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Experimental and ab initio study of the EFG at donor impurities in the Cr2O3:Ta semiconductor.

In this work we report Time- Differential - Perturbed-Angular-Correlation (PAC) experiments on 181Hf(⟶181Ta)-implanted Cr2O3 polycrystalline samples (in their corundum phase) determining the magnitude and symmetry of the electric-field gradient tensor (EFG). The PAC experiments were carried out at 333 K in order to have only the electric quadrupole interaction, since above the Neel temperature (TN=308 K), the system has a paramagnetic behaviour. We performed the PAC measurements after each step of a series of thermal annealings in air in the range 673 K –1273 K, in order to obtain the maximal substitution of Ta impurities at defect free Cr sites in the semiconductor crystal structure. Two hyperfine interactions were detected in the spectra, but only one of them is well-defined and account for the shape of the spectra. This interaction increases its fraction as the annealing temperature and time increase, until it begins to disappear as was the case in the isomorphous Al2O3:181Ta system. The experimental results are compared with ab initio calculations in the framework of the Density Functional Theory (DFT) and with predictions of the Point Charge Model. The ab initio calculations was carried out with the FP-APW+lo method (embodied in the WIEN2K code) with 1:12 of impurity dilution (with respect to the cations). The more intense interaction is also the only one that is in perfect agreement with the ab initio predictions.

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Poster

Primary author: Dr DARRIBA, Germán Nicolás (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.)

Co-authors: RICHARD, Diego (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.); MUÑOZ, Emiliano Luis (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.); ERRICO, Leonardo Antonio (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, Universidad Nacional del Noroeste Bonaerense (UNNOBA), Monteagudo 2772, CP 2700 Pergamino, Argentina.); EVERSHEIM, Paul-Dieter (Helmholtz-Institut für Strahlen- und Kernphysik (H-ISKP),Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany.)

Presenter: Dr DARRIBA, Germán Nicolás (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.)

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