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Structural and Magnetic Properties of Mn-Doped 6H-SiC

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Abstract : n-Type 6H-SiC(0001) substrates were implanted with three fluencies of Mn+ 5x1015 Mn/cm2 (Mn content: 0.7%), 1x1016 (~2 %), and 5x1016 cm–2 (7%) with implantation energy of 80 keV and substrate temperature of 365ºC. The samples were characterized using Rutherford Backscattering and Channeling Spectroscopy (RBS/C), High-Resolution X-Ray Diffraction technique (HRXRD), micro-Raman Spectroscopy (μRS), and Superconducting Quantum Interference Device (SQUID) techniques. The aim of our work is to investigate implantation induced defects with dose and to study any correlation between disorder-composition and magnetic properties. In addition, ab-initio calculations were used to investigate the structural and magnetic properties of Mn-doped 6H-SiC. Various configurations of Mn sites and vacancy types were considered. The calculations showed that a substitutional Mn atom at Si site possesses larger magnetic moment than Mn atom at C site. A model is introduced to explain the dependence of the magnetic structure on site occupation. The magnetic properties of ferromagnetically (FM) and antiferromagnetically (AFM) coupled pairs of Mn atoms with and without neighboring vacancies have also been explored.

Keywords : ab-initio calculations, diluted magnetic semiconductors, magnetic properties, silicon carbide
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