World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:9, No:09, 2015

First Principle Calculation of The Magnetic Properties of Mn-doped 6H-SiC

Authors : M. Al Azri, M. Elzain, K. Bouziane, S. M. Chérif

Abstract : The electronic and magnetic properties of 6H-SiC with Mn impurities have been calculated using ab-initio calculations. Various configurations of Mn sites and Si and C vacancies were considered. The magnetic coupling between the two Mn atoms at substitutional and interstitials sites with and without vacancies is studied as a function of Mn atoms interatomic distance. It was found that the magnetic interaction energy decreases with increasing distance between the magnetic atoms. The energy levels appearing in the band gap due to vacancies and due to Mn impurities are determined. The calculated DOS's are used to analyze the nature of the exchange interaction between the impurities. The band coupling model based on the p-d and d-d level repulsions between Mn and SiC has been used to describe the magnetism observed in each configuration. Furthermore, the impacts of applying U to Mn-d orbital on the magnetic moment have also been investigated. The results are used to understand the experimental data obtained on Mn- 6H-SiC (as-implanted and as –annealed) for various Mn concentration (CMn = 0.7%, 1.6%, 7%).

Keywords : ab-initio calculations, diluted magnetic semiconductors, magnetic properties, silicon carbide
Conference Title : ICMSAPE 2015 : International Conference on Materials Science, Applied Physics and Engineering
Conference Location : Rome, Italy
Conference Dates : September 17-18, 2015