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A First-Principles Study of a New Heusler Alloy

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Abstract: A full-Heusler alloy *Ti₂NiGa* have been investigated by first-principles calculations. The electronic structures and magnetic properties have been obtained. The compound is predicted to be a new half-metal ferrimagnet. The calculations show that there is an energy gap in the minority spin of the band structures, whereas the other spin is strongly metallic, which results in a complete spin polarization of the conduction electrons at the *Fermi* level. This is the obvious feature of a half-metal. The compound has a total magnetic moment of $3.0\mu_B$ per unit cell on first-principles calculations which is in excellent agreement with the *Slater–Pauling* (*SP*) rule. The magnetic moments of *Ti*(A) atom and *Ti*(B) atoms are different. This difference comes from different atom coordination surroundings of *Ti*(A) and *Ti*(B) atoms in crystal structure.

Keywords: Heusler Alloy, Half-Metal Ferromagnet, First-Principles, Band Structure

1. Introduction

With the rapid development of technology, various high-tech areas become increasingly demanding of new functional materials. There are a lot of functional materials have been found in the Heusler alloys. The Heusler alloys Cu_2MnAl and Cu_2MnSn were firstly found by F. Heusler in 1903 [1], though there are no magnetic elements in the alloys, but they show magnetic characteristics. In 1969, a British P. Webster systematically studied the magnetic properties and crystal structure of the Heusler alloys for the first time [2]. Since then, thousands of similar types of intermetallic compounds have been found, these compounds are still in hot research, and new properties are increasingly being found by researchers. The half-metal, which maybe the most important spin injection source in spintronics have been found in Heusler alloys system. Since de Groot et al firstly introduced the concept ''half-metal'' in studying the half-Heusler alloy NiMnSb [3] in 1983, a lot of half-metal ferromagnets (HMFs) have been predicted in several different kinds of compounds: transition-metal oxides, such as CrO_2 [4] and Fe_3O_4; perovskites, such as Ca_2FeMoO_6, Sr_2FeMoO_6, Ca_2FeReO_6; magnetically doped semiconductors such as Mn-doped GaN and GaAs; and the zinc-blended compounds such as MnBi, CrSb, VTe. The so-called half-metal ferromagnet has the character that one spin direction is metallic at the Fermi level while the other is insulating (or semiconducting). The polarization is thus contributed entirely by one spin direction carriers at the Fermi energy. So it is of great interest to investigate HFMs from both theoretical and technical aspects. A lot of new HMFs have been found in Heusler alloy family. $Co_2MnX(X= Si, Ge)$ have been predicted to be HMFs by Ishida et al [5]. Later, Mn_2VAl [6], Co_2CrAl, Co_2CrGa and Co_2FeSi [7-12] have also been reported to exhibit the characteristics of HMFs in their electronic structures. Cr_2MnAl [13], $Cr_2VX(X= Si, Ge, Sb)$ [14], $Cr_2TiX(X= Ga, Si, Sn, Sb)$ [15] have been reported to be or nearly be HMFs. Recently, Ti_2NiAl [16], Ti_2FeGe [17] also have been reported to be new HMFs. However, though atom Ti has similar electronic configuration as Cr, Ti based Heusler alloy family has not been investigated well to explore for new HMFs.

In this paper, we have performed first-principles calculations on the electronic structure of Ti based full-Husler compound Ti_2NiGa and aimed to seek a new HMF.

2. Computational Details

Many full-Heusler compounds have a cubic L_{21} structure.

The structure is usually represented by the generic formula X_2YZ, where X and Y are 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 the crystal positions described with the Wyckoff coordinates are represented 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). Among them, the A and C sites are similar in space surroundings. Usually, the A, C and the B sites are occupied by the X and Y atoms and the D site is occupied by the Z atom. It is known that in a given Heusler alloy, even if the atom is same, the physical properties such as energy and magnetic moment are different when atoms enter different sites. It has been confirmed that atoms with more 3d electrons prefer to occupy the A, C sites and those with fewer tend to occupy B sites [18]. In Ti_2NiGa, because Ni atom has more 3d electrons than Ti atom, Ni atoms prefer to enter site C (1/2, 1/2, 1/2) while Ti atoms prefer to take sites A and B. As a result, a Hg_2CuTi-type L_{21} structure is developed. Ti atoms entering sites A and B are denoted as Ti(A) and Ti(B) respectively and Ni atoms entering site C are denoted as Ni(C). The calculations are applicable and employed for Hg_2CuTi-type Ti_2NiGa in the following study. In one cell of the material, the four Ga atoms form a tetrahedron, and the Ga atoms occupy the four vertex. The crystal structure of the Ti_2NiGa is showed in Figure 1. The spin-polarized electronic structures calculations are carried out by the plane-wave pseudo-potential method [19], which is based on density functional theory that describes the electron-electron interaction [20-22]. A generalized-gradient approximation (GGA) method proposed in 1996 by Perdew, Burke and Emzerhof and the PBE scheme [23] are chosen to dealing with the exchange–correlation potential. Ultrasoft pseudo-potential and a plane-wave cutoff energy of 280eV are used in all calculations. Special k-points generated with 6×6×6 mesh parameters grid are employed in the irreducible Brillouin zone for all calculations. The calculations continue until the energy deviation is less than 10^{-6} eV/atom.
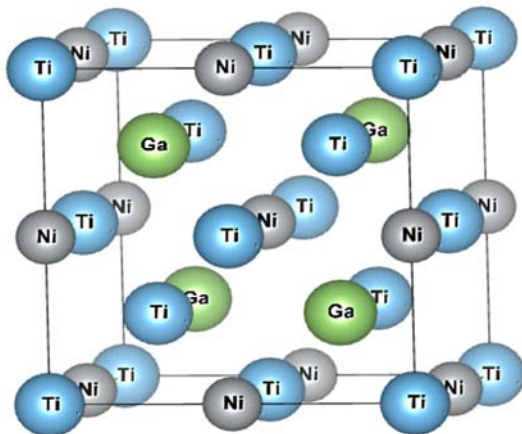

Figure 1. The unit cell of Ti2NiGa with Hg2CuTi-type crystal structure.

3. Results and Discussions

The geometry optimization of the crystal structure has been performed to determine the equilibrium lattice parameters. A diagram (Figure 2) of total energy versus lattice constant is obtained. The lowest total energy locates at a_0=6.18 Å which is considered as the equilibrium lattice parameter. The following calculations are based on the Hg_2CuTi-type structure at a_0.
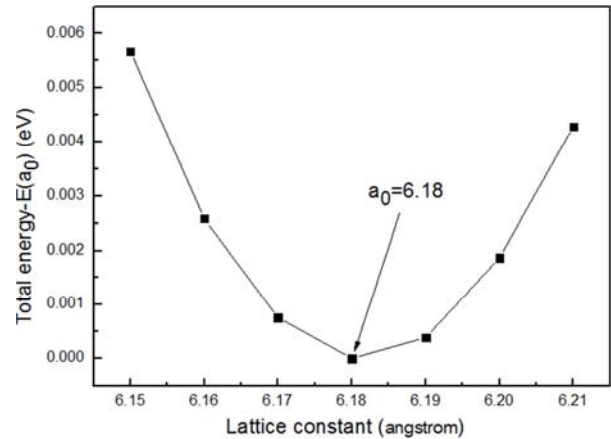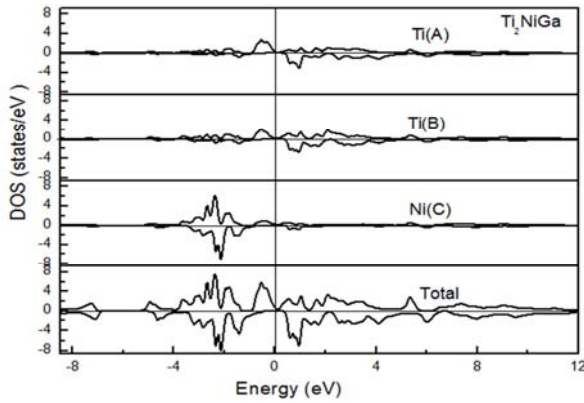

Figure 2. Calculated total energy vs lattice constant for Ti2NiGa full-Heusler compound with Hg2CuTi-type structure. The calculated equilibrium lattice constant is 6.18 Å as indicated by arrow. The energy at equilibrium lattice constant E(a0) is chosen as zero in the vertical axis.

The calculated total moment of Ti_2NiGa is precisely an integral value of $3.0\mu_B$ per unit cell at its equilibrium state, well consistent with the SP rule $M_t = Z_t - 18$ [24-26], where M_t is the total 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 Figure 3. For the total DOS, there is an energy gap about 0.75eV in the minority spin states around the Fermi level, demonstrating a half-metallic feature. The spin states of Ni(C) are mainly below the Fermi level and make a significant contribution to the total density of states. The magnetic moment of Ni(C) is -0.06μ_B, which may be derived from its low exchange splitting in energy band. From the PDOS of Ti (A) and Ti (B), the minority spin states are shown to be mostly concentrated above the Fermi level. In the PDOS of Ti(A), the leading peak at -0.52eV and 0.95eV in the spin-up and spin-down states make a large exchange splitting which leads to a large localized spin magnetic moment 1.96μ_B of Ti(A) and to the polarization of Ti(A) 3d bands away from the Fermi level. In the PDOS of Ti(B), there are no obvious leading peaks for the up and down spin states and the densities are more dispersive on both spin directions which leads to a smaller spin magnetic moment of Ti(B) than that of Ti(A). The shapes of PDOS of Ti (A) and Ti (B) are different which is the similar case in Cr_2MnAl [13]. In Cr_2MnAl, which is also a HMF with Hg_2CuTi-type full-Heusler structure, the shapes of PDOS of Cr(A,C) and Cr(B) are very distinct. The differences of Ti(A) and Ti(B) in DOS shape should come from the atom coordination configuration [25] since Ti(B) atoms are located in a more symmetric coordination in contrast to Ti(A) atoms. The spin magnetic moment of Ti(B) is 1.36μ_B, smaller than

that of Ti(A). The magnetic moment of atom Ga is $-0.26\mu_B$ which is unparallel with those of Ti(A) and Ti(B).

Figure 3. *The calculated total DOS and PDOS for the Hg₂CuTi-type Ti₂NiGa at the equilibrium lattice constant; the upper halves of each panel denote the spin-up states and the lower halves are the spin-down states.*

The spin-dependent energy bands along high-symmetry directions in the Brillouin zone for Ti₂NiGa are shown in Figure 4. It can be seen that the majority spin-dependent band structure is strongly metallic, while the minority shows insulating character. It is obvious that there is an indirect band gap around the Fermi level in minority spin band. The Fermi level lies at 0.46 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 [26]. The non-zero gap indicates that Ti₂NiGa alloy is a typical half-metal.
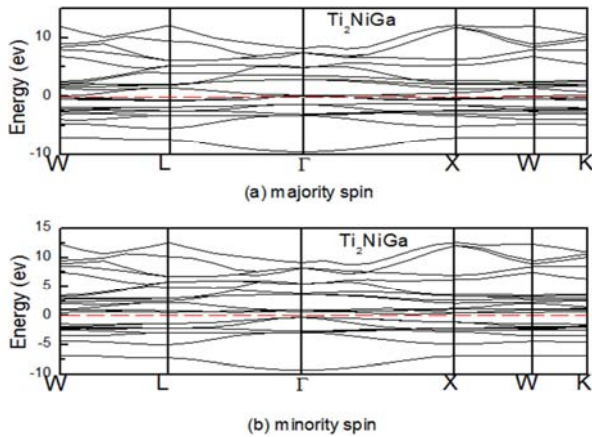
Figure 4. *Majority spin (a) and minority spin (b) band structures for Hg2CuTi-type Ti₂NiGa at the equilibrium lattice constant of 6.18 Å. The zero of energy denotes the position of the Fermi level.*

In the paper, the crystal structure and the electric structure were studied using GGA method, but, one who had the experimental condition could try to prepare the alloy Ti₂NiGa, they would use X-ray diffraction method to confirm the structure, so the calculated X-ray diffraction was done, the data were plotted in the Figure 5. In the figure, the (111) diffraction peak is at 25 degree, and (200) diffraction peak is at 29 degree, the existence of the two diffraction peaks implies

ordered crystal structure exists. Because the Hg₂CuTi-type structure is a high ordered crystal structure, the high order is sensitive to the impurities, so the metal raw materials should be high purity.
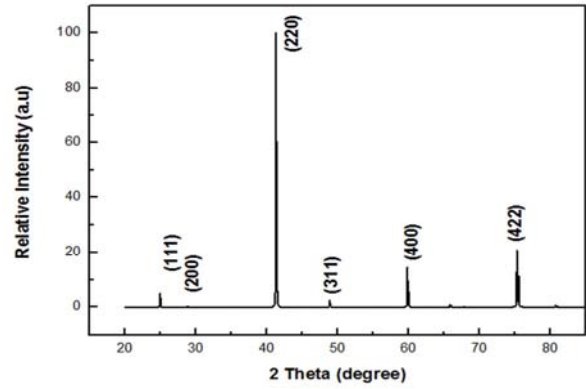
Figure 5. *Calculated X-ray powder diffraction of Ti₂NiGa with Hg2CuTi-type crystal structure.*

4. Conclusion

In summary, Ti₂NiGa with Hg₂CuTi-type structure is confirmed to be a new half-metal ferrimagnet on first-principles calculations and exhibits a promising potential for spintronics and other applications. It has a total moment of $3.0\mu_B$, which is in excellent agreement with the SP rule. The band structures calculations also show the half-metallic character. The magnetic moments of Ti(A) and Ti(B) are $1.96\mu_B$ and $1.36\mu_B$ respectively which are larger that of Ni(C). The differences in magnetic moments between Ti(A) and Ti(B) should come from the different atom coordination configurations in crystal structure.

Acknowledgements

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