EPR Parameters and Local Atom-position Parameters for Co²⁺ Ions in CdS and CdSe Semiconductors

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The EPR parameters (zero-field splitting D and g factors g_{\parallel} , g_{\perp}) of Co^{2+} ions in CdS and CdSe semiconductors are calculated from the high-order perturbation formulas based on the cluster approach for a $3d^7$ ion in trigonal symmetry. These formulas include the contribution to the EPR parameters from both the spin-orbit coupling parameter of the $3d^7$ ion and that of the ligand. From the calculations, the local atom-position parameters u (which are different from the corresponding values in the host crystals) for the Co^{2+} impurity centers in both semiconductors are estimated. The results are discussed.

Key words: Electron Paramagnetic Resonance; Local Atom-Position Parameter; Crystal- and Ligand- Field Theory; Co²⁺; CdS; CdSe.