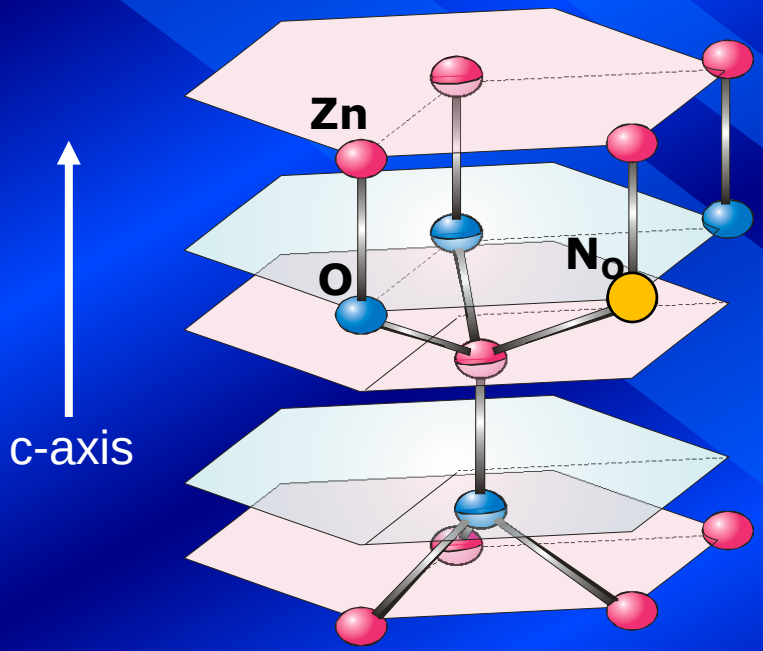
Donor-Acceptor Complexes in ZnO

M. Türker, M. Deicher, H. Wolf, and Th. Wichert

Universität des Saarlandes
Technische Physik, 66123 Saarbrücken

The ISOLDE Collaboration
CERN, Geneva, Switzerland

Zinc Oxide



E_G = 3.37 eV at RT

$E_{exciton\ binding}$ = 60 meV

Bulk crystal

Easy to dope n-type

Difficult to dope p-type

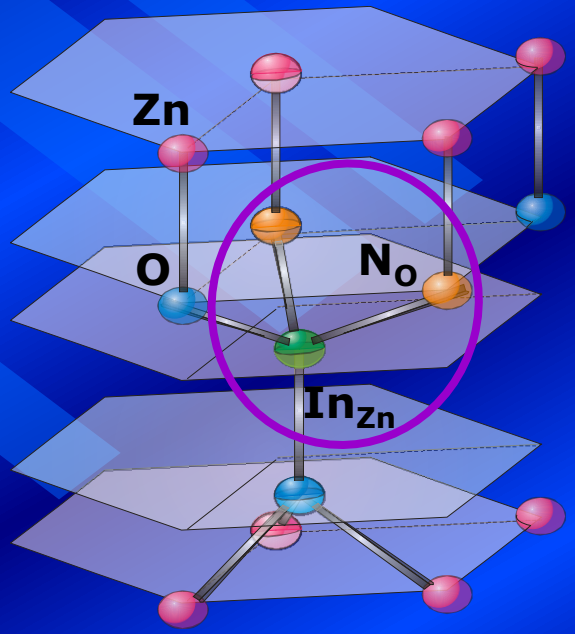
How to enhance p-type doping?

Donor-Acceptor Codoping
Yamamoto and Katayama-Yoshida
Physica B 302 (2001) 155

Donor-Acceptor Cluster-Doping
Wang and Zunger
Physical Review Letters 90 (2003) 256401

		IIIA	IVA	VA	VIA	VIIA
		B	C	N	O	F
IB	IIB	Al	Si	P	S	Cl
Cu	Zn	Ga	Ge	As	Se	Br
Ag	Cd	In	Sn	Sb	Te	I
Au	Hg	Tl	Pb	Bi	Po	At

possible
In-N_2 complex



How to enhance p-type doping?

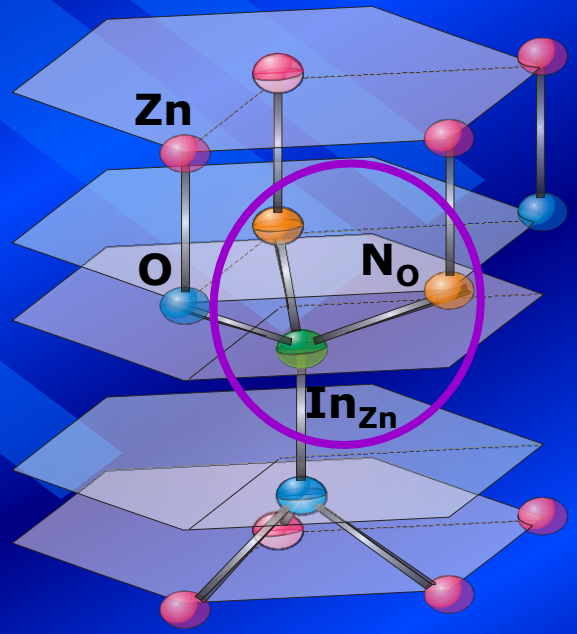
Donor-Acceptor Codoping

Yamamoto and Katayama-Yoshida
Physica B 302 (2001) 155

Donor-Acceptor Cluster-Doping

Wang and Zunger
Physical Review Letters 90 (2003) 256401

possible
In-N_2 complex



Electrical properties of ZnO films

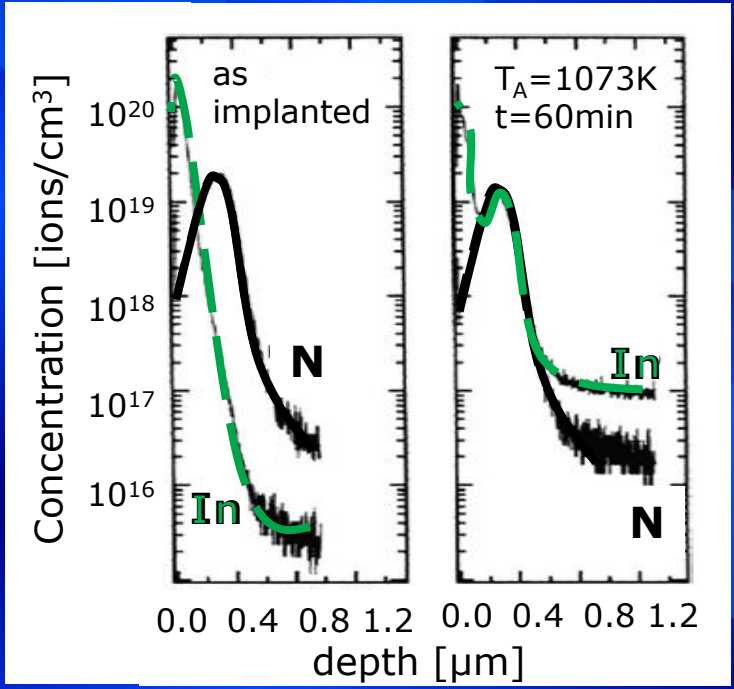
Sample	Carrier type	Carrier concentration
N doped	p	3.25×10^{14} cm^{-3}
In-N_x codoped	p	3.51×10^{17} cm^{-3}

Chen, Lu, Ye, Lin, Zhao, Ye, Li, and Zhu
Applied Physics Letters 87 (2005) 252106

increase by factor 1000

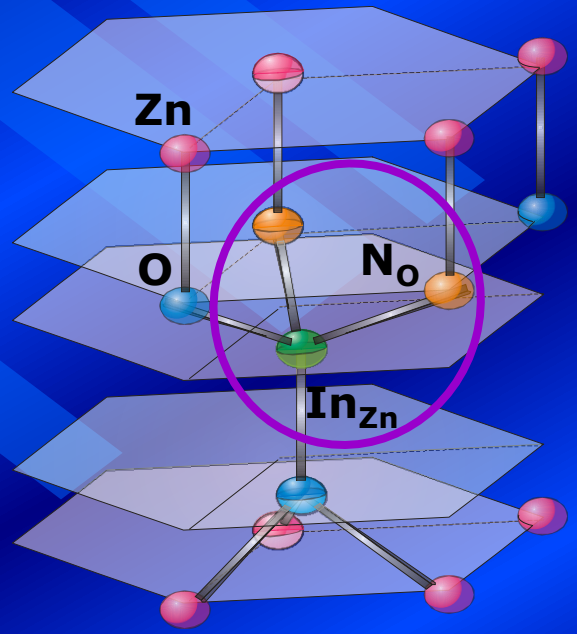
Codoping with In and N by implantation

SIMS depth profiling



Park, Sakaguchi, Ohashi, Hishita, and Haneda
Applied Surface Science 203-204 (2003) 359

possible
In-N_2 complex



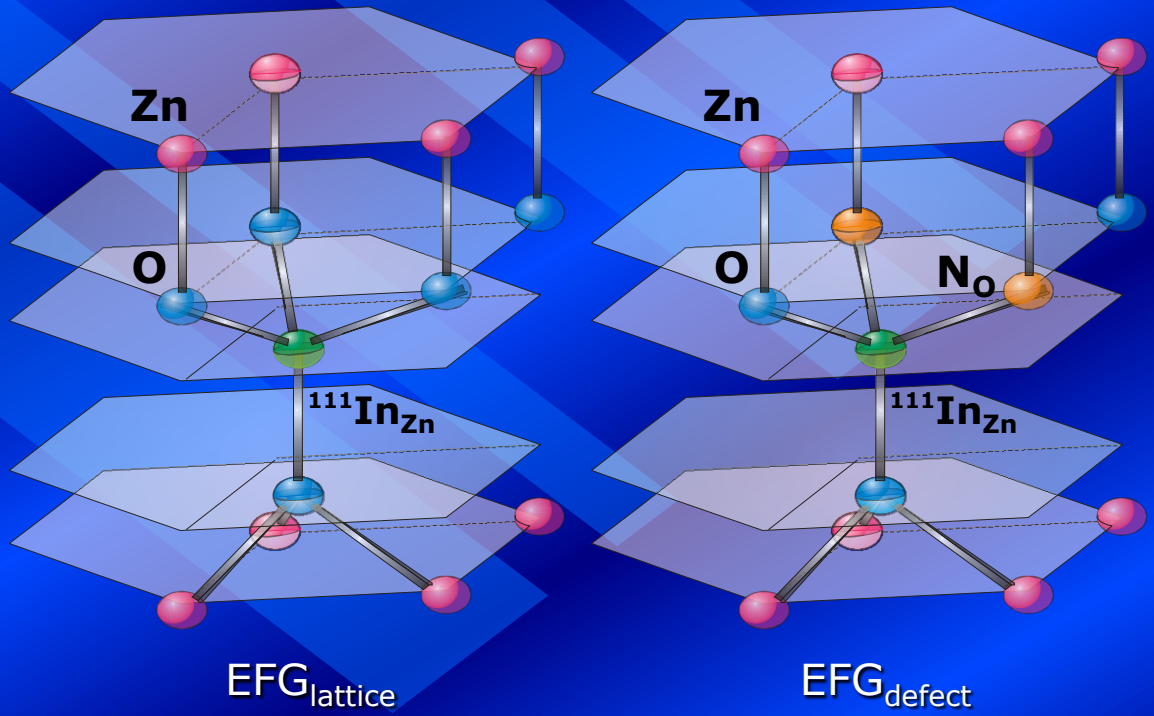
Perturbed Angular Correlation (PAC)

Electrical
field gradient V_{ij}

- strength V_{zz}
- symmetry $\eta = \frac{V_{xx} - V_{yy}}{V_{zz}}$
- orientation

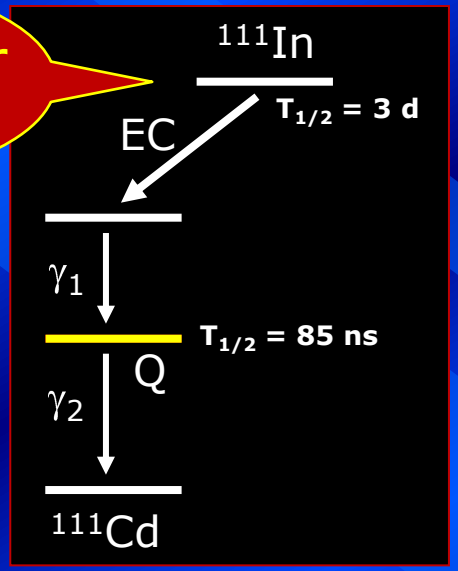
$EFG \sim r^{-3}$

- microscopic local



Perturbed Angular Correlation (PAC)

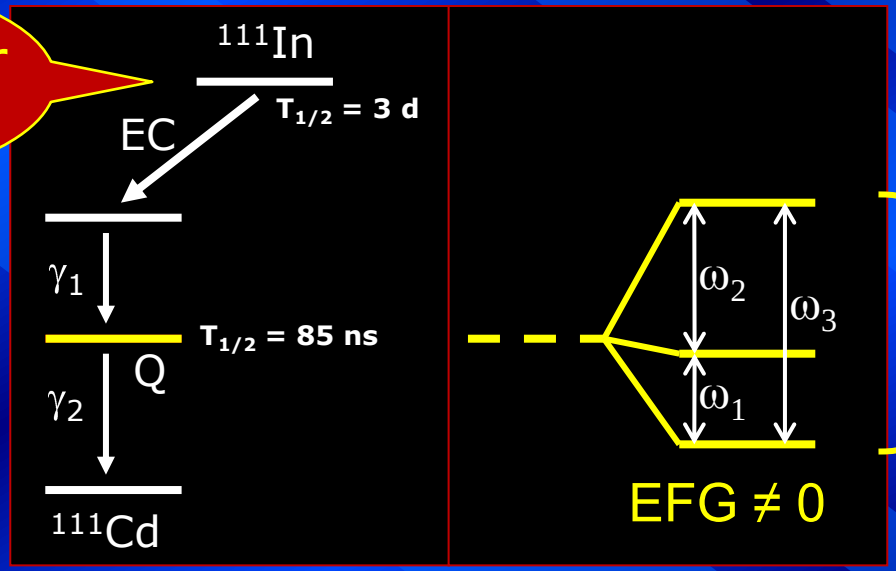
Donor-acceptor interaction



Observation

Perturbed Angular Correlation (PAC)

Donor-acceptor interaction



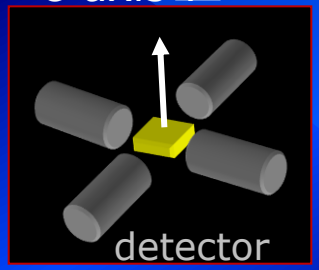
Observation

$$\nu_Q = \frac{10}{3\pi}\,\omega_1 = \frac{e\,Q\,V_{zz}}{h}$$

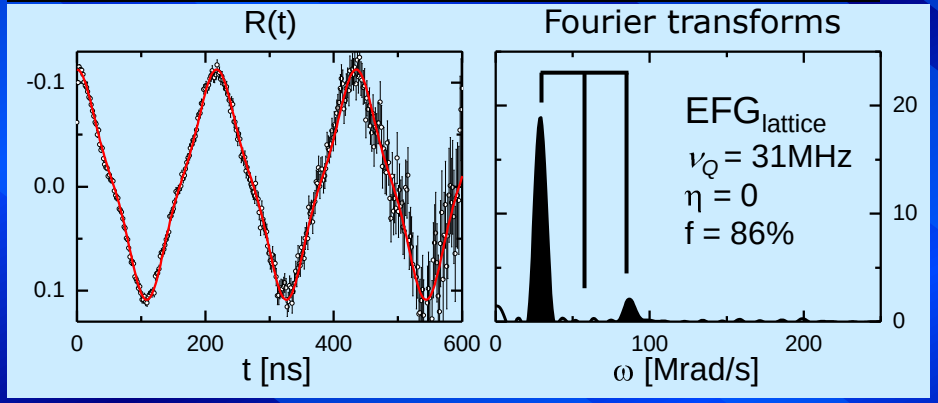
ν_Q: quadrupole coupling constant

Intrinsic $EFG_{lattice}$ of ZnO

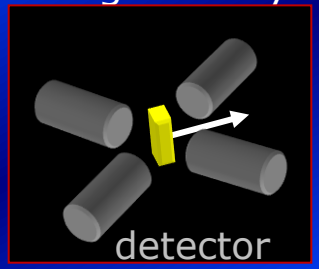
c-axis

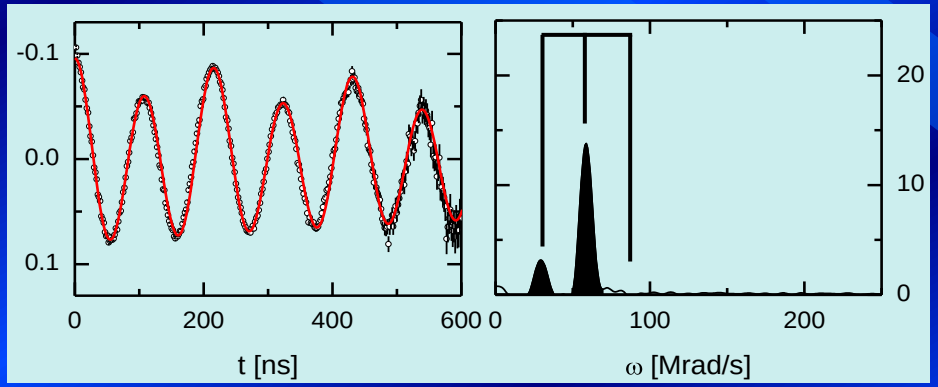


^{111}In implantation; T_A = 1100K t_A = 30min



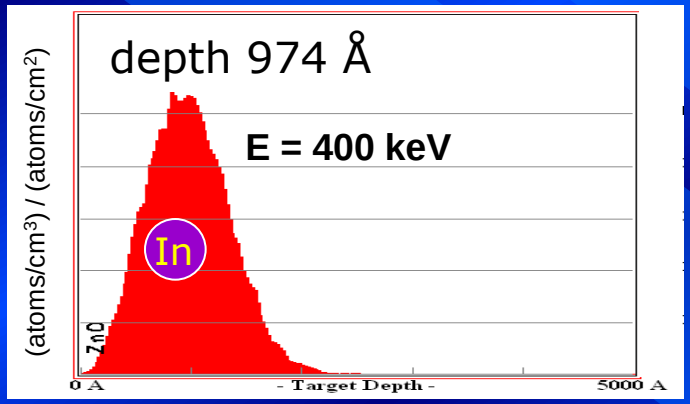
45 -geometry

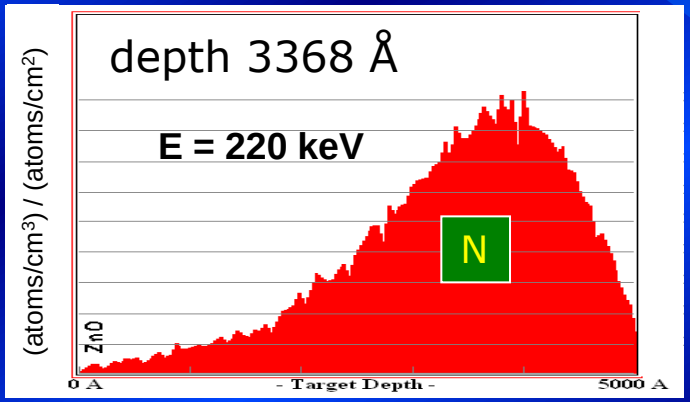




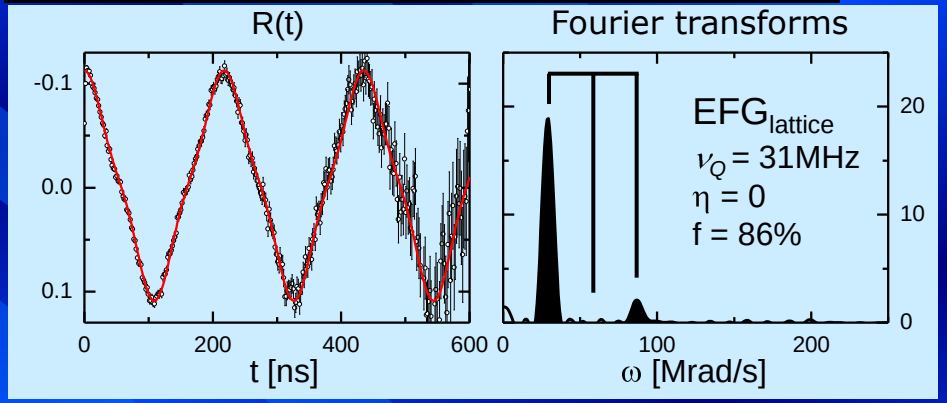
Codoping of ZnO

Indium penetration in ZnO



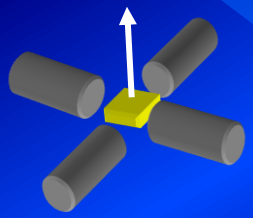


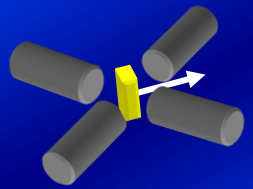
^{111}In implantation; T_A = 1100K t_A = 30min

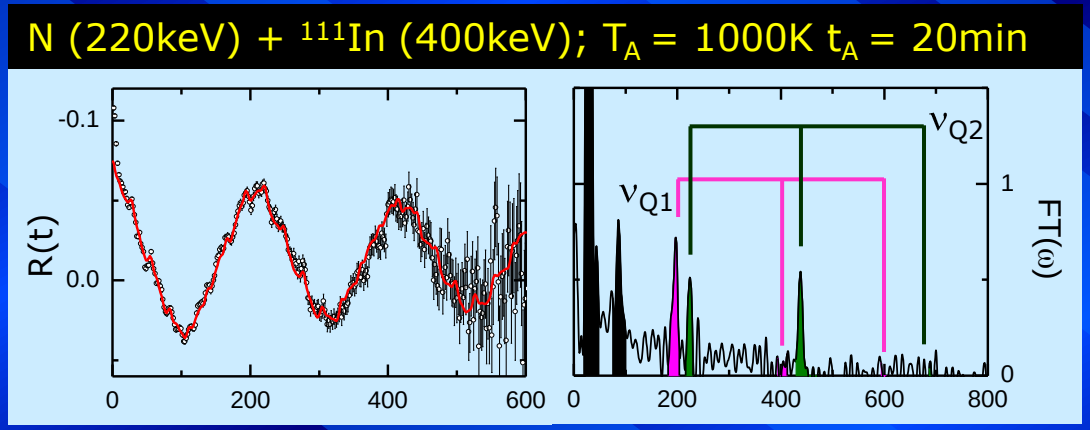


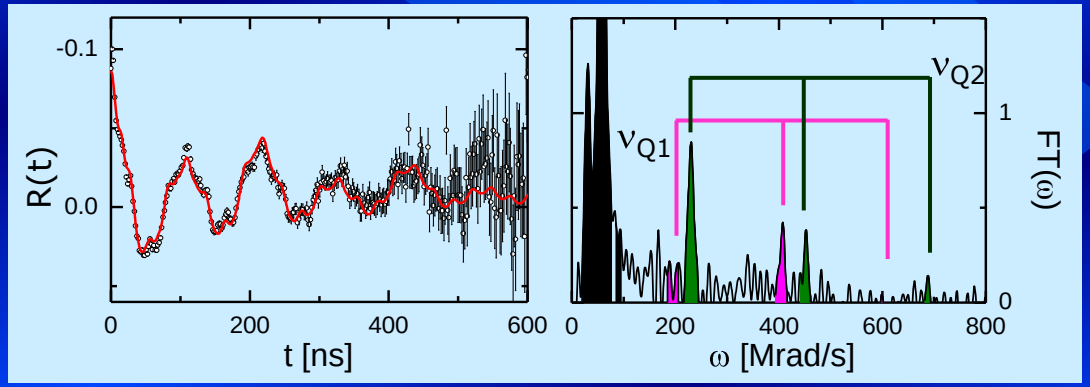
Group V	energy	penetration depth
N	220keV	3368Å
P	400keV	3179Å
As		
Sb	400keV	1228Å

Indium-Nitrogen codoping of ZnO

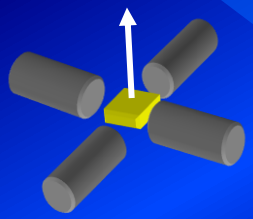


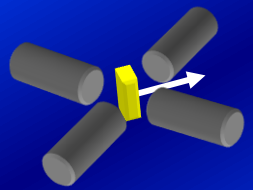




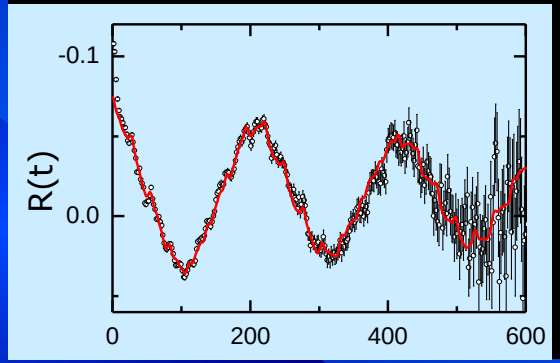


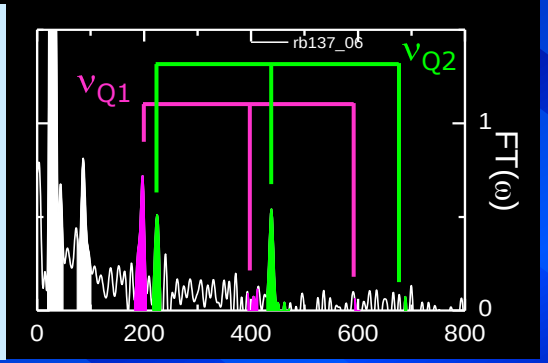
Indium-Nitrogen codoping of ZnO

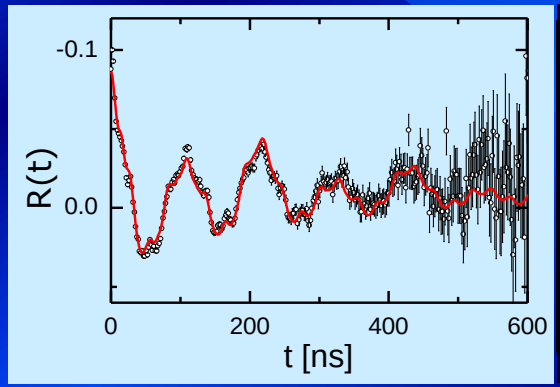


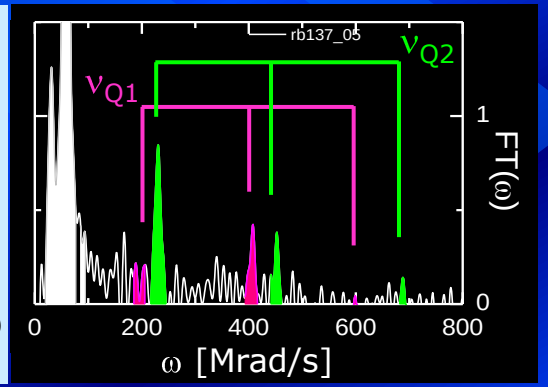


N (220keV) + ^{111}In (400keV); T_A = 1000K t_A = 20min



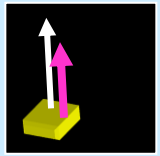




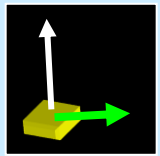


2 axial symmetrical EFG_{defect}:

c-axis oriented
ν_{Q1}=209(1)MHz
η=0
f=2%

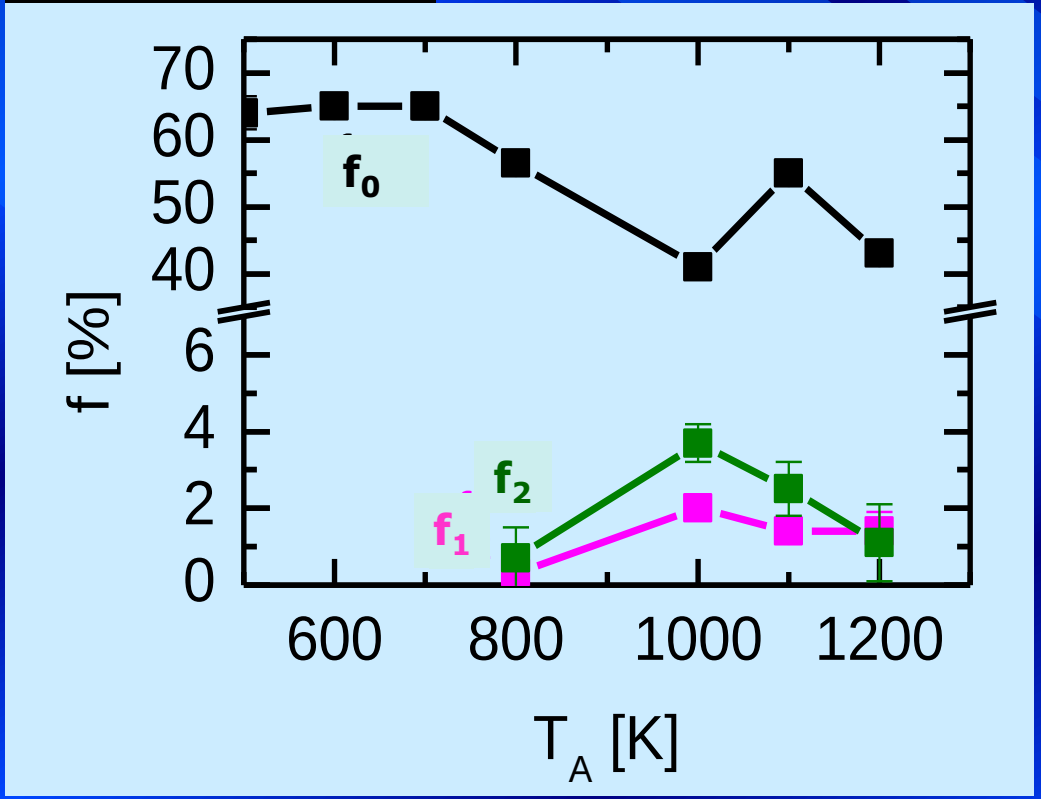


basal plane oriented
ν_{Q2}=234(1)MHz
$\eta \leq 0$
f=5%

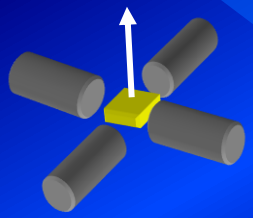


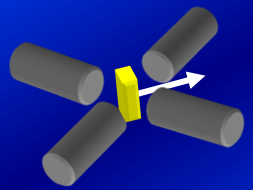
Indium-Nitrogen codoping of ZnO

Isochronic annealing

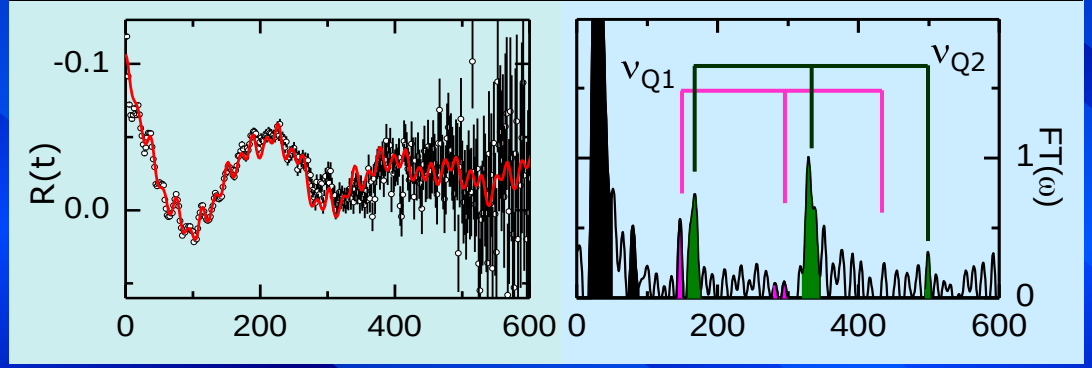


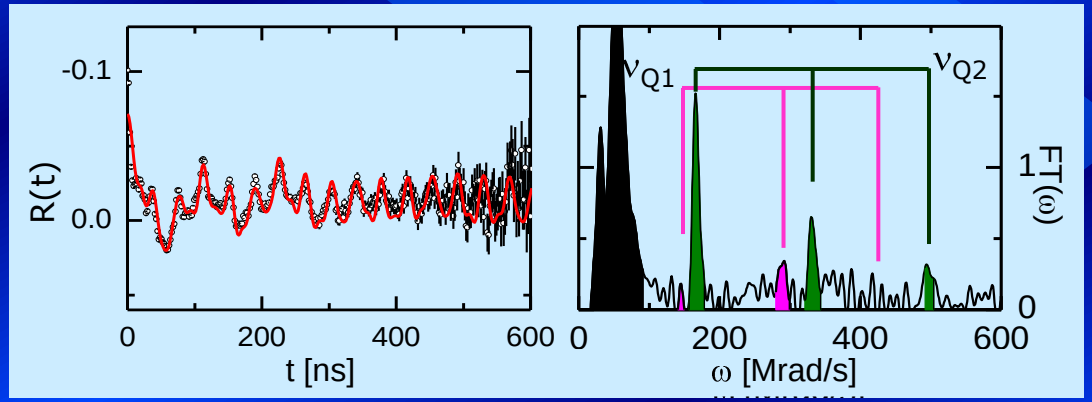
Indium-Phosphorus codoping of ZnO





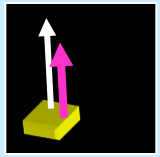
P (400keV) + ^{111}In (400keV); T_A = 800K t_A = 60min



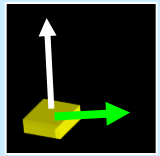


2 axial symmetrical EFG_{defect}:

c-axis oriented
ν_{Q1}=153(1)MHz
η=0
f=2%



basal plane oriented
ν_{Q2}=176(1)MHz
$\eta \leq 0$
f=10%



Formation of Indium-Acceptor-Pairs in II-VI semiconductors

	wurtzite	cubic			theoretical
	ZnO	*ZnSe	*ZnTe	*CdTe	**CdTe
^{111}In – N	209 234	271	262	280	274
^{111}In – P	153 176	219	222	212	224
^{111}In – As		196	199	186	190
^{111}In – Sb	169	156	167	153	162

* Ostheimer, Jost, Filz, Lauer, Wolf, and Wichert
Applied Physics Letters 69 (1996) 2840

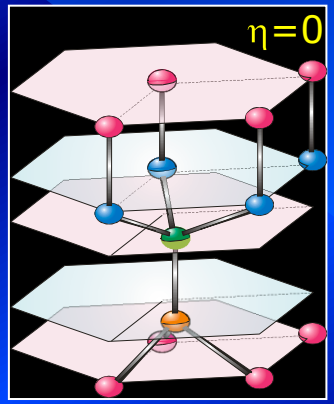
** Lany, Ostheimer, Wolf, and Wichert
Hyperfine Interactions 136/137 (2001) 619

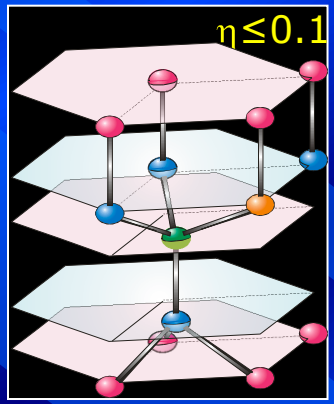
Formation of Indium-Acceptor-Pairs in Zinc Oxide

	ν_Q [MHz]	f [%]	η	Orientation
^{111}In – N	209 (1)	2	0	c-axis
	239 (1)	5	≤0.1	basal plane
^{111}In – P	155 (1)	2	0	c-axis
	175 (1)	10	≤0.1	basal plane
^{111}In – Sb	169 (1)	/	/	/
		9	≤0.1	basal plane

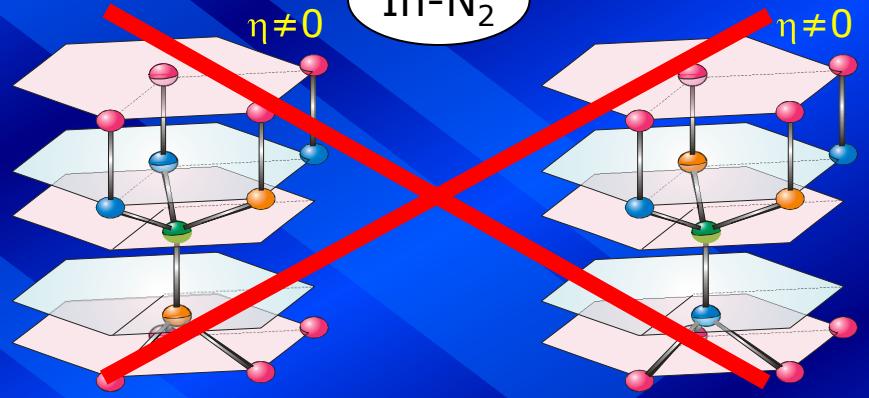
Possible configurations of In-N_x Complexes

In-N_1

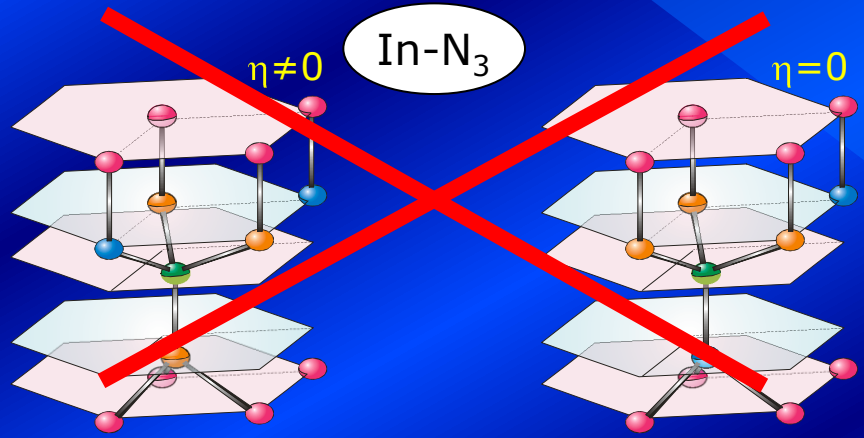




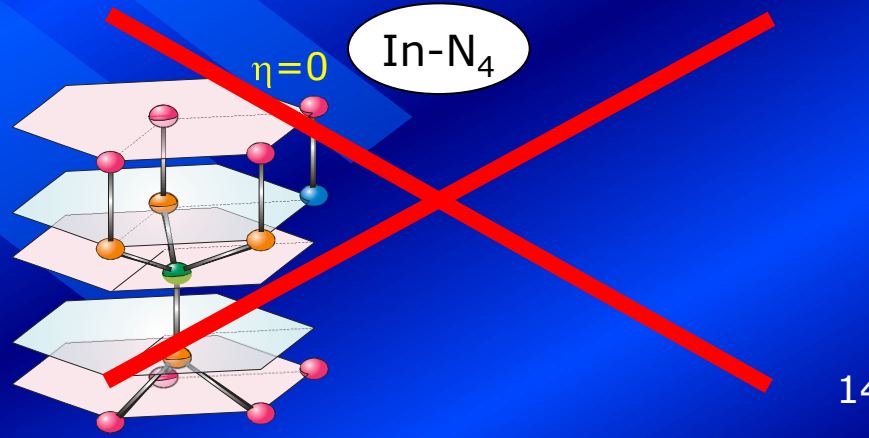
In-N_2



In-N_3



In-N_4



Summary

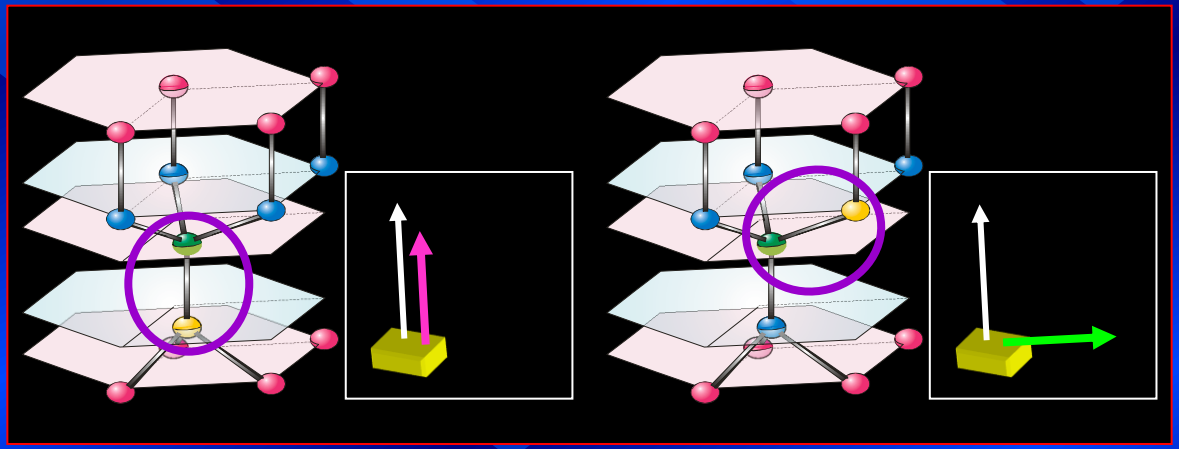
Donor–acceptor codoping of ZnO by ion implantation

Aim: analysis of the microscopic environment on atomic level

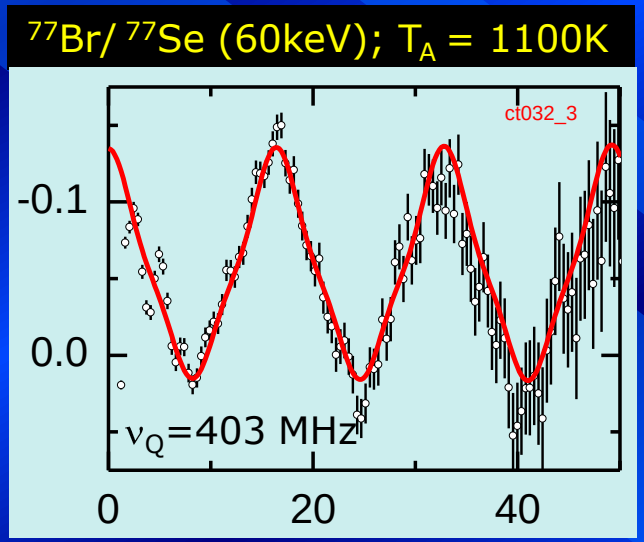
Tool: Perturbed Angular Correlation to obtain structural information

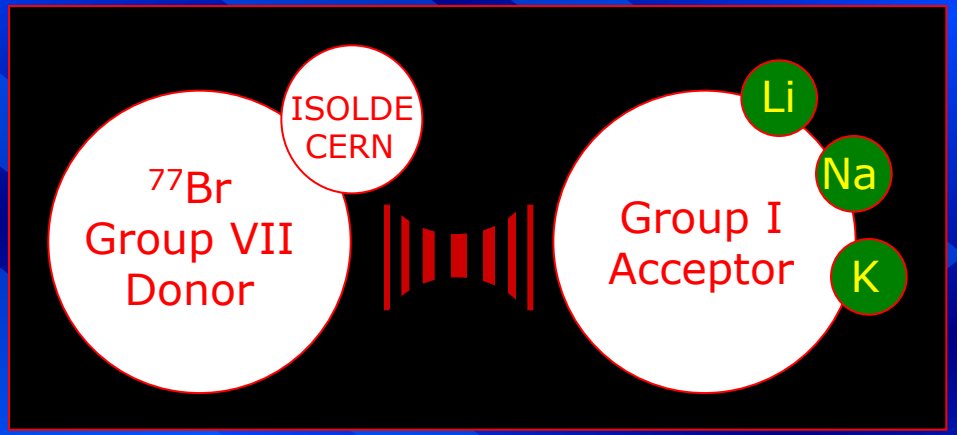
PAC

- In-N_1: 2 EFG
- In-P_1: 2 EFG



Work in progress





Implantations: Michael Uhrmacher and Daniel Jürgens (U Göttingen)

Financial support by BMBF 05KK7TS1