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

During the last 25 years, several Time-Differential Perturbed-Angular-Correlation (PAC) experiments have observed dynamic hyperfine interactions when the probe isotope 111Cd, obtained after the electron-capture (EC) decay of its parent 111In 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 111In isotope. This relaxation must occurs during the time-window of the intermediate sensitive nuclear state of the gamma-gamma 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 111Cd 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 111Cd 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 111In-diffused polycrystalline ZnO have been performed in order to measure the EFG at (111In (EC)–>) 111Cd 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.

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yes

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poster contribution

Summary

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).

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