"After-effects" in ^{111}In(→^{111}Cd)-doped Al_2O_3 semiconductor: a modelization from first principles

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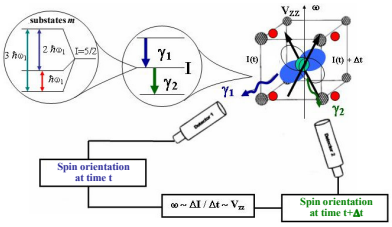
PERTURBED γ-γ ANGULAR CORRELATIONS (PAC) and the ELECTRON-CAPTURE "AFTER-EFFECTS" (ECAE)

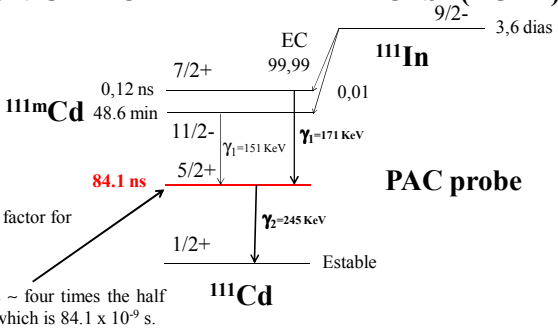


In PAC experiments we measure coincidences $C(90°,t)$ and $C(180°,t)$ between γ_1 and γ_2 detected with 90° and 180° angular positions of the detectors, respectively. The PAC spectrum hs the form:

$$R(t)=2\frac{C(180^\circ,t)-C(90^\circ,t)}{C(180^\circ,t)-2C(90^\circ,t)}\approx A_{22}G_{22}(t)$$

$$R(t)\approx A_{22}^{exp}\left(S_{20}(\eta)+\sum_{n=1}^{3}S_{2n}(\eta)\cos(\omega_n t)e^{-\delta\omega_n t}\right)$$

perturbation factor for polycrystals



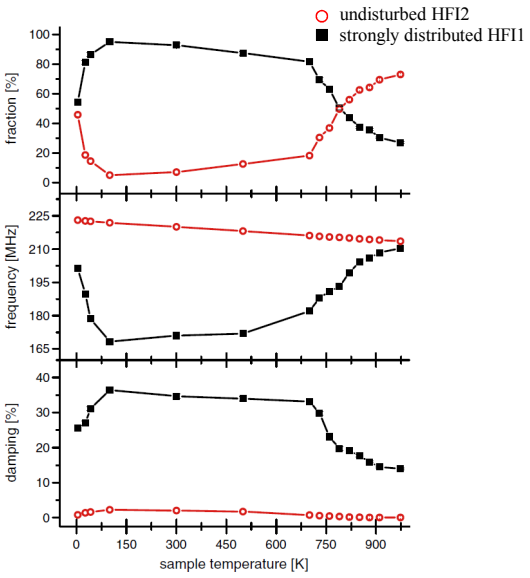
Time window of the measurement for ^{111}Cd is ~ four times the half life of the intermediate sensitive nuclear level, which is 84.1 x 10^{-9} s.

After the ^{111}In electron capture (EC) decay and subsequent Auger processes the ^{111}Cd probe-atom reaches a highly ionized state (6-8 electron holes in the outer shells) in less than 10^{-14} s and which is recovered, in a metallic host, in less than 10^{-12}s, not affecting the quadrupole interaction between the probe´s nuclear quadrupole moment and the external electric-field gradient (EFG).

In insulating environments, at least a single acceptor state at ^{111}Cd can survive during the PAC window of the measurement. Depending on the host, different electronic relaxation processes among different charge states of ^{111}Cd can occur (fast fluctuations, unidirectional relaxation, etc., called here ECAE), giving rise to *dynamic* hyperfine interactions.

PAC EXPERIMENTAL RESULTS

^{111}In(→^{111}Cd) implanted α-Al_2O_3 singlecrystal



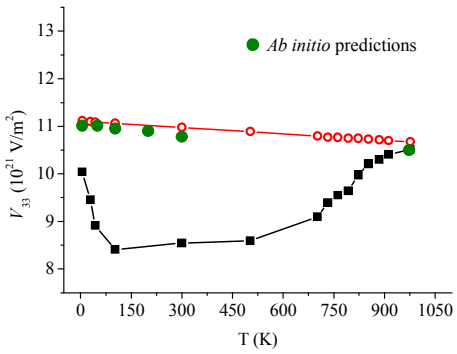
J. Penner and R. Vianden, Hyp. Int. **158**, 389 (2004).

Ab initio PREDICTIONS

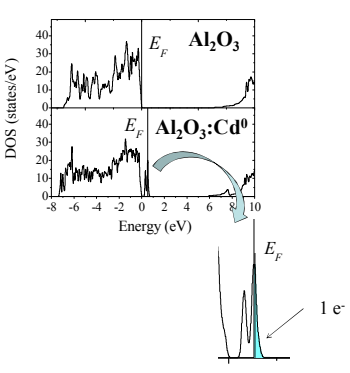
The calculations were performed using the Full-Potential Augmented Plane-Wave plus Local Orbitals (FP-APW+lo) DFT method, implemented in the WIEN2k code. When an Al atom is replaced by Cd in the supercell (SC), a single acceptor impurity level is introduced in the band gap of Al_2O_3, near the top of the valence band.

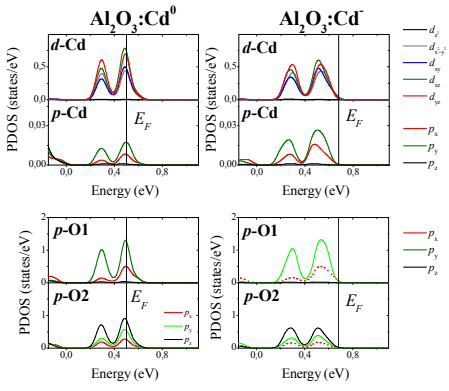
As we demonstrated in Ref. [1], the undisturbed HFI2 corresponds to ^{111}Cd localized at defect-free substitutional Al sites when 1 electron is added to the supercell (system labeled Al_2O_3:Cd^-), i.e. when the acceptor level is ionized (impurity level completely filled).

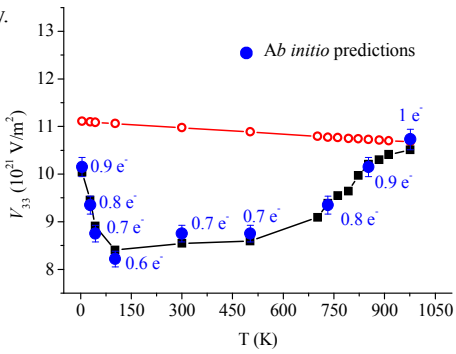
To study the temperature dependence of the undisturbed HFI2 interaction, we performed APW+lo calculations in the system Al_2O_3:Cd^- using experimental lattice parameters as a function of temperature. A perfect agreement is obtained.



To describe the different electronic configurations of the ^{111}Cd probe-atom which are involved in the generation of the *dynamic* hyperfine interactions we simulated different charge states of the impurity, adding charge between 0 to 1 electron to the system Al_2O_3:Cd^0 (in which a neutral Al is replaced by a neutral Cd in the SC), i.e. until filling completely the acceptor level introduced by the impurity.







To describe the strongly dampened interaction HFI1, we used in the calculations the experimental lattice parameter measured at room temperature. The error bar is an estimation of the variation of the predicted EFG in case the experimental lattice parameter at each temperature had been used.

CONCLUSIONES

- ❑ The undisturbed EFG temperature dependence of HFI2 was perfectly reproduced by the calculations.
- ❑ We propose that the EFG temperature dependence in the case of the strongly dampened HFI1 is originated in very subtle electronic charge state variations of the Cd impurity very close to the Fermi level position for which the acceptor state is ionized (completely filled).
- ❑ The strong EFG variation upon this subtle changes are due to the non uniform filling of the different *p* and *d* orbital symmetries of the Cd atom.

REFERENCES

[1] G. N. Darriba, M. Rentería, H. M. Petrilli, and L. V. C. Assali, Phys. Rev. B **86**, 075203 (2012).