Investigation of the Spin Hamiltonian Parameters and the Local Structure of Two Ni\(^{3+}\) Centers in KTaO\(_3\)

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The spin Hamiltonian anisotropic \(g\) factors \(g_{||}\) and \(g_{\perp}\) and the local structures of the Ni\(^{3+}\) centers I and II in KTaO\(_3\) are theoretically investigated by using the perturbation formulas of the spin Hamiltonian parameters for 3d\(^7\) ions in tetragonally distorted octahedrons and dodecahedrons. By analyzing the electron paramagnetic resonance data of the studied systems, the centers I and II can be attributed to Ni\(^{3+}\) ions occupying octahedral Ta\(^{5+}\) (associated with a nearest-neighbour oxygen vacancy \(V_O\) along the \(C_4\) axis) and the dodecahedral K\(^+\) (associated with a nearest-neighbour interstitial oxygen \(O_I\) along the \(C_4\) axis) sites, respectively. Based on these studies, it is found that at the center I the impurity Ni\(^{3+}\) is displaced away from \(V_O\) by \(\Delta Z_I \approx -0.31(2) \ \text{Å}\) along the \(C_4\) axis. At the center II a large off-center displacement, \(\Delta Z_{II} \approx 1.12(2) \ \text{Å}\), towards the \(O_I\) along the \(C_4\) axis is obtained, due to Ni\(^{3+}\)-O\(_I\) covalent bonding.

Key words: Electron Paramagnetic Resonance; Defect Structures; Crystal- and Ligand-field Theory; Ni\(^{3+}\); KTaO\(_3\).