Contribution ID: **19** Type: **Oral Presentation**

Density Functional Based Investigation on Electronic Properties of Fe-Ni Invars

The present talk focuses on the computed results of electronic band structure, electronic density of states, electronic charge density plots and Fermi surfaces of Fe-Ni invar materials namely L12 FeNi3, taenite L10 FeNi, L12 Fe3Ni, D03 Fe3Ni, Z1 Fe3Ni, D03 FeNi3 and tetrataenite L10 FeNi. The investigation carried out based on the density functional theory as implemented in Quantum Espresso. As Fe and Ni are well known ferromagnetic transition metals, the combination of Fe and Ni i.e. Fe-Ni invar like materials exhibit complex magnetic behaviour.

The electronic band structures of all the seven Fe-Ni phases under consideration are not showing any energy gap at Fermi level hence predicts metallic behaviour for them. All electronic bands are well dispersive in nature which concludes the high electron mobility in the Invar like systems. It is concluded from the PDOS of Fe-Ni phases under consideration that d-Fe and d-Ni electrons significantly contribute to the total electronic density of states. The structural stability of the intermetallic compound is also predicted from the position of EF on the deep valley (pseudo gap) in the PDOS. The position of EF in the PDOS of L12 FeNi3 and taenite L10 FeNi predicts structural stability of L12 FeNi3 and taenite L10 FeNi at 0 K. From the DOS of L12 FeNi3 and D03 FeNi3, it is concluded that L12 FeNi3 is highly stable compared to D03 FeNi3. The charge density plots for L12 FeNi3, taenite L10 FeNi and L12 Fe3Ni predict comparatively strong metallic bonding between Fe and Ni compared to between the Fe-Fe metal atoms. The L12 Fe3Ni shows weak metallic bonding between Ni-Ni compared to Fe-Ni metal atoms. The taenite L10 FeNi exhibit slightly strong metallic bonding between Fe and Ni atoms compared to that in L12 FeNi3 and L12 Fe3Ni. In D03 Fe3Ni, Fe metal atoms at a far distance predict comparatively strong metallic bonding between them in comparison to nearest Fe-Fe atoms while the same strong metallic bonding is also observed for two far Ni-Ni metal atoms in D03 FeNi3. Z1 Fe3Ni suggests weak metallic bonding between Fe-Ni compared to that of Fe-Fe and Ni-Ni metal atoms. The complicated shape of comprehensive Fermi surfaces are observed for most of the Fe-Ni phases which occurred from the merging of all individual Fermi surfaces due to corresponding band crossing at Fermi level EF.

Thus the preset talk will cover very exhaustive and large number of results obtained at our group on electronic properties of L12 FeNi3, taenite L10 FeNi, L12 Fe3Ni, D03 Fe3Ni, Z1 Fe3Ni, D03 FeNi3 and tetrataenite L10 FeNi by employing density functional theory.

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Session Classification: Material Physics

Track Classification: Material Physics