Zero-field Splitting and Local Lattice Distortions for Fe^{3+} Ions in Some I_b-III_b-VI_2 Semiconductors

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The EPR zero-field splitting D for Fe^{3+} ions in some I_b-III_b-VI_2 semiconductors is calculated with the superposition model. The calculated D values, when using the local rotation angles $\tau(Fe^{3+})$ for Fe^{3+} in $CuGaS_2$ and $AgGaS_2$ crystals, are consistent with the observed values, whereas for Fe^{3+} in $CuAlS_2$ crystal they are not. The calculated results are discussed. The local lattice distortions except the local rotation angles τ for Fe^{3+} in $CuAlS_2$ are suggested.

Key words: Electron Paramagnetic Resonance; Local Lattice Distortion; Superposition Model; Fe^{3+}; $CuMS_2$(M = Al, Ga, In); $AgGaS_2$.