

EPR Parameters of the Trigonal $\text{Fe}_{\text{Ga}}^+ - \text{S}_{\text{P}}$ Pair Defect in n-Type GaP Codoped with Iron and Sulphur

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Z. Naturforsch. **60a**, 753 – 755 (2005); received April 6, 2005

The EPR parameters (g factors g_{\parallel} , g_{\perp} , and zero-field splitting D) of a trigonal Fe^+ center (which is assigned to a donor-acceptor pair defect $\text{Fe}_{\text{Ga}}^+ - \text{S}_{\text{P}}$ caused by S^{2-} at a nearest-neighbor P^{3-} site of an Fe_{Ga}^+ impurity) in n-type GaP codoped with iron and sulphur are calculated from high-order perturbation formulas based on the two spin-orbit coupling parameter model for the EPR parameters of a $3d^7$ ion in trigonal symmetry. The calculated results agree well with the observed values, suggesting that the assignment is suitable.

Key words: Electron Paramagnetic Resonance; Pair Defect; Crystal- and Ligand-field Theory; Fe^+ ; GaP.