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 $\tau$ 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$_2$. 