Perturbed Angular Correlation Studies in SrTiO₃ Single Crystals

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The quadrupole hyperfine interactions of 111 Cd/ 111 In probe nuclei in single-crystalline SrTiO₃ perovskite samples were investigated using Perturbed Angular Correlation spectroscopy. Three electric field gradients were detected and their fractions and hyperfine parameters were measured in the temperature range from 26 to 700 K. The fraction f_0 having a vanishing quadrupole frequency, as expected for 111 Cd on substitutional sites in a cubic lattice, starts to develop around 300 K and reaches 100% at 700 K. Two well-defined EFG's having closely lying quadrupole frequencies and asymmetry parameters of $\omega_{\rm Q1}=49.1(3)$ Mrad/s, $\eta_1=0.10(2)$ and $\omega_{\rm Q2}=51.8(3)$ Mrad/s, $\eta_2=0.12(2)$, at room temperature, were identified in the temperature range from 250 to 530 K, and their (100) orientation in the lattice was determined. They are associated with electronic defects at the probe atoms.

Key words: Perturbed Angular Correlations; SrTiO₃; Single Crystal; Electronic Defects; Perovskite.