@physics.ox.ac.uk	Oxford University	UNITED KINGDOM
SUZUKI, Kunifumi	suzuki.k.bd@m.titech.ac.jp	Tokyo Institute of Technology	JAPAN
TANIGAKI, Minoru	tanigaki@rri.kyoto-u.ac.jp	Research Reactor Institute	JAPAN
TERAO, Hiromitsu	htterao@yahoo.co.jp	Tokushima University	JAPAN
THAKUR, Pardeep Kumar	thakur@esrf.fr	ESRF	FRANCE
TIMMERS, HEIKO	h.timmers@adfa.edu.au	UNSW@ADFA	AUSTRALIA
TRUJILLO HERRERA, Wiliam	william@cbpf.br	Brazilian Center for Research in Physics	BRAZIL
TüRKER, Muhammed	m.tuerker@tech-phys.uni-sb.de	Universität des Saarlandes	GERMANY
VALENTINI, Riccardo	riccardo.valentini@cern.ch	Helmholtz - Institut für Strahlen- und Kernphysik der Universität Bonn	GERMANY
VIANDEN, Reiner	vianden@hiskp.uni-bonn.de	HISKP	GERMANY
WORTMANN, Gerhard	wortmann@physik.upb.de	Physics Department, University of Paderborn	GERMANY
YAMADA, Yasuhiro	yyasu@rs.kagu.tus.ac.jp	Tokyo University of Science	JAPAN
YOSHIDA, Yutaka	yoshida@sist.ac.jp	Shizuoka Institute of Science and Technology	JAPAN
YUAN, Daqing	yuandaqing@gmail.com	CIAE	CHINA
ZACATE, Matthew	zacatem1@nku.edu	Northern Kentucky University	UNITED STATES OF AMERICA
ZHANG, Guilin	glzhang@sinap.ac.cn	Shanghai Institute of Applied Physics	CHINA
ZHENG, Yongnan	zhengyn@ciae.ac.cn	China Institute of Atomic Energy	CHINA
ZHU, Shengyun	zhusy@ciae.ac.cn	CIAE	CHINA