Theoretical Investigations of the Defect Structure and the g Factors of a Tetragonal Ni^{3+} Center in $PbTiO_3$

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The defect structure and the anisotropic g factors of a tetragonal Ni^{3+} center in $PbTiO_3$ are theoretically investigated from improved perturbation formulas of the g factors for a $3d^7$ ion with low spin $S = 1/2$ in tetragonally elongated octahedra, established in this work. Based on the studies, the distance between the impurity Ni^{3+} and the center of the oxygen octahedron is found to be about 0.14 Å, which is smaller than that (≈ 0.3 Å) for the host Ti^{4+} site due to the inward shift (≈ 0.16 Å) towards the center of the oxygen octahedron. The theoretical g factors based on the above defect structure agree well with the observed values.

Key words: Defect Structures; Electron Paramagnetic Resonance; Crystal-Fields and Spin Hamiltonian; Ni^{3+}; $PbTiO_3$.