

## Half-Metallic Ferromagnetism in Ternary Zinc Blende Fe/In<sub>0.5</sub>Ga<sub>0.5</sub> as/in Psuperlattice: First-Principles Study

**Authors :** N. Berrouachedi, M. Bouslama, S. Rioual, B. Lescop, J. Langlois

**Abstract :** Using first-principles calculations within the LSDA (Local Spin Density Approximation) method based on density functional theory (DFT), the electronic structure and magnetic properties of zinc blende Fe/In<sub>0.5</sub>Ga<sub>0.5</sub>As/InPsuperlattice are investigated. This compound are found to be half -metallic ferromagnets with a total magnetic moment of 2.25 $\mu$ B per Fe. In addition to this, we reported the DRX measurements of the thick iron sample before and after annealing. One should note, after the annealing treatment at a higher temperature, the disappearance of the peak associated to the Fe(001) plane. In contrast to this report, we observed after the annealing at low temperature the additional peaks attributed to the presence of indium and Fe<sub>2</sub>As. This suggests a subsequent process consisting in a strong migration of atoms followed with crystallization at the higher temperature. To investigate the origin of magnetism and electronic structure in these zb compounds, we calculated the total and partial DOS of FeInP. One can see that  $\mu_{total}=4.24\mu$ B and  $\mu_{Fe}=3.27\mu$ B in contrast  $\mu_{In}=0.021\mu$ B and  $\mu_{P}=0.049\mu$ B. These results predicted that FeInP compound do belong to the class of zb half metallic HM ferromagnets with a pseudo gap = 0.93 eV are more promising materials for spintronics devices.

**Keywords :** zincblend structure, half metallic ferromagnet, spin moments, total and partial DOS, DRX, Wien2k

**Conference Title :** ICSRD 2020 : International Conference on Scientific Research and Development

**Conference Location :** Chicago, United States

**Conference Dates :** December 12-13, 2020