World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:13, No:05, 2019

Occurrence of Half-Metallicity by Sb-Substitution in Non-Magnetic Fe_2TiSn

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Abstract : Fe_2TiSn is a non-magnetic full Heusler alloy with a small gap (~ 0.07 eV) at the Fermi level. The electronic structure is highly symmetric in both the spin bands and a small percentage of substitution of holes or electrons can push the system towards spin polarization. A stable 100% spin polarization or half-metallicity is very desirable in the field of spintronics, making Fe_2TiSn a highly attractive material. However, this composition suffers from an inherent anti-site disorder between Fe and Ti sites. This paper reports on the method adopted to control the anti-site disorder and the realization of the half-metallic ground state in Fe_2TiSn, achieved by chemical substitution. Here, Sb was substituted at Sn site to obtain $Fe_2TiSn_{1-x}Sb_x$ compositions with x = 0, 0.1, 0.25, 0.5 and 0.6. All prepared compositions with $x \leq 0.6$ exhibit long-range $L2_1$ ordering and a decrease in Fe – Ti anti-site disorder. The transport and magnetic properties of $Fe_2TiSn_{1-x}Sb_x$ compositions were investigated as a function of temperature in the range, 5 K to 400 K. Electrical resistivity, magnetization, and Hall voltage measurements were carried out. All the experimental results indicate the presence of the half-metallic ground state in $x \geq 0.25$ compositions. However, the value of saturation magnetization is small, indicating the presence of compensated magnetic moments. The observed magnetic moments' values are in close agreement with the Slater–Pauling rule in half-metallic systems. Magnetic interactions in $Fe_2TiSn_{1-x}Sb_x$ are understood from the local crystal structural perspective using extended X-ray absorption fine structure (EXAFS) spectroscopy. The changes in bond distances extracted from EXAFS analysis can be correlated with the hybridization between constituent atoms and hence the RKKY type magnetic interactions that govern the magnetic ground state of these alloys. To complement the experimental findings, first principle electronic structure calculations were also undertaken. The spin-polarized DOS complies with the experimental results for $Fe_2TiSn_{1-x}Sb_x$. Substitution of Sb (an electron excess element) at Sn–site shifts the majority spin band to the lower energy side of Fermi level, thus making the system 100% spin polarized and inducing long-range magnetic order in an otherwise non-magnetic Fe_2TiSn. The present study concludes that a stable half-metallic system can be realized in Fe_2TiSn with ≥ 50% Sb – substitution at Sn – site.

Keywords : antisite disorder, EXAFS, Full Heusler alloy, half metallic ferrimagnetism, RKKY interactions
Conference Title : ICM 2019 : International Conference on Magnetism
Conference Location : Paris, France
Conference Dates : May 16-17, 2019