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Pressure effect of magnetic and electronic properties of Mn_2PtGa Heusler alloy

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ABSTRACT

First-principles calculations are performed to investigate pressure effects on structure, magnetism, martensitic phase transition and Curie temperatures of Mn_2PtGa Heusler alloy in framework of the density functional theory. It is shown that Mn_2PtGa prefer to crystallize in the inverse Heusler type structure. Besides, we predict an extraordinary occurrence of pressure induced metallic ferrimagnetism to half-metallic ferromagnetism transition in cubic phase of Mn_2PtGa alloy under hydrostatic pressure up to 43 GPa and the half-metallic ferromagnetism is found to be robust even the lattice further compression to 90 GPa. However, with the pressure up to 100 GPa, the spin-down gap starts to close and the half metallicity begin to disappear, while with the pressure increasing from 100 GPa to 300 GPa, the alloy returns to metallic characteristic. In addition, the energy difference between the austenitic and martensitic phases is found to increase with increasing pressure followed by a decrease when pressure reaches to 43 GPa, which implies a variation trend of martensitic phase transition temperature. Furthermore, Curie temperatures in both austenitic and martensitic phases are estimated under pressure by using the standard mean-field approximation which agrees well with the theoretical results in literature. The robustness of the half metallicity, magnetic transition and the high Curie temperature under pressure make Mn_2PtGa alloy a promising candidate for applications in spintronic devices.

1. Introductions

The researches on ferromagnetic shape memory Heulser alloys have attracted considerable attention due to the diverse functional properties such as shape memory effect [1–3], magnetocaloric effect [4,5], giant magnetoresistance [6–9], and exchange bias effect [8,10,11] since the discovery of Ni_2MnGa alloy [12]. In recent years, a new class of Mn_2-based Heusler compounds stabilized in the inverse Hg_2CuTi structure with high Curie temperature and extraordinary magnetic sub-lattices are attractive candidates for spin-torque devices [13,14]. Among them, Mn_2PtGa alloy draw many researchers' attention for the unusual first-order ferrimagnetism to anti-ferromagnetism phase transition below Curie temperature and large exchange bias due to the exchange anisotropy induced by the ferrimagnetic clusters embedded in ferromagnetic host [15,16]. Apart from the above mentioned, martensitic transformation can also be observed from the high-temperature cubic structure to the tetragonal structure at low-temperature. It is reported that the martensitic phase transition temperature, Curie temperature and magnetic properties are highly dependent on the composition and external strain [6,17]. Hence, we can expect that there is a vast amount of work, searching for new improved properties in this Heusler family. As we all known, the hydrostatic pressure is an important factor to understand and explore the new physical properties of the magnetic systems. In the literature, the effects of pressure applied on Heusler alloys properties have been studied extensively [6,18,19], because the external pressure can modify the Mn–Mn distance. Nevertheless, the exchange interaction between magnetic atoms is sensitive to the interatomic distances to affect the magnetic properties and accompanied structural and physical natures, such as half-metallic characteristic. Since discovery of half-metallic ferromagnetism, many more systems were characterized as half-metallic by the band structure theory, such as the full Heusler alloys Mn_2RhZ (Z = Si, Ge) [20], Co_2XSi (X = Fe, Mn) [21], $Co_2CrGa_{1-x}Si_x$ [22], Co_2YAl (Y = Fe, Ti) [23], Co_2YZ (Z = P, As, Sb, and Bi) [24] and half-Heusler alloys CoCrZ (Z = Al, Ga) [25], CoVSb [26]. Although relevant researches have expanded to the similar system of the Mn_2XY (X = Transition metal elements, Y = Main group elements), in order to explore the new physical natures in Heusler alloys of Mn_2PtGa, in this letter, we

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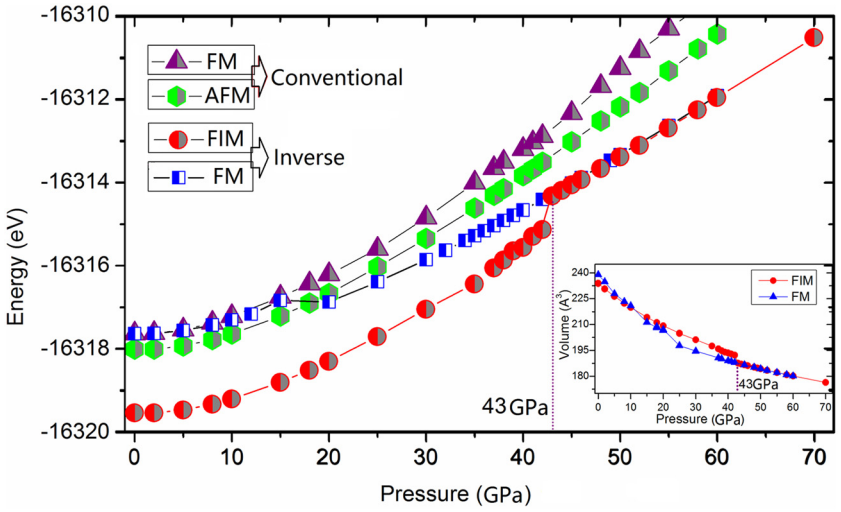

Fig. 1. Total energy curves as a function of pressure for Mn_2PtGa with different magnetic configurations in the inverse and conventional structures.

have performed a more systematic spin-polarized first-principles calculations to check the physical properties at ambient and elevated high pressure. Under the application of hydrostatic pressure, the structural, magnetic and electronic properties as well as the Curie temperature and martensitic transition temperature are investigated. Particular attention must be paid to the prediction of a metallic ferrimagnetism to half-metallic ferromagnetism transition with the pressure up to 43 GPa. All of the results with pressure effects are presented and discussed in the paper.

2. Computational details

The optimization of geometrical structures, electronic band structure and magnetic properties are carried out using first-principles calculations based on the density functional theory, as implemented in the CASTEP code [27]. The exchange and correlation potentials were described by using generalized-gradient approximation (GGA) in the parameterization of Perdew–Burke–Ernzerhof (PBE) functional scheme [28]. The interactions between the valence electrons and ion core were described by the ultra-soft pseudo-potentials. The atomic configurations used to generate the ultra-soft pseudo-potentials are $3d^5\ 4s^2$ for Mn, $5d^9\ 6s^1$ for Pt and $3d^{10}\ 4s^2\ 4p^1$ for Ga, respectively. To ensure the convergence of calculations, we have tested the cut-off energy and k-points grid. It is found the energy cut-off of 420 eV for plane wave expansion and the Brillouin-zone sample of $4 \times 4 \times 4$ k-points will ensure the self-consistent convergence. All the calculations converge with the energy and force tolerance criterion of 10^{-6} eV and 0.01 eV/Å, respectively. A k-point sampling of $12 \times 12 \times 12$ is set in the Brillouin zone integrations based on the Monkhorst–Pack scheme [29] for electronic band structure calculations. To estimate the Curie temperatures, we map the system on the Heisenberg model within the standard mean-field approximation (MFA) approach [30,31].

3. Results and discussion

Generally, Heusler alloy will exhibit two types of structures, namely, conventional and inverse structures. For the conventional structure, the X atoms occupy (0.25, 0.25, 0.25) and (0.75, 0.75, 0.75) sublattices, the Y atom occupies (0.50, 0.50, 0.50) site and group element Z locates at (0.00, 0.00, 0.00), respectively. In the case of inverse structure, X, X, Y and Z occupy the sublattices in the form of (0.25, 0.25, 0.25), (0.50, 0.50, 0.50), (0.75, 0.75, 0.75) and (0.00, 0.00, 0.00), respectively.

We firstly perform the total energy calculations as a function of pressure in the conventional and inverse structures, respectively. Two possible initial magnetic ordering types have been taken into account in our calculations: (a) the antiferromagnetic (AFM) structure with the spin of Mn(1) antiparallel to that of Mn(2); (b) the ferromagnetic (FM) structure with the spin of Mn(1) parallel to that of Mn(2). After calculating with the initial spin configurations, all the structures converge into corresponding ground states. It's worth noting in the inverse alloy, initial magnetic configuration in AFM evolved into a ferrimagenetic ordering (FIM) structure after geometry optimization. The obtained total energies as a function of pressure are plotted in Fig. 1. It can be seen obviously from the energy curves, the FIM configuration in the inverse Heusler alloy is the most stable ground state at ambient and elevated pressure regions up to 43 GPa. While the pressure is above 43 GPa, the Mn_2PtGa inverse Heusler alloy prefers to be stable in "FM" configuration. (Here, the "FM" configuration is actually a strong FIM. To describe conveniently, this stronger FIM configuration is still defined as FM with double quotations because it is evolved from the initial FM structure.) However, it is difficult to crystallize in the conventional structure for the relatively high energy. Therefore, in the following discussions, we will focus on the inverse structure. The calculated pressure–volume relation is displayed in the inset of Fig. 1. The volume of Heusler alloy Mn_2PtGa decreases as pressure increases. In particular, we can find the volume variation have a sudden jump at the pressure of 43 GPa, which is accordance with the jump point of energy trends above. This kind of behavior comes down to the strong coupling between magnetism and crystallographic structure. With the pressure up to the critical point of 43 GPa, the magnetic moment jumps arising from stronger ferrimagnetic interaction, which is often accompanied by a change in energy and volume.

The effects of pressure on the total magnetic moments with initial FM and FIM configurations are presented in Fig. 2(a). In the case of FIM situation, one can see the magnetic moment increases slowly and suddenly jumps up to 3 μB with the pressure elevated up to 43 GPa, which indicates the magnetic phase transition occurring from a weak FIM to a stronger FIM state. Meanwhile, the atom-resolved magnetic moments of Mn(1), Mn(2), Ga and Pt are plotted in Fig. 2(b), (c), (d), and (e), respectively. As can be seen, the total magnetic moment is mainly contributed by Mn(1) and Mn(2) atoms, whose spin moments are opposite to each other. While for the magnetic moments of Ga and Pt, there are no significant contributions to the system magnetism as the very small values with the pressure changing. It is noteworthy that the two

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