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Martensitic transformation, electronic structure and magnetism in D0₃-ordered Heusler Mn₃Z (Z = B, Al, Ga, Ge, Sb) alloys

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Recently, 50-nm Heusler Mn₃Al thin films were experimentally synthesized by Jamer *et al.* [*Phys. Rev. Appl.* (2017), **7**, 064036] and the nominal zero moment, *i.e.* the fully compensated ferrimagnetic property, of these thin films was confirmed. That work motivated the current investigation on the martensitic transformation, electronic structure and magnetism of D0₃-ordered Mn₃Al using first-principles calculations. Owing to tetragonal distortion, the martensitic transformation only occurs with tensile strain rather than with compressive strain and the half-metallic-type Mn₃Al becomes a magnetic metal. Consequently, Mn₃Al shows great potential for application as a ferromagnetic shape memory alloy. Moreover, not only did the martensitic transformation occur in Mn₃Al, it was also observed in similar D0₃-ordered Mn₃Z (Z = B, Ga, Ge, Sb) compounds.

1. Introduction

Heusler alloys have been widely and actively investigated for over a century. Because of their abundant composition and excellent physical properties, they show great potential in many fields, such as in spin-gapless semiconductors (Liu *et al.*, 2008; Skaftouros *et al.*, 2013; Wang & Jin, 2015; Gao & Yao, 2013; Jamer *et al.*, 2015; Bainsla *et al.*, 2015a,b; Xu *et al.*, 2013), topological insulators (Khan *et al.*, 2007; Hou *et al.*, 2015), superconductors (Wernick *et al.*, 1983; Tafti *et al.*, 2013; Winterlik *et al.*, 2009, 2008; Nakajima *et al.*, 2015), shape memory alloys (SMAs) (Oikawa *et al.*, 2002; Fujita *et al.*, 2000; Sutou *et al.*, 2004; Liu *et al.*, 2005), and thermoelectric materials (Katayama *et al.*, 2003; Lue & Kuo, 2002; Lue *et al.*, 2007; Xia *et al.*, 2000). Normally, Heusler alloys possess a high-ordered cubic structure. Additionally, they follow a typical X₂YZ (XYZ) stoichiometry, where X and Y represent transition metal elements, and Z is usually occupied by IIIA, IVA and VA group elements. The differences in the site preference lead to different crystal structures in Heusler alloys, such as L2₁-ordered (Masumoto & Watanabe, 1972; Sakuraba *et al.*, 2005) and C_{1b}-ordered alloys (Masumoto & Watanabe, 1972). Because some solid defects generally exist in the Heusler alloy lattice, such as anti-sites and vacancies, it is necessary to find a suitable structure to decrease the affection toward these defects. In this case, researchers proposed a new crystal structure, the cubic D0₃-ordered structure. The D0₃-ordered Heusler alloy displays a site preference of XXXZ, *i.e.* a stoichiometry of X₃Z. It naturally eliminates the anti-site defects

between the transition metal elements in the lattice because it contains only one kind of transition metal element. Thus, $D0_3$ -ordered Heusler alloys may have more stable physical properties and their synthetic obstacles can be reduced. Many $D0_3$ -ordered Heusler alloys (Liu *et al.*, 2014; Zhang *et al.*, 2012; Yamada *et al.*, 2012) have been theoretically and experimentally proposed.

Martensitic transformation plays an important role in SMAs and other intelligent magnetic materials (IMMs), thus receiving increased attention from researchers. As a kind of diffusionless transformation, martensitic transformation occurs without long-range diffusion and the homogeneous movement of atoms results in lattice structural changes (usually a change from face-centered to a tetragonal lattice structure). Based on the martensitic transformation, IMMs can thus be further divided into three types: temperature-induced, stress-induced and magnetic field-induced alloys. Consequently, we can use the structural tetragonal distortion to obtain martensitic transformation and to investigate its potential application in SMAs. Additionally, the natural ferromagnetism of the thermoelastic Heusler SMA can endow itself with a much higher magnetostriction than traditional magnetostrictive materials. This kind of SMA is called a ferromagnetic shape memory alloy (FSMA). As a typical FSMA, the Mn_2NiAl (Luo *et al.*, 2010) system has been well studied and understood, and it exhibits the possibility of achieving martensitic transformation in Mn_2NiAl -series materials and has inspired researchers to focus on Mn-based Heusler compounds. Because of this promising prospect, it is necessary to investigate more homologous materials.

Recently, Jamer *et al.* (2017) reported compensated ferrimagnetism in zero-moment 50-nm Heusler Mn_3Al thin films, as determined experimentally. Motivated by their article, we surprisingly found that the fully compensated ferrimagnetic Mn_3Al may possess a potential martensitic transformation. More importantly, 50-nm Mn_3Al thin films have been experimentally synthesized by Jamer *et al.* (2017). Thus, to follow their work and expand the investigation of their properties is useful. Additionally, we strongly believe that the similar Mn_3Z ($Z = B, Ga, Si, Ge, Sb$) structures may also have martensitic transformation, and in this work, we confirmed this *via* calculations, except for Mn_3Si .

2. Computational methods

The electronic properties of Mn_3Z ($Z = Al, B, Ga, Si, Ge, Sb$) were computed using the pseudopotential method with a plane-wave basis set (Payne *et al.*, 1992) on the basis of Cambridge Serial Total Energy Package (CASTEP) code (Segall *et al.*, 2002). The ultrasoft pseudo potential (Vanderbilt, 1990) was employed to describe the interactions between the atomic core and the valence electrons. The electronic exchange–correlation energy was treated as the Perdew–Burke–Ernzerhof (PBE) functional of the generalized gradient approximation (GGA) (Perdew *et al.*, 1996). We point out that GGA in the scheme of PBE has been widely used to study the electronic properties of Heusler-based alloys, and

this method can reasonably describe electronic structures. The plane-wave basis set cut-off used was as 450 eV. A Brillouin zone was integrated by meshes of $12 \times 12 \times 12$ k-points in cubic austenite and nonmodulated tetragonal martensitic structures. The convergence of tolerance for the calculations was selected as a difference in total energy within 5×10^{-7} eV per atom. All of these employed parameters confirm good convergences for the total energy. The computed sets ensure the precision of the following calculated results.

3. Results and discussion

3.1. Optimized crystal structure

Generally, Heusler alloys possess a stoichiometry of X_2YZ or XYZ , where X and Y represent transition metal elements, and Z is usually occupied by main group elements; these types of stoichiometry for the Heusler alloys are called full-Heusler and half-Heusler alloys, respectively. As a special full-Heusler alloy, in Wyckoff coordinates, Mn_3Al follows X_2YZ site preference in the cubic lattice, the Mn atoms in Mn_3Al occupy the A (0, 0, 0), B (0.25, 0.25, 0.25) and C (0.5, 0.5, 0.5) positions, and, therefore, Al sits in the D (0.75, 0.75, 0.75) position. Additionally, this kind of atomic ordering is called a $D0_3$ -

Figure 1
Illustration of the (a) cubic and (b) tetragonal $D0_3$ -ordered lattice structures of the Mn_3Al Heusler alloy.

Figure 2
Calculated total energies for Mn_3Al with cubic-type lattice constants as a function of the c/a ratio. The 5.8782, 5.82, 5.7618 and 5.7036 Å lattice constants are for the case of $c/a = 1.0$.

ordered binary intermetallic compound (space group, $F43/m$, No. 216). The corresponding optimized geometric structure shows a face-centered lattice with an equilibrium lattice constant of $a = b = c = 5.82 \text{ \AA}$, as shown in Fig. 1.

Here, to determine the martensitic transformation, electronic structure and magnetism of Mn_3Al , we adopted a tetragonal distortion effect to realize the martensitic phase and investigate the corresponding changes in its physical properties. The parameter of c/a was defined as the ratio of the lattice constant of the c -axis to that of the a -axis under tetragonal distortion. Because the Mn (A) and Mn (C) possess the same neighboring environment, these atoms display the same electronic and magnetic behaviors; thus, we will adopt a representation of Mn (A/C) to exhibit both type atoms in the following discussion.

3.2. Martensitic transformation in Mn_3Al

As we know, tetrahedral distortion via the Bain path is a suitable method (Winterlik *et al.*, 2012) to study martensitic transformation *via* first-principles calculations. Bain paths judge whether martensitic transformation will occur or not; in these alloys according to the relationship between ΔE_M and the c/a ratios [c and a are shown in Fig. 1(a)]. ΔE_M is the difference in energy between the ground state and the martensitic phases, and the total energy is set to zero at a c/a ratio = 1, which is called the austenitic phase. By relaxing the c/a ratios, the minimum total energy can be obtained in the tetragonal distortion, which is called the martensitic phase. Of note, a similar method to predict possible martensitic transformation in Heusler alloys *via* theory has been widely used, *e.g.* Faleev *et al.* (2017a) calculated the tetragonal distortion in 286 Heusler alloys and identified many possible martensitic transformations among them.

We calculated the corresponding total energy as a function of c/a at a volume expansion of 0%, $\pm 1\%$ and -2% based on the equilibrium cubic lattice of Mn_3Al , as shown in Fig. 2. As shown, the possible martensitic transformations can be tuned by changing the lattice constants. For Mn_3Al alloys with 5.7036 and 5.7618 $\text{\AA}$ lattice constants, although two minima can be found in the E_M - c/a curve, the cubic-type austenitic phase is most stable. For the direction

along $c/a > 1$, the brown and blue lines reveal that the phase represented by the right-hand side minimum has a higher total energy than the austenitic phase. This indicates that these phases are energetically unfavorable, *i.e.* phase transformations are unlikely to occur in either modules. For Mn_3Al alloys with 5.82 and 5.8782 $\text{\AA}$ lattice constants, the left-hand side one is located at c/a of 1.0, which means in the austenitic phase. Along the direction of $c/a < 1$, the energies of all these lattices quickly increase, indicating no phase transformation occurs in the compression case. However, the lattices represented by the red and black lines show that the deeper local energy minima appear on the $c/a > 1$ side. The right-hand side 'deep' minimum indicates that a degree of tetragonal tensile distortion can relax the total energy and this distortion in the unit-cell geometry is energetically favorable. Thus, the martensitic phases are able to be realized at a c/a ratio of approximately 1.3 and become more and more stable with volume expansion. Meanwhile, the martensitic transformation temperature (T_M) is related to the value of ΔE_M (Barman *et al.*, 2008), and a relatively large ΔE_M can induce a high T_M . Therefore, for

Figure 3

Band structures (a, c) and the corresponding DOS (b, d) for austenitic and martensitic Mn_3Al , respectively. ($a = b = c = 5.82 \text{ \AA}$). Energies at the Fermi level are set to zero.

Mn₃Al, the martensitic phase may tend to be more stable and possess a high transformation temperature in a larger lattice constant cubic structure compared with the equilibrium structure.

We calculated the band structures of austenitic-type Mn₃Al based on the equilibrium cubic lattice, and the results are shown in Fig. 3(a). The bands in the spin-up channel cross the Fermi level, whereas the bands in the spin-down channel show a semiconducting gap of approximately 0.330 eV, *i.e.* this system was confirmed to be half-metallic. The corresponding total density of states (DOS) are shown in Fig. 3(b). From the total DOS, the half-metallic properties of the Mn₃Al system were also confirmed. The Fermi level is located near the top of the peak, indicating a potentially energetic instability in the austenitic phase. To further investigate the electronic structure of austenite Mn₃Al, we calculated the partial DOS (PDOS). The corresponding PDOS of Mn (A/C) shows a relatively large spin-splitting near the Fermi level, and thus contributes to the magnetic moment with a value of approximately $-2.64 \mu_B$. For Al (D), the delocalized states of Al ignored the contribution for magnetism. For Mn (B), we found two clear peaks of states in two spin directions induced by strong exchange splitting that completely offset the magnetic moment contribution from Mn (A/C) and Al (D), thus making Mn₃Al appear to have fully compensated ferrimagnetism in agreement with the experimental results of Jamer *et al.* (2017).

To further investigate the relative stability of its unit-cell geometry originating from the electronics and the changes in other physical properties, the electronic structure and magnetism of the corresponding martensitic Mn₃Al (where $c/a = 1.31$) were also computed, and the results are shown in Fig. 3. Compared with the half-metallic type band structures of the austenite-type Mn₃Al, the martensite-type Mn₃Al converted to a complete metal. We presented the martensitic DOS of cubic type Mn₃Al with an equilibrium lattice constant of 5.82 Å. In martensite, the symmetries of *d* orbitals broken under the tetragonal distortion would lower the energy states down near the Fermi level, which can improve the phase stability, as shown in Fig. 3. For PDOS, we found that the peaks for Mn (B) slightly decrease compared with those of austenite; additionally, the same situations occurred in Mn (A/C) and Al (D) PDOS. This explains the fact that the energetically favorable martensite may be related to the Jahn–Teller effect (Faleev *et al.*, 2017a; Hong *et al.*, 1990). Overall, the above-mentioned results confirm the relative stability of the unit-cell geometry and the martensitic phase of Mn₃Al.

Furthermore, the magnetic moment as a function of c/a is illustrated in Fig. 4. As the volume compresses, the total magnetic moment of the system will increase. Moreover, along the $c/a > 1$ direction, as the c/a ratio increases, the total magnetic moment values decreased from fully compensated zero to a range of approximately $-1.6 \mu_B$ to $-1.8 \mu_B$. Along the direction of $c/a < 1$, the trend for the total magnetic moment is decreasing, and this decrease changes steeply along with the increase in the original cubic lattice constant.

Interestingly, according to Fig. 2, between the austenitic and the martensitic phases, all these types of Mn₃Al lattices show

an energy peak close to a $c/a = 1.1$. As shown in Fig. 4, near the point of this energy peak, the corresponding net magnetic moment will exhibit a steep slope which is mainly induced by Mn atoms.

As shown by results of the calculated magnetic moments, the fully compensated ferrimagnetic (FCF) state of cubic Mn₃Al is broken, and the magnetic structure of this system is transferred to a common ferrimagnetic state for the martensitic phase. For this transformation, the magnetism analysis

Figure 4

The total/partial magnetic moments as a function of c/a ratio for cubic lattices with different volume expansion ratios.

shows that the main contribution of total magnetic moment was derived from the d orbitals of Mn atoms. Overall, the above discussion indicates that Mn_3Al has a possible energetically favorable martensitic phase with ferrimagnetism and may be applied in magnetostrictive materials such as a FSMA.

4. Outlook for Mn_3Z ($\text{Z} = \text{B}, \text{Ga}, \text{Si}, \text{Ge}, \text{Sb}$)

To expand the results we obtained for Mn_3Al , we also made some attempts regarding D_{03} -ordered Mn_3Z ($\text{Z} = \text{B}, \text{Ga}, \text{Si}, \text{Ge}, \text{Sb}$). Surprisingly, we noticed that not only does the martensitic transformation that is induced by the tetragonal distortion *via* the Bain path occur in Mn_3Al , it can also be found to occur in Mn_3Z . We calculated the energy differences, $\Delta E = E_{\text{tetragonal}} - E_{\text{cubic}}$, as a function of the c/a ratio for Mn_3Z ($\text{Z} = \text{B}, \text{Ga}, \text{Si}, \text{Ge}, \text{Sb}$) for volume expansions of 0%, $\pm 1\%$, and $\pm 2\%$ based on the equilibrium cubic lattice of Mn_3Z . The results are shown in Fig. 5.

According to our calculations, for the equilibrium lattice, the energetically favorable martensitic phases in the above-illustrated alloys occurred *via* tetragonal distortion in the same manner that was found for Mn_3Al . However, Mn_3Si possesses an energetically unfavorable local minimum on the $c/a > 1$ side and, hence, loses its martensitic transformation. Meanwhile, when a different volume expansion is exerted, the ΔE_{M} changes. The volume expansion is always favorable for stabilizing the martensitic phase, whereas the volume compression will decrease its stability and even destroy the martensitic transformation. Additionally, the volume expansion leads to the left-hand side local minimum, and the energy peak moves toward the $c/a < 1$ side. The Mn_3Ga system thus possesses two local minima on both sides of $c/a = 1$. The left-hand side

minimum is a metastable phase and the right-hand side one confirms that this system can relax the total energy according to tensile distortion and thus obtains the martensitic transformation at the point where $c/a = 1.330$. However, the volume expansion leads to a possible martensitic transformation that occurs in Mn_3Si , but the relatively low ΔE_{M} value indicates an unstable martensitic phase and a low transformation temperature. Thus, Mn_3Si is not a suitable candidate to be an FSMA. In Table 1, for the equilibrium lattice case, the ΔE_{M} for Mn_3Z ($\text{Z} = \text{B}, \text{Ga}, \text{Ge}, \text{Sb}$) and its magnetic phase, total magnetic moment (M_{t}), partial magnetic moments and corresponding c/a ratio are provided. Mn_3Ga has the largest ΔE_{M} , and Mn_3B has the lowest one. For Mn_3Z , the c/a value is closely related to the degree of the shape-memory effect (Entel *et al.*, 2013); thus, an alloy that possesses a large c/a ratio is favorable for transformation strain. However, the low c/a ratio of Mn_3Ga may affect its performances as an FSMA. The largest c/a ratio observed is 1.435 for Mn_3Sb and it has a relatively large ΔE_{M} value of -0.143 eV, which ensures that a high T_{M} can be obtained. This strongly indicates that Mn_3Sb is a good FSMA candidate. Based on the above-mentioned considerations, the martensitic transformations are also likely to be realized in Mn_3B , Mn_3Ga and Mn_3Ge .

Moreover, we noticed that energy peaks on the curves can be still found between the austenitic and martensitic phases at a c/a ratio between 1.10 and 1.17. The facts are similar to what we had obtained for Mn_3Al . One interesting fact is that the amplitude of the energy peaks increased along with substitution of IIIA group elements by IVA and VA group elements, and generally, the energy peak for the $\text{Z} = \text{IVA}$ alloy is 0.105 eV (Mn_3Ge), whereas the original peaks for $\text{Z} = \text{IIIA}$ are 0.060 eV (Mn_3B), 0.026 eV (Mn_3Al), and 0.004 eV

Figure 5
 ΔE as a function of c/a ratio for Mn_3Z ($\text{Z} = \text{B}, \text{Ga}, \text{Si}, \text{Ge}$ and Sb). The c/a ratio of cubic austenite was set as $c/a = 1.0$.

Table 1
Total energy differences (ΔE_M) between martensite and austenite, corresponding martensitic c/a ratio, total magnetic moment (M_t), and partial magnetic moments for martensite-type Mn_3Z ($Z = B, Ga, Ge$ and Sb).

	Magnetic phase	ΔE_M (eV)	c/a	M_t (μ_B)	Mn (A/C) (μ_B)	Mn (B) (μ_B)	Z (μ_B)	Stable phase
Mn_3B	Ferrimagnetic	-0.059	1.350	-1.505	-2.15	2.67	0.13	Martensite
Mn_3Ga	Ferrimagnetic	-0.227	1.330	-1.775	-2.79	3.68	0.12	Martensite
Mn_3Ge	Ferrimagnetic	-0.090	1.345	-0.987	-2.31	3.56	0.07	Martensite
Mn_3Sb	Ferrimagnetic	-0.143	1.435	-1.172	-2.43	3.68	0.00	Martensite

(Mn_3Ga), respectively. Additionally, for Mn_3Sb , which contains a VA group Sb atom occupying the D site, an energy peak at 0.120 eV is present. In particular, the energy peak for Mn_3Si is the highest at approximately 0.193 eV. Furthermore, for Mn_3B/Mn_3Ga and Mn_3Si/Mn_3Ge compounds, their ΔE_M are related to Z atoms. Namely, the lighter Z elements that are in the same group, the smaller the absolute value of ΔE_M and, thus, the stability of the corresponding martensitic phase will be lower. The disappearance of the martensitic phase in Mn_3Si may be related to the above-mentioned phenomena. The electronic structures and magnetism of these Mn_3Z alloys in the austenitic and martensitic (tetragonal phase for Mn_3Si) phases were calculated to investigate their physical properties, which are provided in Figs. 6 and 7. The equi-

Table 2
Cubic-type equilibrium lattice constants (a), magnetic phase, total magnetic moments (M_t) and partial magnetic moments for austenitic Mn_3Z ($Z = B, Ga, Si, Ge$ and Sb).

Alloy	a (Å)	Magnetic phase	M_t (μ_B)	Mn (A/C) (μ_B)	Mn (B) (μ_B)	Z (μ_B)
Mn_3B	5.458	FCF	0.0	-1.50	2.87	0.20
Mn_3Ga	5.872	FCF	0.0	-2.07	3.96	0.19
Mn_3Si	5.692	Ferrimagnetic	1.0	-1.23	3.32	0.14
Mn_3Ge	5.791	Ferrimagnetic	1.0	-1.32	3.50	0.15
Mn_3Sb	6.019	Ferrimagnetic	2.0	-0.83	3.55	0.11

rium lattice constants (a), magnetic phase, total magnetic moments (M_t) and partial magnetic moments for austenitic Mn_3Z ($Z = B, Ga, Si, Ge, Sb$) are given in Table 2. Combined with the band structures and the total DOS, Mn_3Sb shows a half-metallic phase with a M_t of 2 μ_B ; Mn_3Si and Mn_3Ge are present as near half-metals with a total M_t of 1.0 μ_B , whereas the others are in a metallic state. The given M_t (Table 2) and DOS indicate the fully compensated ferromagnetism only occurs in austenitic Mn_3B and Mn_3Ga , which is similar to Mn_3Al . All these alloys also follow the well known Slater–Pauling rule (Faleev *et al.*, 2017a). All these features were broken under the tetragonal transformation, and all of the alloys were converted to the metallic phase with a large M_t . For Mn_3Ga , Mn_3Ge and Mn_3Sb , the stability of their tetragonal phase has been iden-

Figure 6
Band structures and total DOS for austenitic (a) Mn_3B , (b) Mn_3Ga , (c) Mn_3Si , (d) Mn_3Ge and (e) Mn_3Sb . The energies at the Fermi level were set to zero. The obtained equilibrium cubic-type lattice constants are given in Table 2.

Figure 7
Band structures and total DOS of martensitic-type (a) Mn_3B , (b) Mn_3Ga , (c) Mn_3Si , (d) Mn_3Ge and (e) Mn_3Sb . The energies at the Fermi level were set to zero. For the case of Mn_3Si , no martensitic transformation occurred, and the electronic structures of Mn_3Si are shown with a c/a ratio of 1.335.

Figure 8
The total magnetic moments of Mn_3Z ($Z = \text{B}, \text{Ga}, \text{Si}, \text{Ge}$ and Sb) as a function of the c/a ratio.

tified; additionally, a recipe for finding tetragonal Heusler compounds with perpendicular magnetic anisotropy has been suggested, see Faleev *et al.* (2017b). Furthermore, for these alloys, the total magnetic moment as a function of the c/a ratio is shown in Fig. 8. Based on this, the steep slope still occurred in addition to the appearance of local energy peaks, which is similar what was found for Mn_3Al at a c/a ratio of approximately 1.10–1.17.

5. Conclusion

We built a D0_3 -ordered Heusler alloy, Mn_3Al , for calculations. Its martensitic transformation and its corresponding physical properties were fully investigated in this study *via* first-principles calculations. To examine the possibility and stability of the martensitic phase, the ΔE_{M} was primarily computed. The lower energy of the tetragonal phase revealed that a martensite phase can feasibly be realized by exerting tetragonal tensile distortion on its cubic austenite phase. However, the martensitic transformation in Mn_3Al does not appear at smaller cubic lattice constants compared with the equilibrium lattice parameter. Furthermore, its fully compensated ferrimagnetism and novel half-metallic phase is destroyed during the martensitic transformation and converts to be a normal magnetic metal phase. Consequently, this demonstrates that Mn_3Al has a potential application as an FSMA.

We also considered substituting the D-site element to build a series of D0_3 -ordered Mn_3Z ($Z = \text{B}, \text{Ga}, \text{Si}, \text{Ge}, \text{Sb}$) alloys in the future. Their equilibrium lattice structures were also computed with the help of GGA in the scheme of PBE. Interestingly, almost all the alloys with the equilibrium cubic lattice achieved the martensitic transformation under tetragonal tensile distortion, except for Mn_3Si . The volume expansion for the equilibrium cubic lattices is energetically favorable to stabilize the martensitic phase when exerting tetragonal tensile distortion to convert to the martensitic phase, whereas volume compression cannot. Meanwhile, we found that Mn_3Sb has a half-metallic phase in the austenitic phase, and the austenitic Mn_3B and Mn_3Ga displayed fully

compensated ferrimagnetism. In the martensitic phase, these alloys all converted to magnetic metals. The relatively large ΔE_{M} and the large c/a ratio of Mn_3Sb ensure its potential for martensitic transformation. These results provide meaningful candidates for searching for FSMAs. Furthermore, the synthesis of Mn_3Al thin films reminds us that it is necessary to experimentally investigate other D0_3 -ordered Mn_3Z alloys.

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