Theoretical Explanation of the EPR Parameters of Tetragonal Ti^{3+} Centers in ZnSe and $CdS_{0.75}Se_{0.25}$ Semiconductors

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The electron paramagnetic resonance (EPR) parameters (g factors $g_\parallel$, $g_\perp$ and hyperfine structure constants $A_\parallel$, $A_\perp$) of the tetragonal Ti^{3+} centers in ZnSe and $CdS_{0.75}Se_{0.25}$ semiconductors are calculated from high-order perturbation formulas based on the cluster approach. In these formulas, both the contribution from the spin-orbit coupling parameters of the central $3d^n$ ion and that of ligands are considered. The calculated results show reasonable agreement with the observed values. The defect structures of the tetragonal Ti^{3+} centers in both semiconductors caused by the static Jahn-Teller effect are suggested.

Key words: Crystal- and Ligand-Field Theory; Electron Paramagnetic Resonance; Local Lattice Distortion; II-VI Semiconductors; Ti^{3+}.