

Theoretical Studies of the EPR Parameters and the Local Structure of the Tetragonal Fe^+ Center in KTaO_3

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The EPR parameters (zero-field splitting D and g factors g_{\parallel} and g_{\perp}) and the local structure for the tetragonal Fe^+ center in KTaO_3 are theoretically studied by using the perturbation formulas of the EPR parameters for a $3d^7$ ion in tetragonally distorted dodecahedra. Based on these studies, we find that the impurity Fe^+ may not locate on the regular dodecahedral K^+ site but suffer a large off-center displacement ΔZ ($\approx 0.43 \text{ \AA}$) along one of the $\langle 100 \rangle$ (or C_4) axes, which is responsible for the large tetragonal distortion of the impurity center. The displacement ΔZ obtained in this work is comparable with that ($\approx 0.46 \text{ \AA}$) of a similar monovalent Li^+ on K^+ site of KTaO_3 obtained from the nuclear quadrupole shift and can be regarded as reasonable. The calculated g factors, particularly the anisotropy $\Delta g (= g_{\perp} - g_{\parallel})$ based on the above displacement, agree with the observed values.

Key words: Defect Structures; Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-fields; Fe^+ ; KTaO_3