

## Dynamic hyperfine interactions in $^{111}\text{In}$ -doped $\text{In}_2\text{O}_3$ revisited: PAC experiments and *ab initio* theoretical support

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In this work, we report recent Time-Differential  $\gamma$ - $\gamma$  Perturbed-Angular-Correlations (PAC) experiments performed on  $^{111}\text{In}$ -diffused  $\text{In}_2\text{O}_3$  polycrystalline samples in order to revisit the dynamic hyperfine interactions reported in the literature at  $^{111}\text{Cd}$  impurity sites in this semiconductor oxide [1,2] and to investigate in more detail their origin and possible dependence on the local symmetry of each crystallographic site of the *bixbyite* structure. These dynamic hyperfine interactions are attributed to the electronic relaxation processes that occur after the electron-capture (EC) decay of the  $^{111}\text{In}(\rightarrow^{111}\text{Cd})$  nuclei, usually called (ruffle speaking) *after effects*. This type of dynamic interactions, using  $^{111}\text{In}$  as parent isotope of the  $^{111}\text{Cd}$  probe atom, have been observed selectively in *bixbyite* oxides depending if the cations have closed shells (as In, Sc, and Y [1-3]) or partially filled 4f shells (as almost all the lanthanides), in which only static interactions were found [4]. The PAC measurements were performed in air as a function of temperature in the range 10-900 K. The  $R(t)$  spectra presents strong damping when measured at intermediate temperatures (150-500 K). This damping decreases partially in the range 10-150 K and totally at high temperatures (500-900 K), where static electric-field gradients (EFGs) are only present. The spectra were fitted with a dynamic perturbation factor proposed by Bäverstam and coauthors [5]. The experimental results are compared with *ab initio* electronic structure calculations in Cd-doped  $\text{In}_2\text{O}_3$  using the Wien2K code [6]. A scenario based on the EFG dependence on the charge state of the Cd impurity [7], supported by the *ab initio* calculations, is proposed to explain the origin and characteristics of the dynamic hyperfine interactions observed in these experiments.

### References

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