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Ferromagnetic properties of manganese doped iron silicide. ANGEL RUIZ-REYES, LUIS F. FONSECA, University of Puerto Rico, RENAT SABIRIANOV, University of Nebraska at Omaha — We report the synthesis of high quality Iron silicide (FeSi) nanowires via Chemical Vapor Deposition (CVD). The materials exhibits excellent magnetic response at room temperature, especially when doped with manganese showing values of 2.0 X 10-04 emu for the FexMnySi nanowires. SEM and TEM characterization indicates that the synthesized nanowires have a diameter of approximately 80nm. MFM measurements present a clear description of the magnetic domains when the nanowires are doped with manganese. Electron Diffraction and XRD measurements confirms that the nanowires are single crystal forming a simple cubic structure with space group P213. First-principle calculations were performed on (111) FeSi surface using the Vienna ab initio simulation package (VASP). The exchange correlations were treated under the Ceperley-Alder (CA) local density approximation (LDA). The Brillouin Zone was sampled with 8x8x1 k-point grid. A total magnetic moment of about 10 μB was obtained for three different surface configuration in which the Iron atom nearest to the surface present the higher magnetization. To study the effect of Mn doping, Fe atom was replaced for a Mn. Stronger magnetization is presented when the Mn atom is close to the surface. The exchange coupling constant have been evaluated calculating the energy difference between the ferromagnetic and anti-ferromagnetic configurations.

Wai-Ning Mei
University of Nebraska at Omaha

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