Theoretical Investigations of the Spin Hamiltonian Parameters of $ZrSiO_4$:Np^{4+}

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In this work, the spin Hamiltonian (SH) parameters $g_{\|}$ and $g_{\perp}$, and the hyperfine structure constants $A_{\|}$ and $A_{\perp}$ for $ZrSiO_4$:Np^{4+} are investigated on the basis of the perturbation formulas of these parameters for a $5f^3$ ion in tetragonal (D_{2d}) symmetry. In these formulas, the contributions to the SH parameters from the second-order perturbation terms, the admixtures of various energy levels and the covalency effect are taken into account. The related crystal-field parameters are calculated from the superposition model and the local structural data of the Zr^{4+} site occupied by the impurity Np^{4+}. The calculated SH parameters agree reasonably with the experimental data. The validity of the theoretical results is discussed.

Key words: Electron Paramagnetic Resonance (EPR); Crystal-fields and Spin Hamiltonian; Np^{4+}; $ZrSiO_4$.