Theoretical design of tetragonal rare-earth-free alloys with high magnetisation and high magnetic anisotropy

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1. Introduction

The high-performance permanent magnet is widely used in various industrial applications, including in motors for electric vehicles, power generators in wind turbines, and hard disk drives. The development of a new rare-earth free permanent magnet is important due to the cost and limited availability of rare-earth elements. Mn–Ga alloys such as L10-MnGa and D022-Mn3Ga have been attracting much attention as candidates for spintronic materials and rare-earth-free permanent magnets because of their high uniaxial magnetic anisotropy and Curie temperature exceeding 700 K.1–3 Moreover, a high saturation magnetisation is required for the application of permanent magnets. However, the saturation magnetisation of D022-Mn3Ga is small due to ferrimagnetic ordering. We investigated the possibility of developing ferromagnetic Heusler alloys with high magnetic anisotropy and saturation magnetisation using the first-principles calculation. We focused on the effects of Fe substitution for Mn in D022-Mn3Ga as well as the consequent volume expansion; the ferromagnetic tetragonal XA phase is stabilized in Fe2MnGa by an 8% volume expansion. This tetragonal XA-Fe2MnGa has desirable properties for a high-performance permanent magnet, such as high magnetisation (1350 emu cc−1) and perpendicular magnetic anisotropy (2.12 MJ m−3) and Curie temperature (1047 K). In addition, the substitution of Sn and increasing the Ga composition in the Fe2MnGa alloy results in volume expansion, which stabilizes the ferromagnetic tetragonal XA phase.

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2. Material and methods

We investigated the relationship between the ferrimagnetic and ferromagnetic formation energies and volumes for D022-Mn3Ga, Mn3FeGa, and Fe2MnGa, by first-principles density-functional calculations using the Vienna ab-initio simulation package based on the plane-wave basis set and projector augmented wave method.16 We adopted a generalised density gradient approximation (GGA) parameterised by Perdew, Burke and Ernzerhof (PBE) for the exchange-correlation potential.17 The cut-off energy of the plane-wave basis set was 500 eV. A 12 × 12 × 12 k-point mesh was employed for Brillouin zone integrations. The formation energy of Mn3–FeGa alloys is given as

\[ E_f = E_{Mn_3-FeGa} - (3 - x)E_{Mn} - xE_{Fe} - E_{Ga}, \]

where \( E_{Mn_3-FeGa} \) is the total energy of the Mn3–FeGa alloys per formula unit; \( E_{Mn}, E_{Fe}, \) and \( E_{Ga} \) denote the total energies of the bulk Mn, bcc-Fe, and α-Ga per atom, respectively. The magnetic anisotropy energy (MAE) values were estimated based on the magnetic force theorem18 using a 24 × 24 × 24 k-point mesh.

In addition, we evaluated the Heisenberg exchange coupling parameter \( J_{ij} \) between the magnetic atoms as a function of volume using the Liechtenstein formula19 with the spin-polarized relativistic Korringa–Kohn–Rostoker code.20 The angular momentum cut-off was set at 4 in the multiple scattering expansion. We used a 15 × 15 × 15 k-point mesh and 50 energy points on the complex energy path for the self-consistent calculation. We adopted a GGA-PBE for the exchange-correlation potential. A fine k-mesh with 34 × 34 × 34 k-points was adopted for the evaluation of the exchange coupling parameters. The Curie temperature was ordering by substituting Fe for Mn in Mn3Ga and volume expansion.

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estimated from the exchange coupling parameters in the framework based on the mean-field approximation (MFA) for multi-sublattice systems.21,22

Furthermore, we also investigated the stable structure and magnetic property of the Ga-rich Fe2MnGa compound using a supercell approach. To simulate the off-stoichiometric compound, we constructed a 40 atom “special quasi-random structure” (SQS)23 to model the off-stoichiometric Fe2MnGa compound. The SQSs used in this work were generated using the “alloy theory automated toolkit” package.24

3. Results
First, we evaluated the formation energies (\( E_f \)) of the ferromagnetic and ferrimagnetic states in the tetragonal Heusler structure. A tetragonal \( X_2YZ \) Heusler compound can have a regular (\( L_21 \)) or inverse (\( XA \)) Heusler structure, as shown in Fig. 1. Figures 2(a)–2(e) show the volume dependence of \( E_f \) for Mn3Ga, Mn2FeGa, and Fe2MnGa with the tetragonal Heusler structures. For Mn3Ga, the \( E_f \) difference is defined as \( \Delta E_f = E_f(\text{ferro}) - E_f(\text{ferri}) \), where \( E_f(\text{ferro}) \) and \( E_f(\text{ferri}) \) denote the formation energies in the ferromagnetic and ferrimagnetic states, respectively, and the value is 0.39 eV f.u.\(^{-1}\) at the equilibrium volume of each magnetic structure. This value is relatively larger than the elastic energy, and therefore, it is difficult to stabilize the ferromagnetic state of the \( DO_{22} \) structure by volume modulation alone [see Fig. 2(a)]. In Mn2FeGa, the \( \Delta E_f \) values are -0.02 and 0.33 eV f.u.\(^{-1}\) for the \( L_21 \) and \( XA \) structures, respectively.

In the \( L_21 \) structure, the ferromagnetic state becomes stable, but the \( L_21 \) structure is energetically unfavourable as compared with the \( XA \) structure for all the volumes studied here. A discontinuous point is seen in the energy-volume curve of the ferromagnetic \( L_21 \) and \( XA \) phases, as shown in Figs. 2(b), 2(c), which is attributed to the transition from the low-spin to high-spin ferromagnetic phase. The magnetisation is enhanced from 6.16 (5.83) to 7.37 (8.49) \( \mu_B \) f.u.\(^{-1}\) for the \( L_21 \) (\( XA \)) phase at these points. For Fe2MnGa, the \( \Delta E_f \) values are 0.19 and -0.14 eV f.u.\(^{-1}\) for the \( L_21 \) and \( XA \) structures, respectively, and the ferromagnetic \( XA \) phase has formation energy of 0.01 eV f.u.\(^{-1}\), and it is more stable than the ferrimagnetic \( L_21 \) phase. In the ferromagnetic \( XA \) phase, the magnetic moments of the A site Fe, C site Mn, and B site Fe are 2.19, 2.80, and 2.30 \( \mu_B \), respectively, and the magnetisation reaches 1350 emu cc\(^{-1}\).

The tetragonal \( L_21 \)-Mn2FeGa and \( XA-Fe_2MnGa \), wherein the Fe atom occupies the B site, favour the ferrimagnetic state over the ferrimagnetic state. Table I shows the \( J_{ij} \) between the nearest-neighbour magnetic atoms at the A(C) site and the B site. When Mn occupies the B site, the \( J_{ij} \) values are negative, and the ferrimagnetic spin alignment becomes stable. Conversely, the \( J_{ij} \) values become positive when Mn is replaced with Fe at the B site, and the ferrimagnetic spin alignment becomes energetically favourable.

Next, we compared the \( E_f \) and magnetisation of several crystal structures of Mn2FeGa and Fe2MnGa (see Table II). For Mn2FeGa, the ferrimagnetic state in the tetragonal \( XA \) structure is the most energetically favourable, as mentioned in a previous theoretical report.25 For Fe2MnGa, the ferrimagnetic state in the cubic \( L_21 \) structure becomes the most energetically favourable. In the previous theoretical report, the ferromagnetic \( L_21 \) structure becomes more stable than the \( L_21 \) structure.26 However, the \( E_f \) difference between the tetragonal \( XA \) structure with ferromagnetic ordering and the cubic \( L_21 \) structure is very small, 0.016 eV f.u.\(^{-1}\). Figure 3 shows the volume dependence of \( E_f \) for Fe2MnGa with several crystal structures. The equilibrium volumes are 46.09, 48.05, and 49.76 Å\(^3\) f.u.\(^{-1}\) for the cubic \( L_21 \), tetragonal \( L_21 \), and tetragonal \( XA \) structures, respectively, which are different. The ferromagnetic \( XA \) phase is stabilized by the 8% volume expansion from the equilibrium volume of the cubic \( L_21 \) phase. The data in Table II reveal that the \( E_f \) of the ferromagnetic \( DO_{19} \) phase is also close to that of the cubic \( L_21 \). Experimental evidence for bcc to the ferromagnetic hexagonal phase transformation upon thermal annealing has been reported.27

Afterward, we evaluate the Curie temperature and MAE of the tetragonal \( XA-Fe_2MnGa \) compound. The Curie temperature obtained for the \( XA-Fe_2MnGa \) by MFA is 1047 K, which
Table I. Exchange coupling constant, $J_{ij}$, between the nearest-neighbour magnetic atoms for the tetragonal $L_2_1$-$\text{Mn}_2\text{FeGa}$ and $X\text{A}$-$\text{Fe}_2\text{MnGa}$. Positive (negative) $J_{ij}$ denotes ferromagnetic (anti-ferromagnetic) coupling.

| Structure              | $I$ | $J$ | $J_{ij}$ (meV) |
|------------------------|-----|-----|---------------|
| $L_2_1$-$\text{Mn}_2\text{FeGa}$ | Mn(A) | Fe(B) | 7.0 |
| $X\text{A}$-$\text{Mn}_2\text{FeGa}$ | Mn(A) | Mn(B) | -20.4 |
| $L_2_1$-$\text{Fe}_2\text{MnGa}$ | Fe(A) | Mn(B) | -1.5 |
| $X\text{A}$-$\text{Fe}_2\text{MnGa}$ | Fe(A) | Fe(B) | 29.5 |
|                         | Mn(C) | Fe(B) | 3.0 |

is much higher than that for $D0_{22}$-$\text{Mn}_3\text{Ga}$ (730 K). This high Curie temperature is predominantly attributed to the strong ferromagnetic exchange coupling (29.5 meV) between the Fe atoms at the A and B sites (Table I). A high perpendicular MAE of 2.12 MJ m$^{-3}$ is also obtained for $X\text{A}$-$\text{Fe}_2\text{MnGa}$; however, this value is slightly smaller than that for the $D0_{22}$-$\text{Mn}_3\text{Ga}$ (2.80 MJ m$^{-3}$). Additionally, we evaluate the contribution from each constituent atom to the MAE. In $D0_{22}$-$\text{Mn}_3\text{Ga}$, the MAEs of the Mn atom at the A (C) (4d) site and the B (2b) site are evaluated as 0.37 and 0.05 meV atom$^{-1}$, respectively, which agree well with the results of previous first-principles calculations.28) For $X\text{A}$-$\text{Fe}_2\text{MnGa}$, the MAEs of the Fe atom at the A site and the Mn atom at the C site are 0.23 and 0.31 meV atom$^{-1}$, respectively, which are much larger than that of the Fe atom at the B site (0.04 meV atom$^{-1}$). In both $D0_{22}$-$\text{Mn}_3\text{Ga}$ and $X\text{A}$-$\text{Fe}_2\text{MnGa}$, the perpendicular MAE predominantly originates from the Mn and Fe atoms at the A and C sites. However, the MAE from the A-site Fe in $X\text{A}$-$\text{Fe}_2\text{MnGa}$ is smaller than that from the A-site Mn in $D0_{22}$-$\text{Mn}_3\text{Ga}$.

4. Discussion

Volume expansion is necessary for the stabilization of the tetragonal $X\text{A}$-$\text{Fe}_2\text{MnGa}$ compound. We focus on the effect of substituting the Ga atom with other typical elements having a large atomic radius. Figure 4 shows the volume dependence of $E_r$ for $\text{Fe}_2\text{MnGa}_{0.75}\text{Sn}_{0.25}$, where 25% of the Ga atoms are replaced by Sn atoms. The equilibrium volume of the cubic $L_2_1$ and tetragonal $X\text{A}$ phases expands by 4.1% and 3.6%, respectively, due to the Sn substitution. Due to the lattice expansion, the $E_r$ of the ferromagnetic state in the tetragonal $X\text{A}$ becomes lower than that of the cubic $L_2_1$. The magnetisation, Curie temperature, and MAE of the tetragonal $X\text{A}$-$\text{Fe}_2\text{MnGa}_{0.75}\text{Sn}_{0.25}$ are determined to be 1314 emu cc$^{-1}$, 1049 K, and 2.23 MJ m$^{-3}$, respectively. Thus, $\text{Fe}_2\text{MnGa}_{0.75}\text{Sn}_{0.25}$ is a good candidate for permanent magnet applications. However, the formation energy difference between the cubic $L_2_1$ and tetragonal $X\text{A}$ phases is not enough to stabilize the $X\text{A}$ phase around the Curie temperature.

Next, we evaluated the effect of volume expansion by increasing the Ga composition, which has a larger atomic radius than those of Fe and Mn. First, we determine the site preference of the excess Ga atoms in the Ga-rich $L_2_1$ and $X\text{A}$-$\text{Fe}_2\text{MnGa}$ alloys. We calculated the formation energies of the Fe-deficient alloy with a composition of $\text{Fe}_{1.9}\text{Mn}_{1.0}\text{Ga}_{1.1}$ and the Mn-deficient alloy with a composition of $\text{Fe}_{2.0}\text{Mn}_{0.9}\text{Ga}_{1.1}$. In the present work, we consider 2, 2, 4 and 3 site-occupation configurations for the

Table II. Formation energies and magnetisation ($M_s$) of the $\text{Mn}_2\text{Ga}$, $\text{Mn}_2\text{FeGa}$, and $\text{Fe}_2\text{MnGa}$ alloys with cubic and tetragonal Heusler and hexagonal structures.

| Structure (space group) | Lattice constant (Å) | Magnetic structure | $E_r$ (eV f.u.$^{-1}$) | $M_s$ (μB f.u.$^{-1}$) |
|------------------------|---------------------|--------------------|------------------------|------------------------|
| $\text{Mn}_2\text{FeGa}$ | cubic-$L_2_1$ (Fm3m) | $a = 5.73$ | Ferri. | 0.04 | 1.00 |
|                         | cubic-$X\text{A}$ (F43m) | $a = 5.78$ | Ferri. | 0.12 | 1.04 |
|                         | tetragonal-$L_2_1$ (P42/mcm) | $a = 5.32$, $c = 6.81$ | Ferro. | -0.12 | 5.58 |
|                         | tetragonal-$X\text{A}$ (I-4m2) | $a = 5.23$, $c = 6.96$ | Ferri. | -0.45 | 0.79 |
|                         | $D0_{10}$ (P63/mmc) | $a = 5.49$, $c = 4.14$ | Ferri. | -0.02 | 0.00 |
| $\text{Fe}_2\text{MnGa}$ | cubic-$L_2_1$ (Fm3m) | $a = 5.71$ | Ferri. | -0.35 | 2.04 |
|                         | cubic-$X\text{A}$ (F43m) | $a = 5.78$ | Ferro. | -0.31 | 7.41 |
|                         | tetragonal-$L_2_1$ (P42/mcm) | $a = 5.25$, $c = 7.08$ | Ferri. | -0.30 | 0.14 |
|                         | tetragonal-$X\text{A}$ (I-4m2) | $a = 5.57$, $c = 6.41$ | Ferro. | -0.33 | 7.23 |
|                         | $L_1_1$ (cP4) | $a = 3.58$, $c = 3.86$ | Ferro. | -0.32 | 7.02 |
|                         | $D0_{10}$ (P63/mmc) | $a = 5.16$, $c = 4.16$ | Ferro. | -0.29 | 5.73 |
Here, we use the site occupancy configurations as follows: (I) excess Ga occupying the B site, (II) excess Ga occupying the A site, (III) excess Ga occupying the C site and Mn migrating to the A site, (IV) excess Ga occupying the C site and Mn migrating to the B site. Table III shows the relative formation energies for Fe$_1.9$Mn$_1.0$Ga$_1.1$ and Fe$_2.0$Mn$_0.9$Ga$_1.1$. The excess Ga atoms preferably occupy the B site and Mn(Fe) migrating to the A site in the $L_2_1(XA)$ structure.

Next, we estimate the composition dependence of the formation energies $L_2_1$ and $X A$ structures for Fe$_2.0$Mn$_0.9$Ga$_1.1$ and Fe$_2.0$Mn$_0.9$Ga$_1.1$. The excess Ga atoms preferably occupy the B site and Mn(Fe) migrating to the A site in the $L_2_1(XA)$ structure.

We theoretically investigated the stabilization of the ferromagnetic state in tetragonal Heusler alloys. We focused on the effects of Fe atom substitution for Mn and the lattice expansion in the Mn$_3$Ga alloy. When the volume of Fe$_2$MnGa is expanded by about 8%, the ferromagnetic tetragonal $X A$ phase becomes stable. The tetragonal $X A$-Fe$_2$MnGa alloy can be applied in permanent magnets because of its high saturation magnetisation, perpendicular magnetic anisotropy, and Curie temperature. Sn substitution at the Ga sites results in volume expansion so that the ferromagnetic tetragonal $X A$ phase is stabilized. Finally, we examined the stability of the $X A$ phase and magnetic properties of Fe$_2$MnGa in relation to the Ga composition and found that Fe$_2$Mn$_{1.0}$Ga$_{1.5}$ is a good material that can be utilized as a permanent magnet.
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Fig. 6. (Color online) Magnetisation (a), magnetic anisotropy coefficient (b) and Curie temperature (c) of the tetragonal XA Fe2Mn1+Ga1+x+y alloys.