IOP Publishing Physica Scripta
Phys. Scr. 95 (2020) 065803 (5pp) https://doi.org/10.1088/1402-4896/ab7bea

Electronic, magnetic, reentrant and spin compensation phenomena in Fe_2MnGa Heusler alloy

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Received 22 December 2019, revised 28 February 2020
Accepted for publication 3 March 2020
Published 20 March 2020

Abstract

First principles calculations of structural and magnetic properties of the Fe_2MnGa Heusler alloy with face-centered cubic, have been studied using a full potential linearized augmented plane wave within the density-functional theory. Partial and total magnetic moments of Fe, Mn and Ga have been determined as well the bulk modulus using the generalized gradient approximation proposed by Wu and Cohen. Ferromagnetic interactions between next-nearest neighbors, (Fe-Fe, Mn-Mn; $J_{Fe\text{-}Fe} > 0$ and $J_{Mn\text{-}Mn} > 0$) in addition to the ferrimagnetic Fe-Mn ($J_{Fe\text{-}Mn} < 0$) within FMG Heusler alloy are considered. Fe_2MnGa exhibits spin compensation temperatures and a first-order reentrant behavior. The studied system undergoes a first-order phase transition between an ordered ferrimagnetic to a paramagnetic. Transition T_C, compensation T_{Comp} and first order phase transition, T_t points have been determined using Monte Carlo simulation; they are around 750, 400, 684 K, respectively. Magnetic hysteresis cycle has been found for different temperatures; it has been 190, 210 and 230 K.

Keywords: Fe_2MnGa heusler alloy, DFT, monte carlo simulation, first-order reentrant behavior and magnetic hysteresis cycle

(Some figures may appear in colour only in the online journal)

1. Introduction

Heusler materials are used in the electronics industry and in various current technical applications such as sensors, actuators, as spintronic materials, ferromagnetic shape memory alloy, energy conversion, etc [1–5]. Several materials with Heusler type structure present a half-metal features [6, 7]. Electronic structure and magnetic properties of different heuslers materials are investigated by [8]. In other hand, theoretically [9] and experimentally [10, 11], show that the L_{12}-type structure is the stable configuration with group space Pm3m. It has been shown that, unlike most Heusler stoichiometric alloys, bulk Fe_2MnGa crystallizes in the face-centered cubic lattice of the L_{12} (Cu_3Au) type with a transition temperature of 800 K [9].

The magnetic moment of Fe_2MnGa is 2 μ_B (μ_B is Bohr magneton) [12, 13] and it is interesting to look for its magnetic properties at low temperature and to compare them with the theoretical results. In previous works, the magnetic and electronic properties of Ni_2MnGa [14] and Mn_2NiAl [15, 16] compounds, have been investigated. The physical properties of Zr_2MnIn and Zr_2MnGa are studied using density functional theory (DFT) based first principle calculations [17, 18]. In recent work [19], ground state total energy calculations confirms the structural stability of anti-ferromagnetic phase of Zr_2MnAl over ferromagnetic phase.

Table 1. Calculated lattice parameter, bulk modulus and values of exchanges interactions of Fe_2MnGa Heusler.

Fe_2MnGa Heusler	a (Å)	B (GPa)	$J_{Fe\text{-}Fe}$(K)	$J_{Fe\text{-}Mn}$(K)	$J_{Mn\text{-}Mn}$(K)
Our results	3.60	207.232	+63.2	−53.3	+69.3
Experimental	3.697 [4], 3.701 [8]	—	—	—	—
Theoretical	3.644 [21]	—	—	—	—

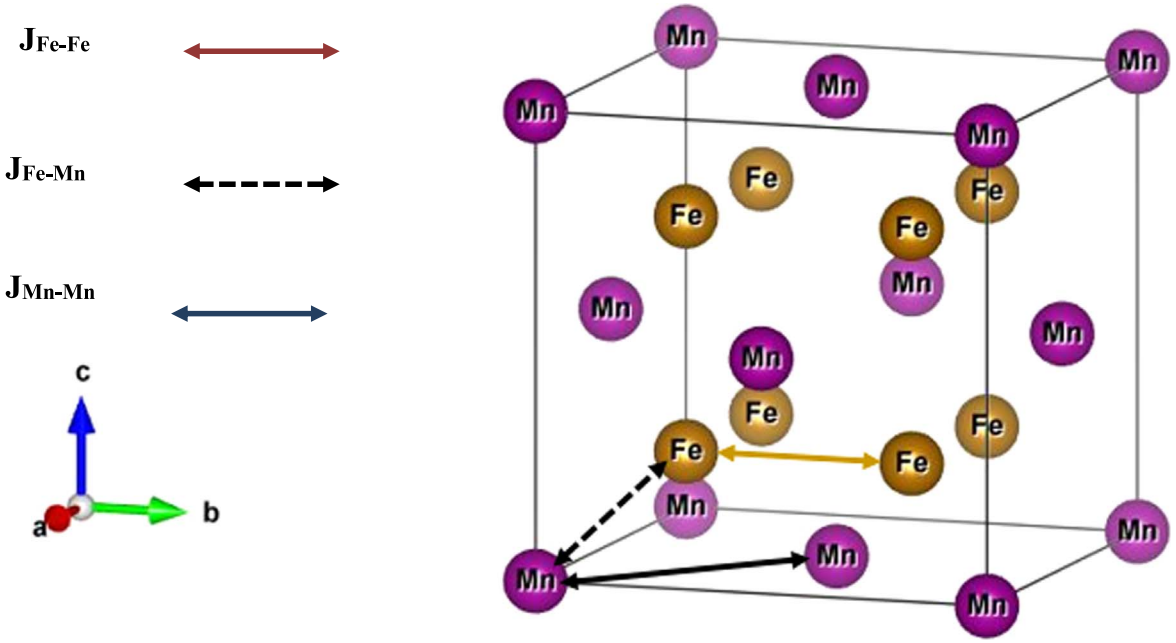

Figure 1. Fe_2MnGa Heusler alloys.

In the present work, the electronic and magnetic properties of Fe_2MnGa heusler have been investigated using full potential-linearized augmented plane wave (FP-LAPW) method and Monte Carlo simulation.

The paper is organized as follows: sections 2, 3 and 4 describe the calculations method, the adopted model and Monte Carlo simulations respectively. 5 presents the results and discussion and conclusion is given in section 6.

2. *Ab initio* calculations

The FP-LAPW method [20] performing DFT calculations was used to calculate the structural and magnetic properties of Fe_2MnGa Heusler alloy using the local density approximation. FP-LAPW method is used to evaluate the Kohn–Sham equation and energy functional. The space was divided into interstitial and non-overlapping muffin mold spheres centered on the atomic site. The basic function used within each atomic sphere was considered as a linear expansion of the radial solution of a spherical potential multiplied by spherical harmonics. The wave function was taken as an expansion of the plane waves and no potential shape approximation was introduced in the interstitial region, which is consistent with the full potential method. The muffin-tin radii R_{MT} were assumed to be 1.98, 1.85 and 2 a.u for Fe, Mn and Ga, respectively. The plane wave cut off of $K_{\max} = 8.0/R_{MT}$ (R_{MT} is the smallest muffin-tin radius) is chosen for the expansion of the wave functions in the interstitial region, while the charge density was Fourier expanded up to $G_{\max} = 12\ (R_{yd})^{1/2}$. The number of special k points in the irreducible Brillouin zone is 10^4. To ensure proper convergence of the self-consistency calculation, the calculated total energy of the crystal converged to less than 0.1 mRy. The results of crystalline structure parameters for e Fe_2MnGa Heusler of interest are compared with the available experimental and theoretical predictions in table 1.

3. Model and monte carlo simulation

The Hamiltonian of Ising with external magnetic field h is given by:

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j - h\sum_i S_i \qquad (1)$$

where $\langle i, j\rangle$ stands for the first and second nearest neighbor sites (i and j). S_i(or S_j) spins moments and take the values $S_{Fe} = 1$ and $S_{Mn} = 3/2$. The J_{ij} is the exchange interactions can take $J_{Fe\text{-}Fe}$, J_{FeMn} and $J_{Mn\text{-}Mn}$ as given in figure 1. The values of exchange interactions and magnetic moments are obtained by *Ab-initio* calculations and are given in table 1.

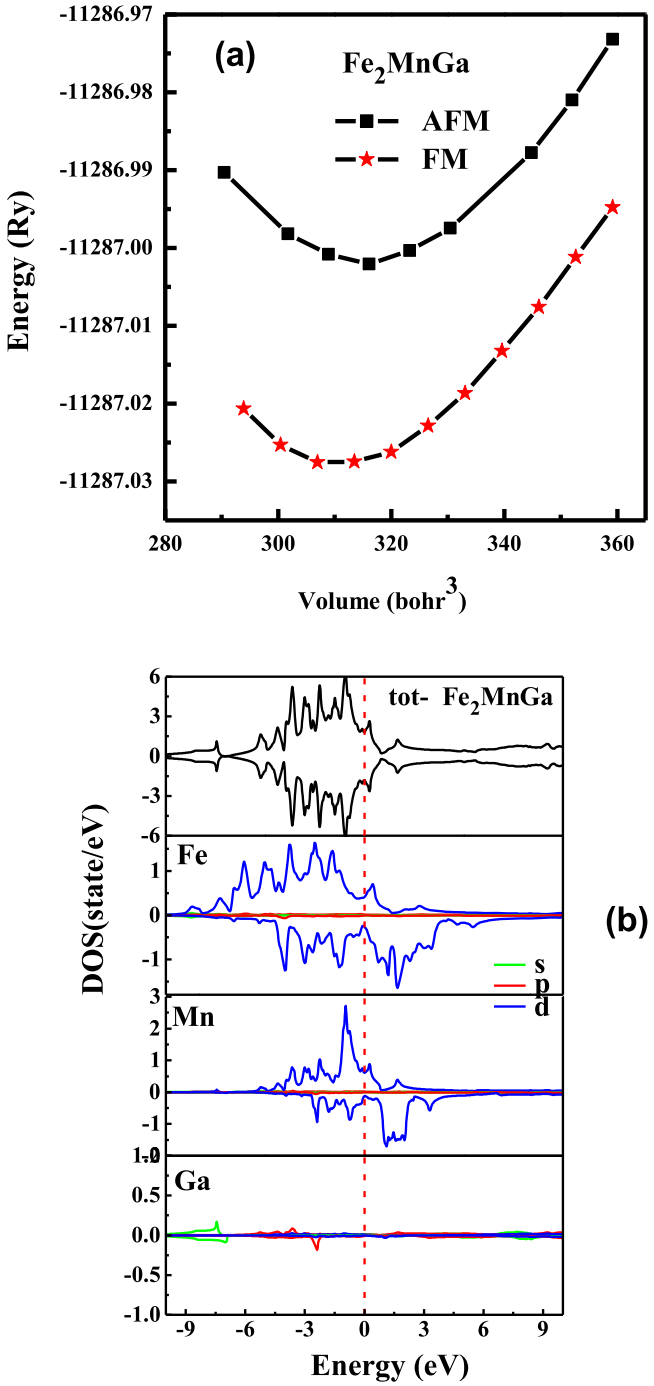

Figure 2. Energy optimization (a) and total and partial densities of state (b) for Fe_2MnGa Heusler.

4. Monte carlo simulations

Monte Carlo is a computational method that uses random sampling to characterize the system behavior. This methodology is helpful when the system characteristics are unknown or there is no practical solution through deterministic methods [21]. The Fe_2MnGa Heusler is assumed to reside in the unit cell and the system consists of the total number of spins $N = 2xN_{Fe} + N_{Mn}$ with $N_{Fe} = 4096$ and $N_{Mn} = 2048$. The Monte Carlo simulations are applied to model the Hamiltonian. In this section, the cyclic boundary conditions is used on the lattice. The flips are accepted or rejected according to a heat-bath algorithm under the standard Metropolis approximation.

Internal energy per site E is,

$$E = \frac{1}{N}\langle H \rangle \tag{2}$$

The total magnetization of Fe_2MnGa Heusler is given by:

$$M = \left\langle \frac{1}{N}\sum_i S_i \right\rangle \tag{3}$$

The total magnetic susceptibility of Fe_2MnGa Heusler is defined as:

$$\chi = \frac{N_{Fe}\chi_{Fe} + N_{Mn}\chi_{Mn}}{N_{Fe} + N_{Mn}} \tag{4}$$

with

$$\begin{aligned} \chi_{Fe} &= \beta(\langle M_{Fe}^2 \rangle - \langle M_{Fe} \rangle^2) \\ \chi_{Mn} &= \beta(\langle M_{Mn}^2 \rangle - \langle M_{Mn} \rangle^2) \end{aligned} \tag{5}$$

where $\beta = \frac{1}{k_B T}$, k_B denotes the Boltzmann constant which is fixed at its unit value, in this work.

5. Results and discussion

Obtained data from *Ab initio* calculations are used as input for the Monte Carlo simulations to compute other magnetic parameters. The stability of the magnetic phase (Ferromagnetic, FM and antiferromagnetic, AFM) of bulk face centered cubic structure with space group Pm-3m (No. 123) for FMG is studied in this section. The optimization of energy in both magnetic configurations FM and AFM using first principal calculations is illustrated in figure 2(a). It is evident that the FM configuration has a low energy than AFM configuration which indicates that the FM is more stable, which in good agreement with the experimental results reported by [9]. On the other hand, the experimental results indicated that the Fe_2MnGa heusle has a large curie temperature around 750 K and that FM-to-AFM phase transformation occurred at room temperature [4]. The calculated values of lattice parameter and bulk modulus compared with other theoretical and experimental values, are given in table 1 [4]. It is clear that the obtained values for lattice parameter are underestimated then experimental and theoretical results reported in the literature, while no values for bulk modulus have been not reported in the literature and thereby can be used as reference for future studies.

The calculated values of total and local magnetic spin moment of the face-centered-cubic ferromagnetic Fe_2MnGa Heusler are reported in table 2, while including some theoretical and experimental data from literature. The total spin magnetic moments (M_{tot}) of the considered compounds, which satisfies a Slater–Pauling type rule proposed by Galanakis and Dederichs [8], for localized magnetic moment systems $M_{tot} = Z_t - 24$, where Z_t is the number of valence electrons in the primitive cell. The obtained value of total

Table 2. Calculated of magnetic moment and spin polarization in Fermi level.

Fe_2MnGa Heusler	M_{Fe} (μ_B)	M_{Mn} (μ_B)	M_{Ga} (μ_B)	M_{tot} (μ_B)	P %
Our results (*Ab initio* calculations)	1.820	2.004	−0.02	5.82	0.089
Experiment [9]	—	—	—	4.86	—
Theoretical [9]	1.97	2.292	−0.092	6.01	0.089

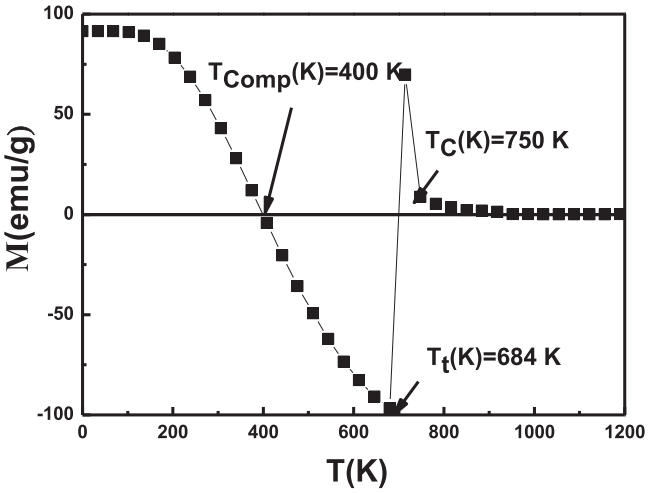

Figure 3. Temperature dependence of magnetization, M(T), calculated in a magnetic field of h = 0 T for Fe_2MnGa Heusler compound.

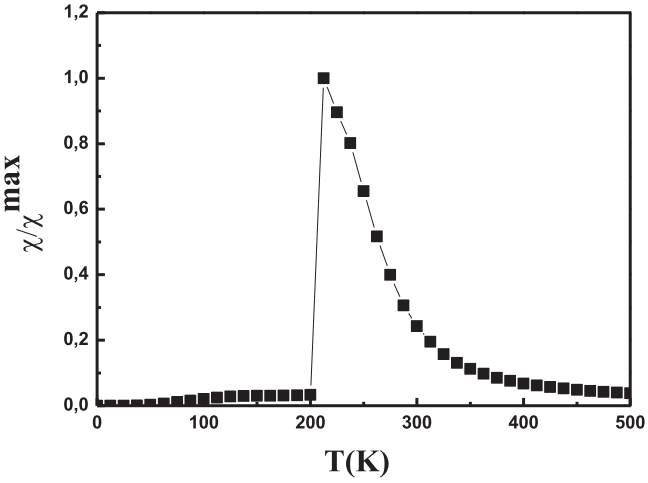

Figure 4. Temperature dependence of normalize magnetic susceptibility, χ/χ^{max}, calculated in a magnetic field of h = 0 T for Fe_2MnGa Heusler compound.

magnetic moment by GGA-08 is 5.82μ_B, whereas the obtained value from Slater–Pauling is 2 μ_B. This difference is due: in our case, we choose the spins are ferrommagnetic but in Slater–Pauling type rule proposed by Galanakis they choose the spins ferrimagnetic. Our value is near to that obtained by experiment results 6.107 μ_B with face-centered cubic lattice [9]. On the other hand, the values for local magnetic moment of (Fe, Mn and Ga) are underestimated in comparison to the theoretical [8] and overestimated than other experimental values [4, 22]. In table 2, it can be noted that the majority contribution in magnetic moment is given in the first

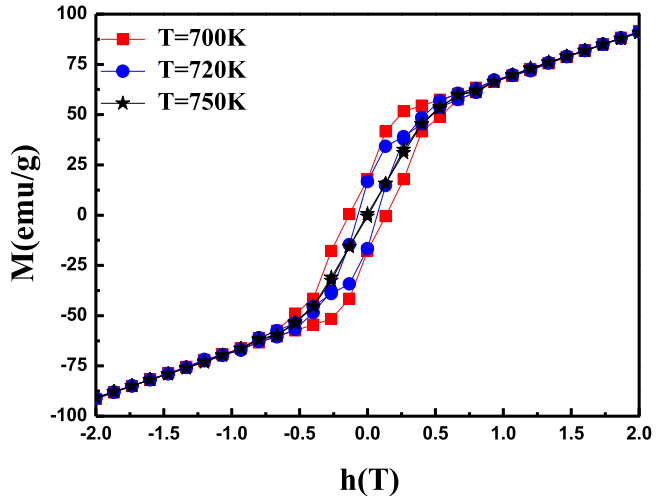

Figure 5. Magnetic hysteresis cycle of Fe_2MnGa Heusler compound with different temperatures T = 190, 210 and 230 K.

Table 3. The obtained values of h_C, M_r a several temperatures T = 700, 720 and 750 K.

Temperatures T(K)	700	720	750
h_C(T)	13.21	6.84	0.53
M_r(T)	0.56	0.53	0.02

order from the Mn atom. Fe atom has the second contribution, while the Ga atom has a very high low contribution. The total and partial densities of states (DOS) of Fe_2MnGa Heusler spin directions are displayed in figure 2(b), where all energies are relative to respective Fermi level. It can be seen that DOS has a very small inhomogeneity between the up and down spins and the s and p states of the Ga atom have a very small contribution in the upper valence band. The bottom of the valence band is occupied only by the state s of Ga included. In the case of X_2YZ Heusler, the state s-Z is generally located in the lowest energy band of the state d of the transition metal atoms (X and Y), which is important because they accept the charges of transition metal atoms, thus effectively reducing d electrons and resulting in the stability of the crystal structure [9]. The main contribution of the resulting DOS comes mainly from the 3d hybridization of Fe and Mn atoms. It is clear that the Fermi level of this compound in the majority spin configuration is almost entirely occupied by the 3d states of the transition metal atoms, with the majority contribution coming from the Fe state, so the strong 3d hybridization −3d is presented in the Fermi Level, indicating that this material has a metallic character in this direction and the Fermi level in

the minority spin configuration exhibited 3d-3d interaction, so that the Fe_2MnGa Heusler is a metal.

The thermal total magnetization is given in figure 3 for a zero magnetic field. The nature of the magnetic phase transition is of second order. The paramagnetic to ferrimagnetic phase transition is observed at transition temperature $T_C = 750$ K. The obtained value of T_C is comparable with that given in [9, 11]. In figure 3, the compensation temperature (i.e., temperatures below the critical point for which the total magnetization is zero while the individual system remain magnetically ordered [22]) and first order phase transition (corresponds to a transition temperature when the system toward from the ordered phase to the disordered phase [23]), the points are noted as $T_{Comp} = 400$ K and $T_t = 684$ K, respectively. It can be observed the appearance of a reentrant phenomenon at $T = T_t$, which is similar to that found in previous works [24, 25]. The compensation temperature appears only due to the different dependences on temperature of the two magnetic atoms Fe and Mn with the magnetizations M_{Fe} and M_{Mn} and does not exhibit any special singularity.

The peak of magnetic susceptibility is situated at the compensation temperature and first order phase transition and transition points corresponding to a transition temperature are deduced from the temperature dependence of magnetization such as given in figure 4. The values obtained are the same as those found in figure 3.

The magnetic hysteresis cycle of Fe_2MnGa Heusler is shown in figure 5 for different temperatures value.

The values of coercivity, h_C, and remanence, M_r, are deduced for different temperatures value (see table 3).

In the previous works [26–28], the monotonic decrease observed on coercivity and remanence generally corresponds to the previously predicted dependencies observed experimentally and may be due to the coexistence of blocked and unblocked particles. The presence of superparmagnetism behavior due to coexistence with thermal fluctuations and also with blocked grains linked to a complex crystal structure of this system.

6. Conclusions

In this study, the magnetic moments carried by Fe, Mn and Ga atoms in Fe_2MnGa Heusler were computed using FP-LAPW calculations and were revealed in accordance with the values previously reported. A detailed study of the spin compensation and reentrant phenomena of Fe_2MnGa Heusler compound has been performed. First order phase transition was revealed, which is due to a reentrant phenomenon produced by the sudden inversion of the magnetic moments, as manifested by the total magnetization. First-order phase transition between an ordered ferrimagnetic phase to a paramagnetic phase was evidenced around the transition temperature. The magnetic coercive field and remanent magnetization were found to decrease with the rise temperature. The superparamagnetic behavior was found at first order phase transition point.

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