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The Electrical Point Charges Model: application boundaries for Electrical Field Gradient calculations at nuclei sites in disordered ^{57}Fe doped ZnO matrixes

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Electric Field Gradients (EFG) at Zn and O sites in disordered ^{57}Fe doped ZnO matrixes arising from ^{57}Mn irradiated ZnO samples with wurtzite crystal structure were simulated through DFT atomistic calculations methods. The ZnO disordered crystal defective structures were simulated by means of overdimensioned unit cells (supercell) containing Zn vacancies at different concentrations with a ^{57}Fe atom per supercell. Previous DFT electron density calculation results in these defective crystalline structures reported in [1] were applied. Electric Point Charge Model (PCM) was also applied to calculate EFG at Zn and O sites in the same ^{57}Fe doped ZnO supercells as before, where Steinheimer antishielding factors γ_∞ values were taken from previously reported ones. A new methodology based on algebraic invariants, as I and D named, of the EFG resulting secular equations for both, DFT and PCM EFG data, were introduced and applied. It was proved that the second degree invariant I is proportional to the electrical quadrupole splitting at ^{57}Fe sites.
It results that a general agreement among Zn and O DFT- and PCM- EFG invariant data statistical distributions was observed, though the best results were achieved at the supercell with higher dimension (3x3x2) and the lowest vacancy concentration, where a good linear correlations among DFT and PCM I and D data were proved and the resulting effective γ_∞ values are very close to the previously reported ones. It was concluded that PCM approach might be applied as an initial numerical assessment for EFG data for high dimensioned supercells.

1. Y. Abreu, et al. Solid State Communications, 185 (2014) 25-29.

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