Electronic Structure, Magnetic and Optical properties of Fe_2 Mn Z (Z=Si, Ge, Sn, Ga)

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Abstract:-

The article describes the electronic structure, magnetic and optical properties of bulk Fe_2Mn Z (Z= Si, Ge, Sn, Ga) of full heusler alloy. The value of total magnetic moment is $3\mu_B$ for Fe_2MnSn and Fe_2MnGe at their equilibrium lattice constant and follows Slater-Pauling curve. Fe_2MnSn posses the largest magnetic moment among the three with the value of $5.73\mu_B$ at equilibrium lattice constant. The magnetic and optical properties of Fe_2MnGa of heusler alloy are discussed in terms of energy band calculation for ordered FCC and L_{21} type structure.

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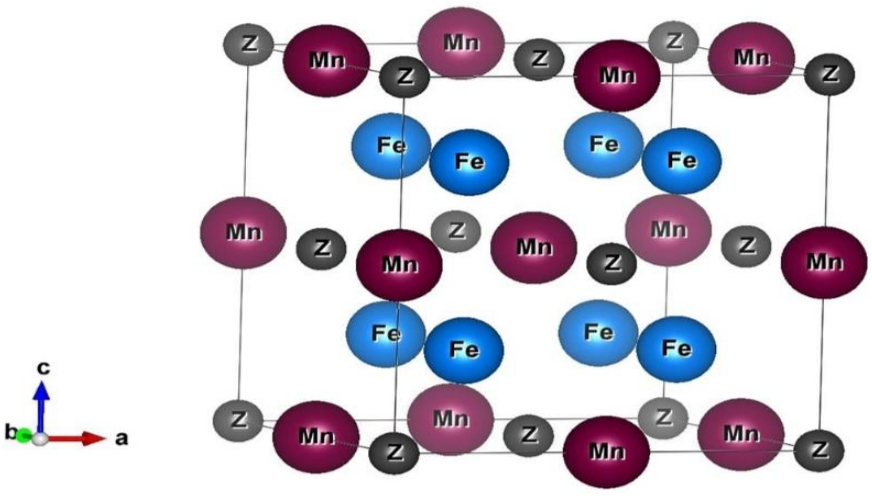
Introduction:-

Heusler alloys possessing half metallic ferromagnetic nature. It has high spin polarization due to presence of a gap Fe_2YZ Heusler alloy with Y which is transition metal (Mn) and with Z as a semiconductor. Good thermoelectric and magnetic properties can be calculated by theatrical calculation of the electronic structure in magnetic order Fe_2MnZ heusler alloy. Yang founded that magnetic moment is affected with pressure in Fe_2MnAl. The structural transformation in Fe_2MnGa is bcc and the electronic structure of Fe_2MnGa alloy is with Fcc-type. Now, the electronic structural, magnetic and optical properties of Fe_2MnZ (Z= Si, Ge, Sn and



Ga).

Electronic Structural Properties :-

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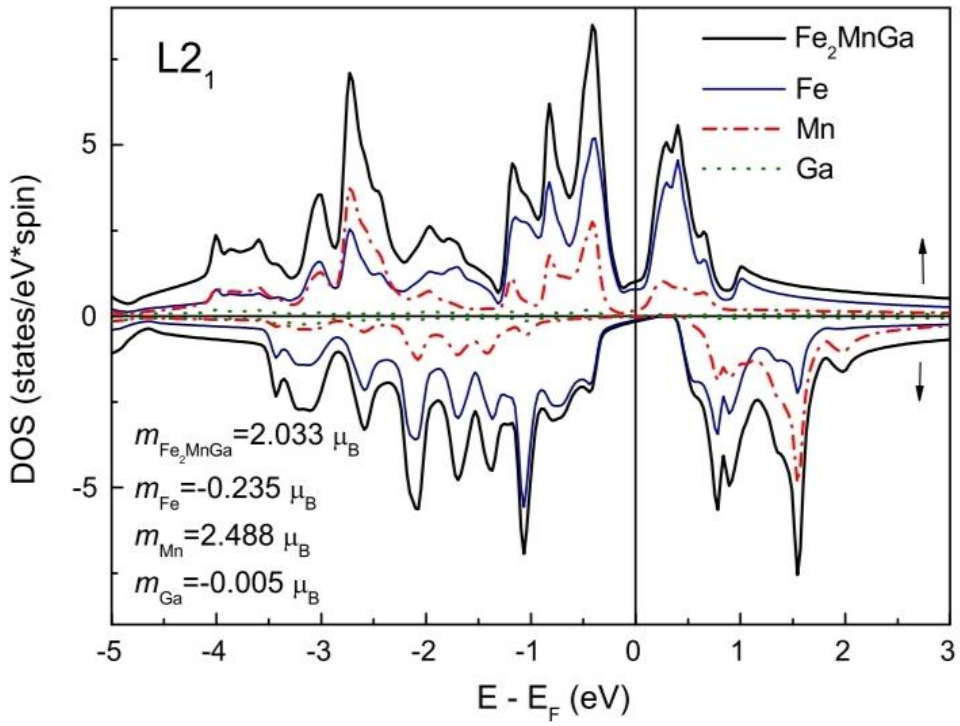
It can be seen that the main contribution is due to the Fe and Mn atoms, which have strongly hybridized states: the most intense DOS peaks formed by both Fe and Mn states coincide in terms of energy. Furthermore, we observe thata main contribution to those hybridized states is due to the Fe and Mn 3d states indicating the covalent character of their interaction. DOS of sp elements of Si, Ge, and Sn have contributed to the lower valence state and higher conduction state in both majority and minority spin bands. The Ga contribution to the total DOS is small i.e. Ga atoms form basically ionic bonds with surrounding atoms. Alloys are said to be true half metallic when value of SP is 100% and is achieved when any one of the DOS from majority and minority spins is equal to zero and other is not equal to zero at E_F. Now Fe_2MnSi shows half-metallic behavior where Fe_2MnGE and Fe_2MnSn are not fully half metallic. The calculated density of electronic states (DOS) for Fe_2MnGa alloy in $L2_1$-phase shows that spin up and spin down states are strongly polarized, since separate peaks of the up and down states . The calculated DOS of spin-up states at E_F is 1.009, while spin-down EF is 0.152. The minority spin band in Fe_2MnSi shows band gap of 0.5ev at EF. The minority spin band in Fe_2MnGe shows band gap of 0.45 eV at E_F. The minority spin band in Fe2MnSn shows band gap of 0.35ev at E_F.As this shows decreasing order at Fe_2MnSi>Fe_2MnGe>Fe_2MnSn. The calculated densities of electronic states for Fe2MnGA alloy is ferro- and ferromagnetic order. The DOS of Fe_2MnGe and Fe_2MnSN shows metallic and ferromagnetic behavior at majority spins.



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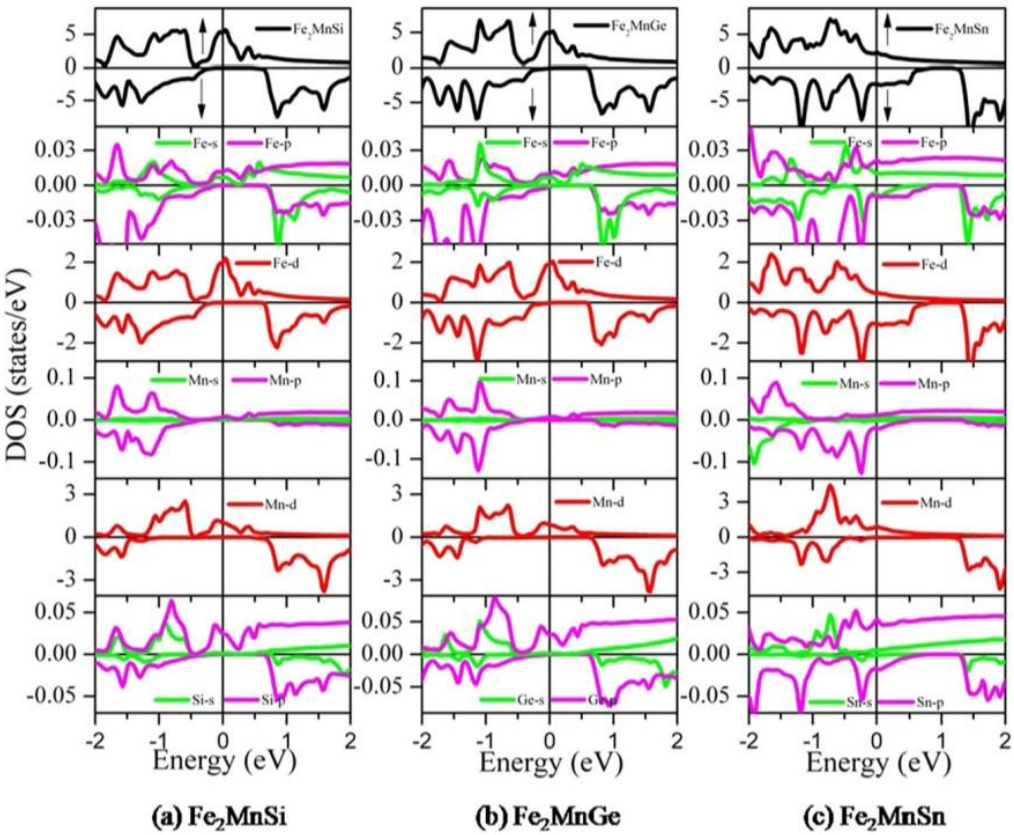

Optical Properties:-

In general, Optical properties of semiconductor materials are observed to exhibit a metal-like behavior at very low frequencies and insulator like at very high frequencies necessitating the study of optical properties with variation in the incident photon energy as has been done in the present work. The results are shown in fig. The main features of the optical absorption spectra are the high level of interband absorption peaks of interband absorption which are observed at different energy points for three alloys (Fe_2MnZ, Z= Si, Ge, and Sn) in the whole spectral range (0-13ev) studied, namely, infrared (IR) (1.24Mev to 1.7ev), visible (1.7 to 3.3ev), and UV (3.3 to 1.24ev). Overall, peaks of different optical Parameter are seen at a lower Photon energy range of energy for Fe_2MnSi. The existence of low-energy gaps in the band spectra of alloys (Fe_2MnZ, Z= Si, Ge, Sn) are correlated to the presence of peaks of these alloys are also found in the energy ranges corresponding to visible and UV parts of spectrum.

Optical conductivity spectra, fig shows that two major peaks are observed for the alloys Fe_2MnZn (Z= Si, Ge, Sn) in the energy range of 2-3 and 7-10ev. The value of Fe_2MnSn is the least among Fe_2MnZ and shifts towards lower energy side while Fe_2MnSi shows high energy points. This shows that of three alloys. Fe_2MnSn is least conductive in visible region.

The trend of reflectivity R (σ) as function of photon energy in fig indicates that all three samples how major peaks below 3ev in IR and visible light region and above 8ev in the UV region. The value of reflectivity is more than 50% for alloys in a range of energy between 0ev and 4ev and from 8ev onwards in the UV region.

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Trends of energy loss L (□) and absorption coefficient I (□) with the incident photon energy show that absorption coefficient and energy loss increase as incident photon energy increases. Maximum energy loss occurs have above 10ev in the UV region for the alloys with Fe_2MnSn shows highest energy loss. This implies that reflectivity is minimum at the point at which energy loss is maximum and vice-versa.

The complex dielectric function E (□) is E(□)= E_1(□)+iE_2(□)

Here E_1(□) and E_2(□) are real and imaginary parts of dielectric function related to the polarization and energy loss resp. and the characteristics freq. is called plasma freq. and defined as that freq. at which the real part of the dielectric function vanishes on E_1(□)=0. The values p of are in the order Fe_2MnSn>Fe_2MnGe>Fe_2MnSi. The peaks of the real and imaginary parts are found in the IR and visible region for alloys. Behavior of E_2 (□) for Fe_2MnSi, Fe_2MnGe, Fe_2MnSn alloys is identical with that of R (σ) with respect to incident photon energy. Negative values of E_1 (□) shows a metallic behavior of all three alloys in visible and UV regions. These alloys have potential for use in optical filters or shielding devices at different freq. region. The value of E_1 (□) shows energy absorption is high in the IR region.

Refractive index n (□) as a function of photon energy of all three alloys.Value of n (□) at zero frequency is 11.33, 11.47 and 11.00 for Fe_2MnSi, Fe_2MnGe and Fe_2MnSn resp. and decreases with increase in photon energy. Fe2MnSn shows lowest value of n (□) among the three at lower energy points from visible to UV region. In the IR region peaks of K (□) for Fe_2MnSi and Fe2MnGe overlap while those of Fe_2MnSn are at high energy.In visible and UV regions peaks of K (□) for Fe_2MnSi and Fe_2MnGE. The maximum value of K (□) is 4 for alloys and decreases with increase in photon energy toward UV region.

In XRD analysis shows in Fe_2MnGa addition to the fundamental [111, 200, 220, 311 and 222] diffraction lines a set of super structure diffraction peaks [100, 110, 210, and 211] clearly indicates the formation of ordered structure in the alloy Fe_2MnGa. At the sometime, as well as these diffraction lines, additional reflections at 2=44.05 and 99.27. Signify the presence of second phase. These can be assigned to the fundamental (220) and (440) reflection of A2-(Or B2 or L21 phase with lattice constant a=0.5808nm), with the volume fraction below 10%. The experimental lattice parameters of Fe_2MnGa HA for Fcc-(a=0.3701nm) and A2(B2 or L21)- phase (a=0.5808) are similar to the calculated parameters a=0.3644 or 0.666nm for fcc-phase or a=0.57nm for L21-Phase, are in good agreement with the data a=0.5685nm or a=0.5688nm. It should be mentioned here that the XRD spectrum as milled powder ofFe_2MnGa did not show any A2-phaserelatedpeaks.

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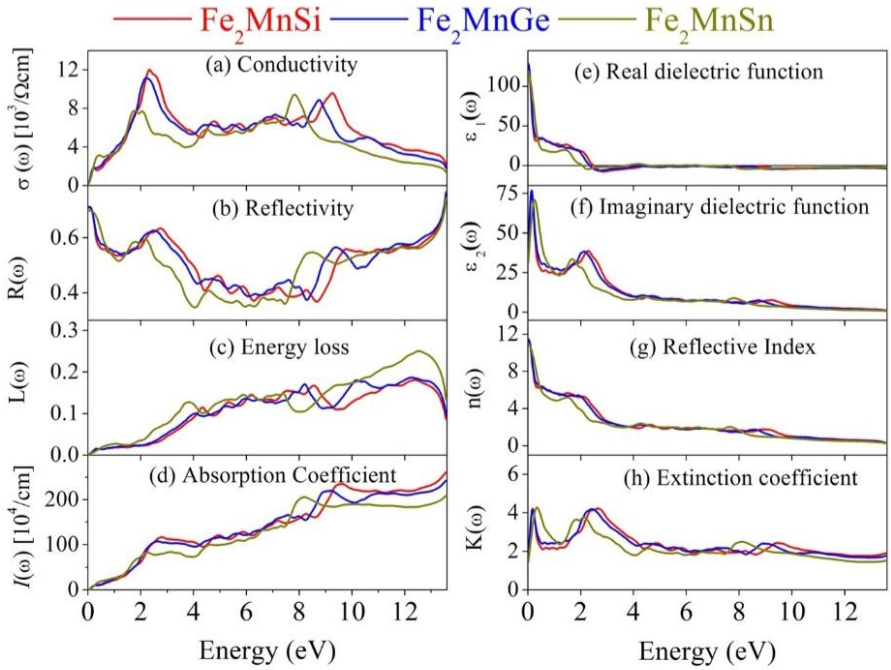

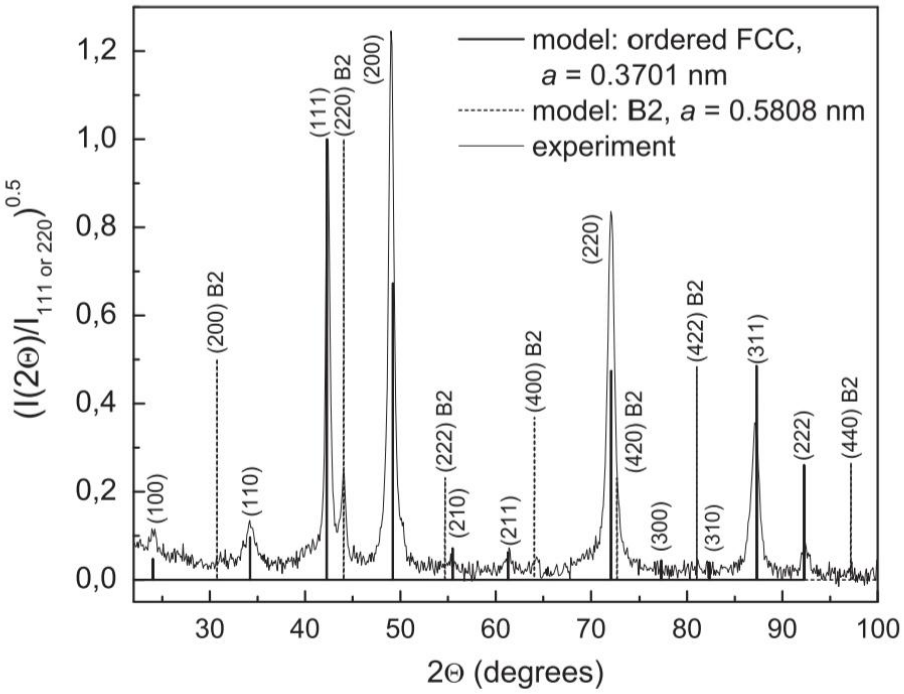

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Magnetic properties:-

The calculated value of total an individual moment for Fe_2MnZ is shown in table. Magnetic moment of Fe increases in the presence of Sn and is the same for Mn atom in all three alloys. While the magnetic moment of the Z-atom is negative and negligible.According to staler-Pauling curve. The magnetic moment per unit cell in multiples of Bohr magneton (μ_B) is given by M total=n-24.

Total and partial magnetic moment in terms of μ_B of Fe_2MnZ Heusler alloys

Sample	Total	2*Fe	Mn	Z
Fe_2MnSi	3.00	0.53	2.49	-0.01
Fe_2MnGe	3.00	0.38	2.61	-0.01
Fe_2MnSn	5.73	3.47	2.45	-0.07

Where N denotes valence electrons in the unit cell. For Fe_2MnZ, there are a total of 27 valence electrons in the unit cell of Fe_2MnZ. For this reason the magnetic moments are the expected from SPC is $3\mu_B$ for all three alloys. While the calculates magnetic moments are the same as that predicted by SPC Fe_2MnSn is 5.73. A calculation of the dependence of the magnetic moment on the value of the lattice constant makes the bend clear. To further explore this aspect we have calculated variation in total and partial magnetic moments with respect to $a_\circ$.

For range of $a_\circ$ from 5.30 to 5.85 Å the total magnetic of all three alloys is $3\mu_B$ and remain constant, which fallows the Slater-Pauling rule for full Heusler alloys. However variation in the individual magnetic moments of Fe and Mn are brought about due to the change in the separation on a change in the lattice constant which affects the interaction and thus hybridization 3d electron is present. Magnetic moment of Fe decreases while it increases for Mn with increase in lattice constant for all alloys. Magnetic moment of Z atoms remains almost zero and doesn't effectively contribute to the total Magnetic moment of Fe_2MSi becomes higher than $3\mu_B$ and does not follow the Slater Pauling rule and Fe moment starts to increases . Although we have plotted the magnetic moment for lattice constants higher than 5.85Å for Fe_2MnSn alone almost the same behavior is observed for Fe_2MnSi and Fe_2MnGe. However the equilibrium lattice constant for Fe_2MnSn is 6.01Å and is the reason that the calculated magnetic moment is much layer than that predicted by SPC . The sudden increase in the lattice parameter after 5.85Å is mainly due to the sharp increase in the moment of the Fe atom due to change in hybridization of the 3d electron brought about by the change in lattice parameter the majority and minority DOS with variation in lattice constant $a_\circ$ for Fe_2Mn(Si, Ge, Sn). The majority spin DOS at Fermi energy levels is almost the same for or 4.86μg at T=2k and $H=10^7$. Some what smaller than predicted by the calculation i.e 6.10μb, but nearly two times larger than that phase melt-spin stoichiometric Fe_2MnGA ribbon Ms=58 $emug^{-1}$ (at T=5K and H=5T). The origin of this discrepancy may be related partly to the degree of atomic disorder in our bulk sample and ribbons, as well as to the presence of some A2-(B2- or $L2_1$) phase with smaller magnetic moment [13,24,25]. At the same time insignificant device from stoichiometry weakly affects the saturation magnetization of Fe_2MnGa alloys near 2:1:1 stoichiometry Ms=93.8$emug^{-1}$ (at T=5k and H=13T).

On the other hand for these slightly off stoichiometric FeMnGa alloys, the magnetization hysteresis loop for 100≤T≤170K temperature ranges. Clearly show the presence of matersitic transformation from parent PMto matersitic FMphase. However, unlike the afford

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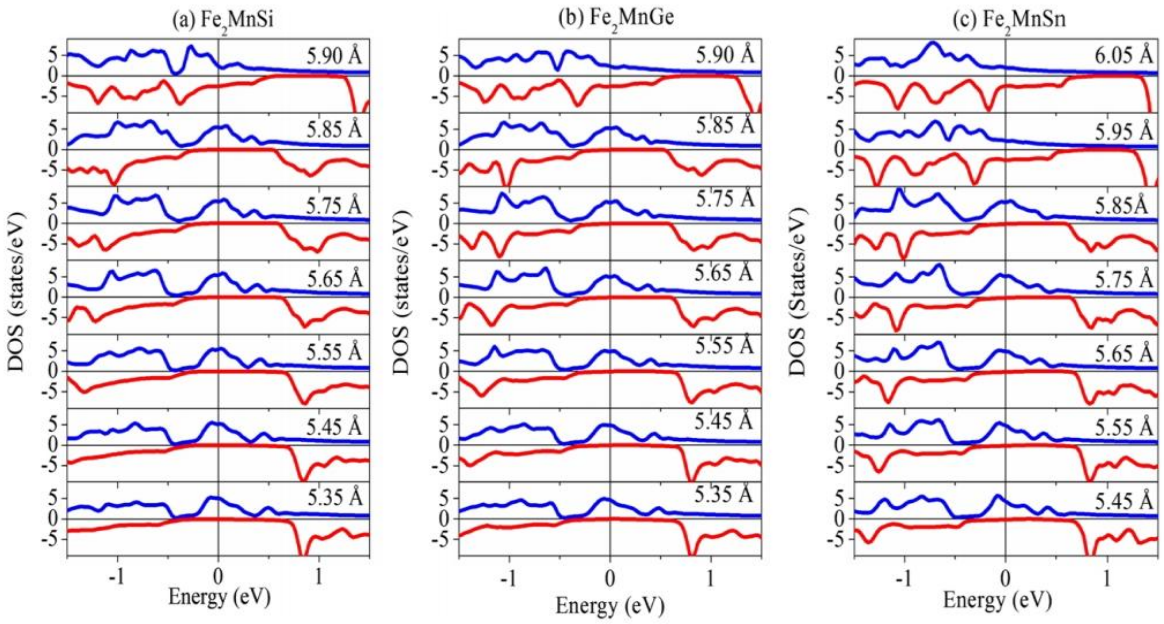
mentioned case, M(H) decencies For Fe_2MnGa bulk alloy do not show any traces of hysteresis in the 2-400K temperature range, indicating the assence of matersitic transformation.

The first peculiarity can be attributed to the FM-PM transition with Curie temperature 7C=800K all range of Lattice constants for all three alloys while it shift towards the valence state in minority spin DOS on decrease in the lattice constant. This indicates that all three alloys exhibit a semiconductor behavior at ranges of lattice constant lesser than the equilibrium lattice constant in theminority DOS.



The temperature dependence of magnetization of bulk Fe_2MnGA alloy taken at different magnetic field behave in a noticeably different way. At low magnetic field, the zero field cooled (ZFC) branch of the M(T) curve for Fe_2MnGa alloy rapidly inc. with temperature, intersecting the zero-line at T=60K. However at $emug^{-1}$ the field cooled (FC) M (T) curve combines two different regions with a decrease and increase in magnetization upon warning. At $emug^{-1}$ magnetization insignificantly increases with temperature. At rather high magnetic field $emug^{-1}$ the magnetization M(H) of Fe_2MnGa alloy behaves typically for ferromagnetic an inc. in temp. Curve a dec. in magnetization. The rapid inc. in magnetization at t=250K from nearly zero up to 29.2$emug^{-1}$on ribbon warning at $emug^{-1}$was attribute by the author to the meta-magnetic transformation in the alloy from AFM to FM phase. No structural transformation at this temperature was observed. The AFM to FM transition in the ribbon is evidenced by the change in the field dependence of magnetization M(H) i.e. an appearance of the linear part of the M(H) curve within the AFM region and its asymmetry with respect the origin.

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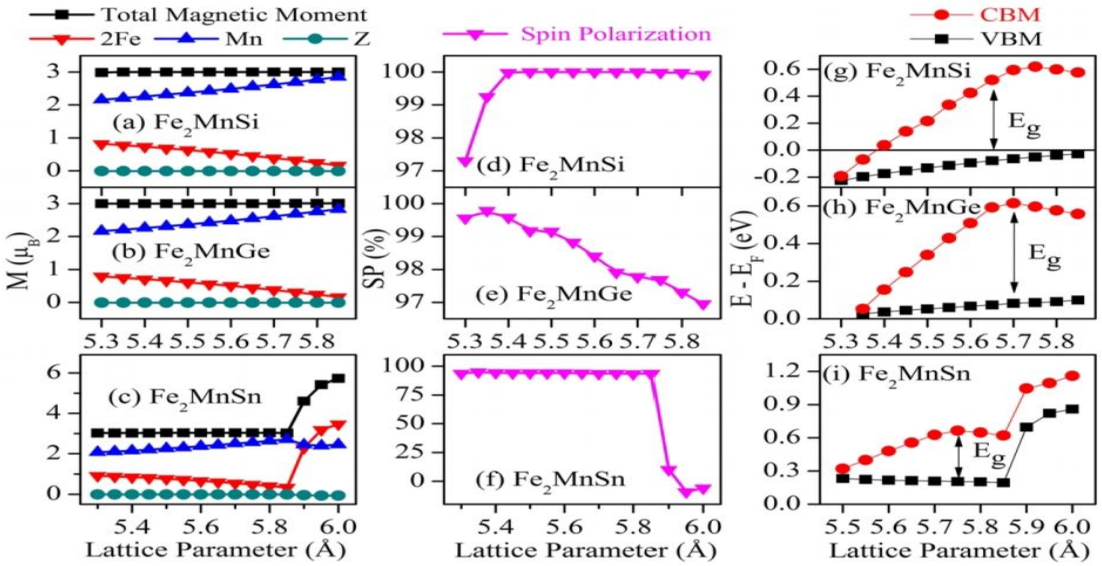

The FC temperature dependence of magnetization of our bulk Fe_2MnGa alloy obtained for $emug^{-1}$ consist of two clear parts i.e. decrease and increase in magnetization with increase in temperature. Such behavior can be explained by different magnitudes and M(T) dependencies of Fcc and Bcc type ordered phases in the alloy. Indeed according to the results of our calculation the magnetic moment of the FM FCC-phase is more than three times large than that of the $L2_1$ phase, At higher there as the M(T) dependence of the BCC ordered impurity phase is masked by the M(T) of the dominant parent phase. The experimental value of the saturation magnetization of our bulk Fe_2MnGa alloy.

Conclusion:

1- This study shows that the total magnetic moment of Fe_2MnZ (Z=Si, Ge, Sn, Ga) remains $3\mu_B$.
2- Good optical conductivity and reflectivity in various regions of the electromagnetic spectrum are observed in these alloys.
3- They show dielectric to metallic transition which has a potential for use in optical filters and photo electronics devices.
4- FeMnGa with a curie temperature of Tc=800K and a saturation magnetization of $4,86\mu_B$ F,U-1 crystallizes in the FCC ordered lattice of $L1_2$.

References:

1- Yin, M., Nash, P., Chen, S.: Enthalpies of formation of selected Fe2YZ heusler compounds. Intermetallics 57, 34-40 (2015)
2- Graf T, Felser C, Parkin SSP. Prog Solid State Chem 2011;39(1)
3- Kokorin VV, Martynov VV, Chernenko Va. Scr Metal Mater 1992;26:295
4- Galanakis I, Dederichs PH, Papanikolau N. Phys Rev B 2002;66174429

eISSN 1303-5150

5- Kikalj A. Comput Mater Sci 2003;28:155
6- Thee JY. J Korean PhysSoc 2003;43:792
7- Blaha P, Schwarz K, Madsen GKH, Kvasnicka D, Luitz J. WIEN2k, an augmented plane wave + local orbitals program for calculating crystal properties. Karl-heinz Schwarz, Techn. UniversitAat Wien, Wien; 2001.
8- M. Pugaczowa-Michalska, A. Go, L. Dobrzynski, Phys. Status Solidi B 242 (2) (2005) 463.
9- S.M. Azar, B.A. Hamad, J.M. Khalifeh, J. Magn. Magn. Mater. 324 (2012) 1776–1785
10- A.H. Reshak, Z. Charifi, H. Baaziz, , J. Magn. Magn. Mater. 326 (2013) 210–216.
11- D. Nanto, D.-S. Yang, S.-C. Yu, Physica B 435 (2014) 54–57
12- K.M. Wong, S.M. Alay-e-Abbas, Y. Fang, A. Shaukat, Y. Lei, J. Appl. Phys. 114 (2013) 034901.
13- W. Kohn, L.J. Sham, Phys. Rev. A 140 (1965) 1133
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eISSN 1303-5150