Defect Structures for Fe^{3+}, Mn^{2+}, and Ni^{3+} Impurities in Wuritzite GaN Crystals

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Electron paramagnetic resonance (EPR) zero-field splittings D for Mn^{2+} and Fe^{3+} in wurtzite GaN crystals are studied from high-order perturbation formulas based on the spin-orbit mechanism in both weak- and strong-field schemes. From these studies it can be seen that the Mn^{2+} or Fe^{3+} impurity does not occupy the exact Ga^{3+} position, but is displaced by ΔR on the C_3' axis. The displacements are confirmed from a study of the superposition model, based on which a normal value of $\overline{b_2}(R_0)$ ($\approx$ –0.34 (15) cm^{-1}) for the Fe^{3+}-N^{3-} combination is suggested. The EPR parameters D, $g_{\|}$ and $g_{\perp}$ for Ni^{3+} in GaN crystals are also studied. It is found that Ni^{3+} is almost not displaced. The impurity displacements in GaN are discussed by considering the valences and radii of these impurity ions and the replaced Ga^{3+} ion. – Pacs: 61.16Hn; 76.30Fc; 71.70Ch

Key words: Defect Structure; EPR; Crystal Field Theory; GaN; Fe^{3+}; Mn^{2+}; Ni^{3+}.