J Supercond Nov Magn (2015) 28:3553–3556
DOI 10.1007/s10948-015-3187-2

ORIGINAL PAPER

V_2NiSe: a First-Principles Study

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Received: 20 May 2015 / Accepted: 23 July 2015 / Published online: 14 August 2015

Abstract The Heusler alloy system is a rich source of functional materials. We studied the ternary alloy V_2NiSe by first-principles calculations to explore for a new functional alloy. We performed geometry optimization for the alloy with Hg_2CuTi-type structure and obtained the equilibrium lattice parameter a_0. The magnetic moment of the compound is 0.707 μ_B in 1-unit cell. The total density of states and the partial density of states were calculated. The band structure was also studied. The magnetic moment of the two vanadium atoms in 1-unit cell in different space positions is different.

Keywords Heusler alloy · Magnetic property · Band structure · Magnetic moment

1 Introduction

Nowadays, new technology and new materials are changing the human life. New materials are rather important because they serve as the foundation of the new technology. In ancient times, humans used natural wood and stone to make tools and then humans learned to make porcelain and smelting technology; especially when the iron and steel smelting technology was invented, humans obtained a kind of widely used material. This material is cheaper for the iron ore reserves are very great and mining of iron ore is also easier. Steel materials are used in many areas of life, such as building construction, bridges and railway construction, machinery manufacturing, automotive manufacturing, etc. Although the steel is widely used, it is a common material unable to satisfy the demand of new technology's development; functional materials are much important, as far as humans have found many kinds of functional materials, such as semiconductor materials, shape memory alloys, superconductors, energy storage materials, piezoelectric materials, ferroelectric materials, refrigerant, various optical materials, ceramics, etc. Among the functional materials, metal alloy functional material is an important part. An Heusler alloy is an important part of metal alloy functional materials. The Heusler alloys possess a lots of unusual physical and chemical properties, thus having a potential application value. Thus, the Heusler alloy is the hot material system to explore for new functional materials in condensed matter physics and materials science. So far, magnetoresistance effect [1], completely spin-polarized electronic half-metal effect [2], ferromagnetic metal intermetallic compounds composed of non-ferromagnetic elements [3], superconducting Heusler alloys with rare earth elements [4], ferromagnetic shape memory alloys [5–7], and superelastic alloys have been found in the Heusler alloy system. Just recently, martensitic transformation driven by a magnetic field has been found firstly in Heusler alloys [8–10]. All the above properties attract interests of people for the researches of Heusler alloys. In 1903, F. Heusler [11] first reported the Cu_2MnAl and Cu_2MnSn series magnetic alloys with high chemical ordering which were usually called Heusler alloy. Since then, numerous Heusler alloys have been found. However, vanadiumbased Heusler alloys have not been well investigated. In this paper, we have

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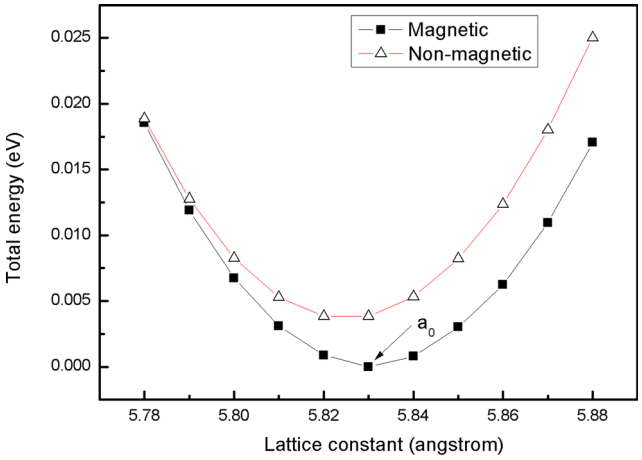

Fig. 1 Calculated total energy at magnetic and non-magnetic states versus lattice constant for V_2NiSe. The equilibrium lattice constant is indicated by an *arrow*. The energy at equilibrium lattice constant ($E(a_0)$) is chosen as zero in the *vertical axis*

performed first-principles calculations of the electronic structure of V-based full-Heusler alloy V_2NiSe.

2 Crystal Structure and Computational Methods

The space structure of Heusler alloy has an O_h symmetry, consisting of four face-centered cubic sub-lattices interpenetrating along the space diagonal with a quarter of the length of the diagonal. Generic formula X_2YZ used represented the structure, where X and Y are transition metal elements and Z is a group element. The structure crystal positions described with the unique sites 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 and C sites 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 stoichiometric ratio, even if the atom is the 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 and C sites and those with fewer tend to occupy the B sites [10]. In V_2NiSe, which is with a Hg_2CuTi-type structure, V atoms enter site A (0, 0, 0) and site B (1/4, 1/4, 1/4) while Ni atoms take site C (1/2, 1/2, 1/2). V atoms entering sites A and B are denoted as V(A) and V(B), respectively. The following calculations are applicable and employed for Hg_2CuTi-type V_2NiSe in the present study. The spin-polarized electronic structure calculations are carried out using the plane-wave pseudo-potential method [12], which is based on density functional theory that describes the electron–electron interaction [13–15]. A generalized gradient approximation (GGA) proposed in 1996 by Perdew, Burke, and Emzerhof and a PBE scheme [16] are chosen to dealing with the exchange–correlation potential. Ultrasoft pseudo-potential and a plane-wave cut-off energy of 500 eV are used in all calculations. Special k-point 1728 is employed in the irreducible Brillouin zone for all calculations. The calculations continue until the energy deviation is less than 10^{-6} eV/atom.

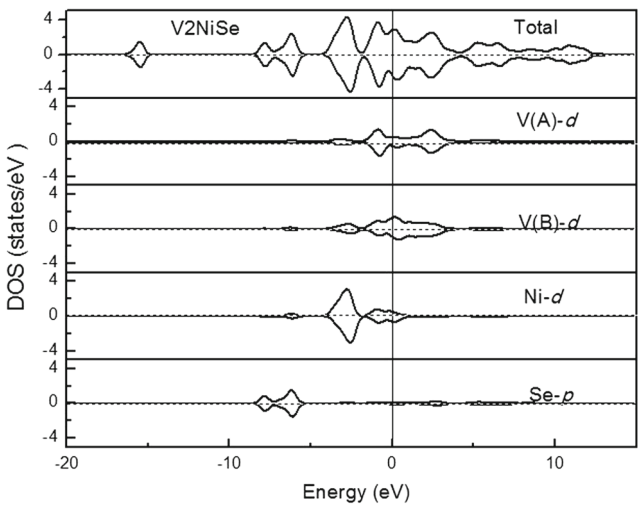

Fig. 2 The calculated total DOS and PDOS for the V_2NiSe at the equilibrium lattice constant. The *upper halves of each panel* denote the spin-up states, and the *lower halves at each fraction map* are the spin-down states

3 Computational Results and Discussions

We have performed geometry optimization on V_2NiSe to determine the equilibrium lattice parameters. The energy at different lattice parameters with magnetic and non-magnetic states is calculated. We found that the magnetic state had lower energy at each equilibrium lattice parameter.

So, for the compound, the lowest total energy ($E(a_0)$) is -5559.856 eV and the corresponding lattice parameter (a_0) is 5.83 Å which is identical to the theoretical equilibrium lattice parameter. A diagram of total energy versus lattice constant (Fig. 1) is obtained. In the figure, the lowest total energy ($E(a_0)$) is chosen as zero in the vertical axis. The following calculations are based on the Hg_2CuTi-type structure at its theoretical equilibrium lattice constant.

The calculated total moment of V_2NiSe is 0.70 μ_B per unit cell at its equilibrium state. The calculated total density of state (DOS) and atom-projected DOS (PDOS) are presented in Fig. 2. The shape of spin states of V(A) and V(B) is not similar which indicates that the interaction of atom V(A) and V(B) is not strong. The shape of PDOS of

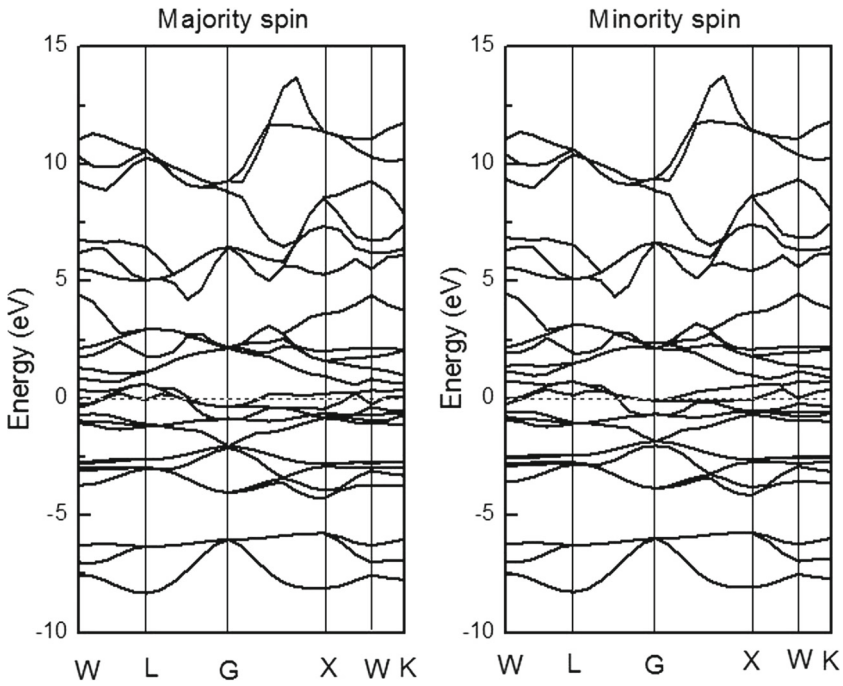

Fig. 3 Majority-spin (**a**) and minority-spin (**b**) band structures of V_2NiSe. The *dash line* denotes the position of the Fermi level

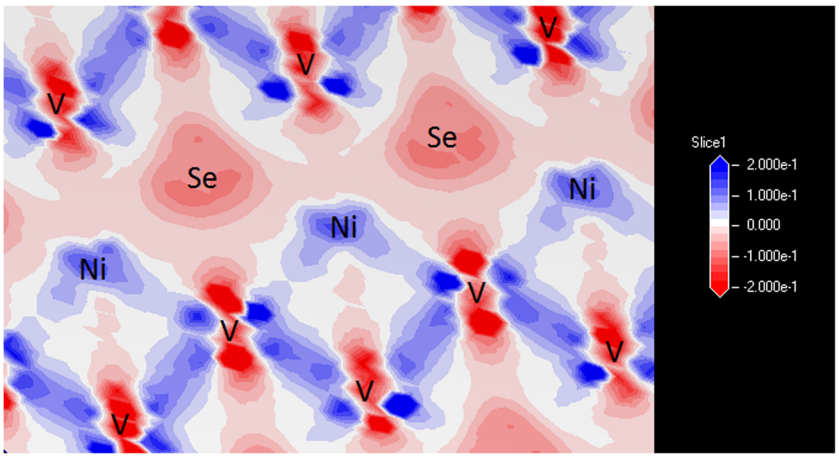

Fig. 4 Difference of electron density of V_2NiSe

V(A) is almost symmetrical, so the magnetic moment of atom V(A) is only $-0.02\ \mu_B$. However, the shape of PDOS of V(B) is with obvious asymmetry and atom V(B) has a larger magnetic moment of $0.46\ \mu_B$. The PDOS shape of atom Ni is nearly symmetrical, which causes a little magnetic moment of $0.24\ \mu_B$. The magnetic moment of atoms V(A) and V(B) is antiparallel, so the alloy is ferrimagnetic. From the PDOS of Ni, the minority-spin states are shown to be mostly concentrated below the Fermi level. The magnetic moment of sp atom Se is $0.02\ \mu_B$. Atom V(A) having a magnetic moment is interesting, and this situation comes from the characteristic spatial occupation of the atoms in the Heusler structure.

The spin-dependent energy bands along high-symmetry directions in the Brillouin zone for V_2NiSe are shown in Fig. 3. In the majority-spin band, the valence band overlaps with conduction band and the Fermi level passes through the overlapping region. So, majority of the band shows a conducting character. In the minority-spin-dependent band, it has a very similar shape with the majority-spin band, showing a metal property.

From the difference of electron density, the bonding situation between atoms, charge distribution, and transfer can be understood, so the difference of electron density of V_2NiSe is obtained. From Fig. 4, one can see that both positive and negative charge densities around atom V are large; electrical

charge is closer to vanadium atoms, showing the metallic bonding properties; adjacent V atoms interact strongly; electrical charge around Ni atom is small; there is d–d exchange between atoms Ni and V; and atom Se provides the bonding state charge.

4 Conclusion

In summary, V_2NiSe alloy with a Hg_2CuTi-type structure is confirmed to be a new Heusler alloy on first-principles calculations and it may have potential applications for high-tech industries. The magnetic state has lower energy than the non-magnetic state at each equilibrium lattice parameter. It has a total moment of 0.70 μ_B. The band structure calculations show a metallic character. The magnetic moment of V(A) and V(B) is -0.02 and 0.46 μ_B, respectively, which is antiparallel, so the alloy is a ferrimagnet.

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