Investigation of the Local Geometry and EPR Parameters of V^{3+} and Cr^{4+} Centers in Al_2O_3 Crystals

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The EPR parameters (zero-field splitting D and g factors $g_{\|}$, $g_{\perp}$) of $3d^2$ V^{3+} and Cr^{4+} centers in Al_2O_3 crystals are calculated by using the diagonalization of the complete energy matrix for $3d^2$ ions in trigonal symmetry. The crystal-field parameters are estimated for the superposition model related to the local geometry (or structure) of the impurity centers. From the calculations, the EPR parameters for both impurity centers are explained and the local structures (characterized by the impurity displacement Δz along the C_3 axis and the displacement Δx of O^{2-} ions in the oxygen triangle between the impurity and the vacant oxygen octahedron along the x-axis, resulting from the electrostatic repulsive force and the electronic cloud overlap) of these impurity centers are estimated. The results are discussed.

Key words: Electron Paramagnetic Resonance; Defect Structure; Crystal-Field Theory; V^{3+}; Cr^{4+}; Al_2O_3.