Calculation of the EPR Parameters and the Local Structure for Fe^{+} on the Zn^{2+} Site of $ZnSiP_2$

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The zero-field splitting D, g factors $g_{\parallel}$ and $g_{\perp}$ and the local structure near Fe^{+} on the Zn^{2+} site of $ZnSiP_2$ are calculated from high-order perturbation formulas of the EPR parameters for a $3d^7$ ion in tetragonally distorted tetrahedra based on the cluster approach. According to these studies, we find that the impurity-ligand bonding angle α_{1oc} related to the fourfold axis is about 58.05° in the studied Fe^{+} impurity center, which is larger than the metal-ligand bonding angle $\alpha_{1h}(\approx 56.65°)$ in pure $ZnSiP_2$. The EPR parameters based on the above angle α_{1oc} agree well with the observed values. The errors of the results are analyzed.

Key words: Electron Paramagnetic Resonance (EPR); Defect Structure; Crystal- and Ligand-field Theory; Fe^{+}; $ZnSiP_2$.