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Half-metallic full-Heusler compound Ti_2NiAl: A first-principles study

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ABSTRACT

Full-Heusler compound Ti_2NiAl with Hg_2CuTi-type structure is demonstrated to be a new half-meltal ferromagnet by first-principles calculations. The compound has a complete (100%) spin polarization around the Fermi level in the total density of state. The band structure calculations show that the majority spin is strongly metallic, while the minority spin shows an insulating behavior. The compound has a total magnetic moment of $-3.0\ \mu_B$ per formula on first-principles calculations which complies well with the Slater–Pauling (SP) rule. Though having different atomic surroundings, the profiles of atom-projected density of states of Ti(*A*) and Ti(*B*) are similar. The half-metallic character is retained when the lattice constant ranging from −12.8% to +4.9%.

1. Introduction

In recent years, spintronics has attracted much attention due to its rapid development [1–4]. One of the crucial aspects for spintronics is the injection source of the high spin-polarized charge carriers. Half-metallic materials, including half-metallic ferromagnets and half-metallic antiferromagnets are the ideal choice. Investigations on half-metallic materials are more concentrated on Heusler alloy family since the conception of half-metal arises from electronic structure calculations for NiMnSb with a half-Huesler structure by de Groot et al. [5]. Since then, some more compounds have been found theoretically as half-metals by means of band structure calculations.

However, the full-Heusler compound is the most studied series. Mn_2VZ (*Z* = Al, Ga, Si, etc.) [6–8], Co_2MSi (M = V, Ti and Cr) [9], Fe_2YSi (Y = Mn, Cr) [10] and Cr_2MnZ (*Z* = P, As, Sb, Bi and Al) [11,12] which are recently found to be half-metals are all full-Heusler compounds. Since the experimental search for half-metals is difficult and the verification of the expected spin polarization is involved, electronic structure calculations have played an important role in this area. Recently, Cr_2 based half-metallic ferromagnets have been found by Galanakis et al. [11] and Li et al. [12].

Though atom Ti has similar electronic configuration as Cr, Ti_2-based full-Heusler half-metalic compounds have not yet been theoretically reported widely. In this work, the density of states, energy bands, and magnetic moment of Ti_2NiAl with Hg_2CuTi-type full-Heusler structure are studied extensively by first-principles calculations.

2. Computational details

Many full-Heusler compounds usually have a cubic $L2_1$ structure. This structure is commonly represented by the generic formula X_2YZ, where *X* and *Y* denote transition metal elements and *Z* is a group III, IV or V element. The structure can be seen as composed of four interpenetrating face-centered-cubic lattices with space positions described with the Wyckoff coordinates denoted as *A* (0, 0, 0), *B* (1/4, 1/4, 1/4), *C* (1/2, 1/2, 1/2), and *D* (3/4, 3/4, 3/4). In Hg_2CuTi-type $L2_1$ structure, *X* atoms occupy sites (*A*, *B*). It has been confirmed that elements with more 3*d* electrons prefer to occupy sites (*A*, *C*) and those with fewer tend to occupy sites *B* [13]. Ni atom has more 3*d* electrons than Ti atom therefore tends to fill site *C*. Similar circumstances have been exhibited in Mn_2-based full-Heusler alloys Mn_2NiGa [14] and Cr_2MnAl [12].

In Hg_2CuTi-type full-Heusler compound Ti_2NiAl, Ti atoms enter sites *A* and *B*, atoms Ni enter sites *C*, and atoms Al occupy sites *D*. Ti atoms entering sites *A* and *B* are denoted as Ti(*A*) and Ti(*B*), respectively and Ni atoms entering sites *C* are denoted as Ni(*C*). The geometry of Ti_2NiAl with Hg_2CuTi-type full-Heusler structure is optimized. The density of states and electric energy bands are calculated by the plane-wave pseudopotential method [15], which is based on density functional theory that describes the electron–electron interaction [16,17].

A generalized-gradient approximation (GGA) functional and the Perdew–Burke–Ernzerhof functional (PBE) scheme are chosen to deal with the exchange and correlation potential in the calculations.

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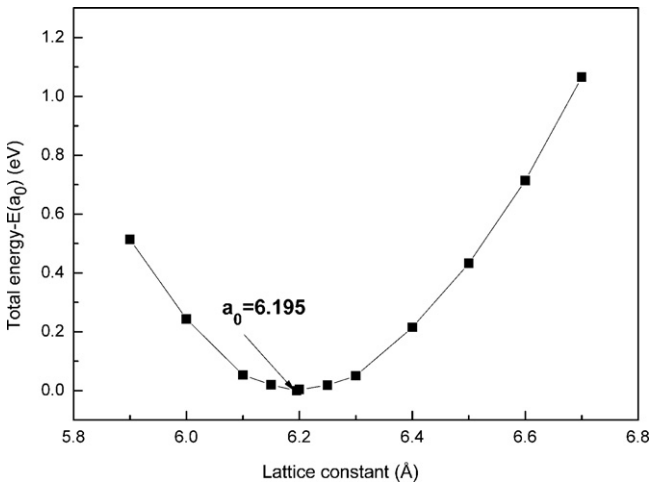

Fig. 1. Calculated total energy vs. the lattice constant for the full-Heusler compound Ti_2NiAl with Hg_2CuTi-type structure. The calculated equilibrium lattice constant for the Hg_2CuTi-type Ti_2NiAl is 6.195 Å, pointed by an arrow in the figure. $E(a_0)$ is the total energy at equilibrium lattice constant and is chosen as zero.

Ultrasoft pseudopotential is used in our calculations. An energy cut-off of 280 eV for the plane-wave expansion and Monkhorst-Pack special k-point mesh $6 \times 6 \times 6$ are used for Brillouin zone integration. The calculations continue until the energy deviation is less than 10^{-6} eV/atom.

3. Results and discussion

The optimized geometry of Ti_2NiAl with Hg_2CuTi-type structure is acquired and a diagram of total energy vs. lattice constant is illustrated in Fig. 1. The equilibrium lattice constant is shown to be 6.195 Å and the corresponding total energy is −4617.59 eV. The following calculations of Ti_2NiAl are based on the Hg_2CuTi-type structure at its theoretical equilibrium lattice constant.

The calculated total magnetic moment of Ti_2NiAl is precisely an integer value of $-3.0\,\mu_B$ per unit cell, well compliant with the SP rule $M_t = Z_t - 24$ [18], where M_t is the total magnetic moment and Z_t is the total number of valence electrons per unit cell. The calculated total density of states (DOS) and atom-projected DOS (PDOS) are presented in Fig. 2. For the total DOS, there is an energy gap of roughly 0.57 eV in the minority spin states around the Fermi level, indicating a half-metallic character and Ti_2NiAl is a true half-metallic ferromagnetism at the equilibrium state. The PDOS of Ni(C) are mainly below the Fermi level and make the largest contribution to the total density of states. For the PDOS of Ti (A) and Ti (B), the minority spin states are mainly situated above the Fermi level. The shapes of PDOS of Ti (A) and Ti (B) are similar although these two atoms have different atomic coordination surroundings.

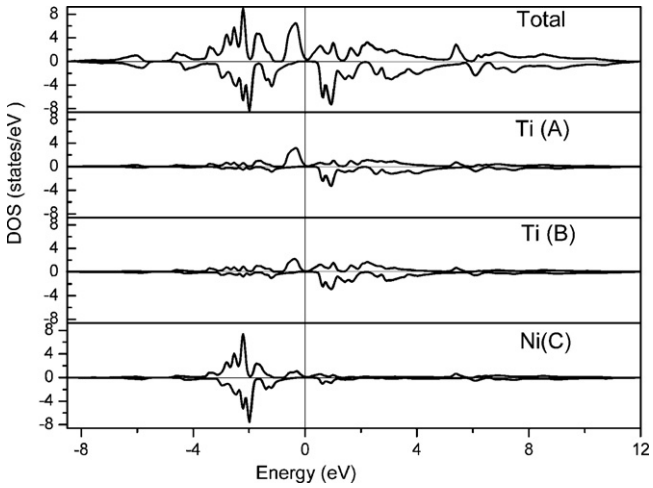

Fig. 2. Calculated total DOS and PDOS for Ti_2NiAl at the corresponding calculated equilibrium lattice constant. The zero energy denotes the position of the Fermi level. The upper halves of each panel display the spin-up states and the lower halves the spin-down states.

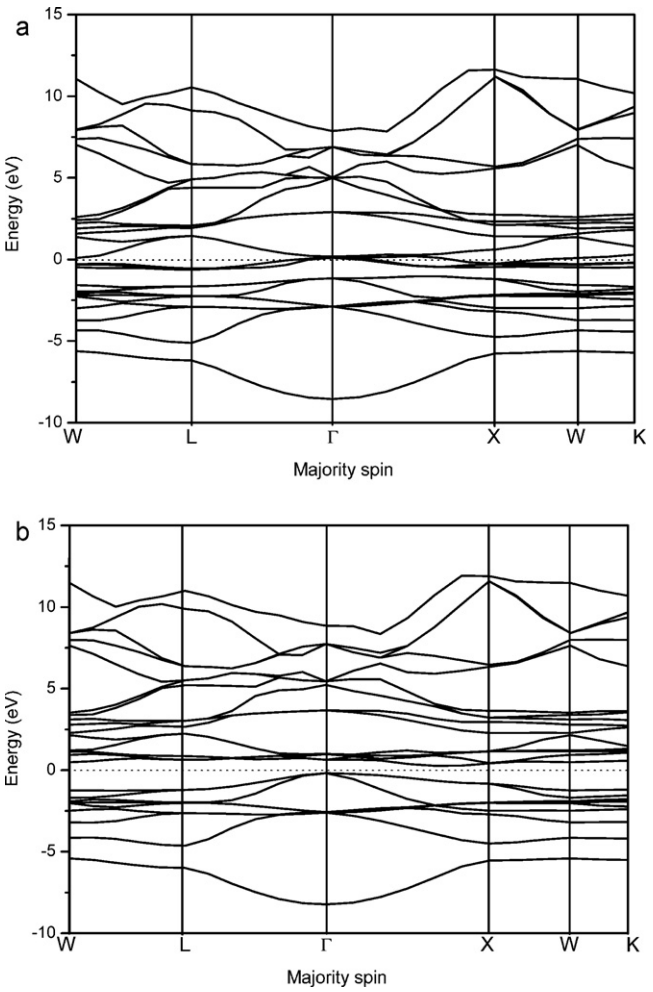

Fig. 3. Calculated band structures of majority spin (a) and minority spin (b) for Ti_2NiAl. The dash dot line denotes the position of the Fermi level.

However, in Cr_2MnAl [12], which is also a Hg_2CuTi-type full-Heusler half-metal, the shapes of PDOS of Cr(A,C) and Cr(B) are very different. In the compound Ti_2NiAl with Hg_2CuTi-type structure, one Ti(A) atom has four nearest Ti(A) and four next-nearest Ti(B) atoms, and one Ti(B) atom has four nearest Ti(B) atoms and four next-nearest Ti(A) atoms. This configuration may cause similar DOS in shape though one Ti(A) atom and one Ti(B) atom have six and four nearest Ni atoms respectively.

There are also small differences between PDOS of Ti(A) and that of Ti(B), since the former have obvious one leading peak on both spin states which become weaker in the latter. In the PDOS of Ti(A), the leading peaks at −0.34 eV and 0.94 eV in the spin-up and spin-down states make a significant exchange splitting which leads to large localized spin magnetic moments of Ti(A) and to the 3d bands of atoms Ti(A) away from the Fermi level. Similar case happens to Ti(B) while the density of states is more dispersive on both spin states which leading to a smaller spin magnetic moment of Ti(B) than that of Ti(A). This divergence is merely the reflection of different Ni coordination surroundings of Ti (A) and Ti(B).

The spin-dependent band structures along high-symmetry directions in the Brillouin zone for Ti_2NiAl are shown in Fig. 3. It can be seen that the majority spin band structure is strongly metallic while the minority spin band structure shows an insulating behavior. It is obvious that there is an indirect band gap around the Fermi level in minority spin band. The Fermi level lies 0.19 eV above the minority spin valence band maximum (VBM) which is the minimum energy required to flip a minority spin electron from the VBM to the majority spin Fermi level, which is very important and often referred to as the "spin-flip gap (HM gap)" [19]. The non-zero HM gap reveals that Ti_2NiAl alloy is a typical half-metal ferromagnetism.

The influence of lattice constant on half-metallic character is also investigated. It is shown that in a −12.8% to +4.9% range of lattice constant the half-metallic character is not affected. This is very useful in the practical applications of this compound because lattice distortion is often inevitably introduced in the production process.

4. Conclusion

In summary, the Ti_2NiAl with Hg_2CuTi-type structure is demonstrated to be a stable full-Heusler compound with an equilibrium lattice constant of 6.195 Å based on first-principles calculations. The computation results of the density of states, electronic bands and magnetic moment have clearly proved that a typical half-metallic ferromagnet with a total magnetic moment of $-3.0\ \mu_B$ per unit cell complies well with the SP rule. The half-metallic character is not affected when the lattice constant changing from −12.8% to +4.9%, implying a promising potential in spintronics and other applications. However, as our knowledge, there have not been reports on ferromagnetism in Ti–Ni–Al Heusler phase. But our results based on first principles calculations present a new half-metallic ferromagnet. So, farther experiments should be performed and more attentions should be paid on the magnetic properties of Ti–Ni–Al ternary system.

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