PALS Measurements and Ab Initio/DFT Calculations for Positron Traps Identification on Zn-Based Nanopowders

Germán N. Darriba, Marcos Meyer, Mario Rentería and Laura C. Damonte

Departamento de Física and Instituto de Física La Plata (IFLP, CONICET La Plata), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, 1900 La Plata, Argentina

*email: damonte@fisica.unlp.edu.ar

Positron annihilation lifetime spectroscopy (PALS) was applied to study different positron traps induced by mechanical work and doping in three different Zn-based semiconductors. These experimental data were complemented by a precise theoretical ab initio calculation in the framework of the Density Functional Theory (DFT). In this approach the equilibrium structures of the doped systems (i.e., final atomic positions) were obtained applying the Full-Potential Augmented Plane Wave plus local orbitals (FP-APW + lo) method, embodied in the WIEN2k code. The Multigrid Instead of the K-spAce (MIKA) program was then used to predict the characteristic semiconductor lifetimes at these equilibrium structures. Also, in order to evaluate the effects produced by the structural relaxations on the lifetime, we predict the annihilation lifetimes for the non-relaxed systems. With the aim to elucidate electronic distortions introduced by the different defects (Al substitutional, Zn vacancies) in the semiconductor the electronic density of states (DOS) were evaluated. The calculations predict that Al substitutes the Zn atom in the ZnTe and ZnSe lattice and a zinc vacancy must appear in order to recover the semiconductor character, as suggest the experimental results. The characteristic positron annihilation lifetimes for the doped samples are obtained for both systems and compared with those measured. This theoretical approach helps us to deeper understand the origin and characteristics of different positrons traps.