EPR Parameters and Local Atom-position Parameters for Co$^{2+}$ Ions in CdS and CdSe Semiconductors

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Z. Naturforsch. 59a, 783 – 786 (2004); received July 9, 2004

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 3$d^7$ ion in trigonal symmetry. These formulas include the contribution to the EPR parameters from both the spin-orbit coupling parameter of the 3$d^7$ 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; Co$^{2+}$; CdS; CdSe.