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Electronic and magnetic properties of Cr-Mn-Ni-Al compound with LiMgPdSb-type structure

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ABSTRACT

We investigate the electronic and magnetic properties of Cr-Mn-Ni-Al compound with a LiMgPdSn-type structure in three different atomic arrangement configurations (AAC) by using the first-principles calculations. It was found that Cr-Mn-Ni-Al compound with type I AAC exhibits a spin-gapless semiconductive characteristic. The type II AAC is the most stable one and exhibits an especial band structure where the Fermi level slightly crosses the top of the valence bands in spin-up channel and the bottom of conductive bands in spin-down channel, which leads to the electronic transport with the spin-resolved carrier type. The Cr-Mn-Ni-Al compound shows an ordinary metallic behavior in type III AAC. The three nonequivalent atomic arrangement configurations of Cr-Mn-Ni-Al are all in ferromagnetic ground state under their equilibrium lattice parameters.

1. Introduction

Spin-gapless semiconductors (SGS), as a new concept in spintronics, were first reported theoretically and verified experimentally in doped Pb-based oxide materials by Wang in 2008 [1,2]. They uniquely merges the properties of zero-gap semiconductor and half-metallic (HM) ferromagnets, and can be regarded as the combination of them. There are four possible band structure configurations with spin-gapless features as shown in Fig. 1(a)–(d). For the first case (Fig. 1(a)), one spin channel is gapless, while the other spin channel is semiconducting. In the second case (b), one spin channel is gapless, and the other spin channel is semiconducting with the top of the valence band next to the Fermi level. In the third case (c), one spin channel is gapless while the bottom of the conduction band for the other spin channel touches the Fermi level, which is separated from its corresponding valence band by a gap. In the fourth case (d), there is a gap between the conduction and valence bands for both the majority and minority electrons, while there is no gap between the majority electrons in the valence band and the minority electrons in the conduction band. From these spin-gapless semiconductor band structures, one can see that no energy is required to excite electrons from the valence band to the conduction band and not only the excited electrons but also the holes can be completely spin-polarized. The special band structure of SGS leads to some novel transport properties and new functionalities of spintronic devices.

In recent several years, several different classes of materials have been theoretically and experimentally reported to be new SGSs, such as N-doped zigzag grapheme nanoribbons [3], zigzag silicone nanoribbons with asymmetric sp^2–sp^3 edges [4], and several binary, ternary and quaternary Heusler compounds [5–11]. Among them, Heusler compound is one of the most important one. Heusler compound Mn_2CoAl [4], which was previously calculated to be a half-metallic ferromagnet by our previous work [12], has been realized to be a SGS experimentally. A series of inverse Heusler compounds [5] and DO_3-type Heusler compounds [5] were found to be promising candidates for SGSs. Most recently, I. Galanakis [9] and Xu et al. [8] show theoretically that five quaternary Heusler compounds: CoFeMnSi, CoFeCrAl, CoMnCrSi, CoFeVSi and FeMnCrSb would be probable SGSs. They also reveal a semi-empirical general rule: the spin-gapless feature should occurs in the Heusler compounds with the total valence electrons number of 26 or 28. Heusler compounds are a huge family that has been applied in many areas due to their multi-function and numerous properties [13]. In the present work, we substitute one of the Mn atom with Cr atom in the Mn_2NiAl Heusler compound, which has been predicted to be a ferromagnetic shape-memory alloy (FSMA) [14], forming a new quaternary Heusler compound: Cr-Mn-Ni-Al with the total valence electrons number of 26. It follows the semi-empirical general rule that has been mentioned in reference 12. Cr-Mn-Ni-Al compound have three different atomic arrangement configurations (AAC). In this paper, we investigate the electronic and magnetic properties of Cr-Mn-Ni-Al compound with three different atomic arrangement configurations.

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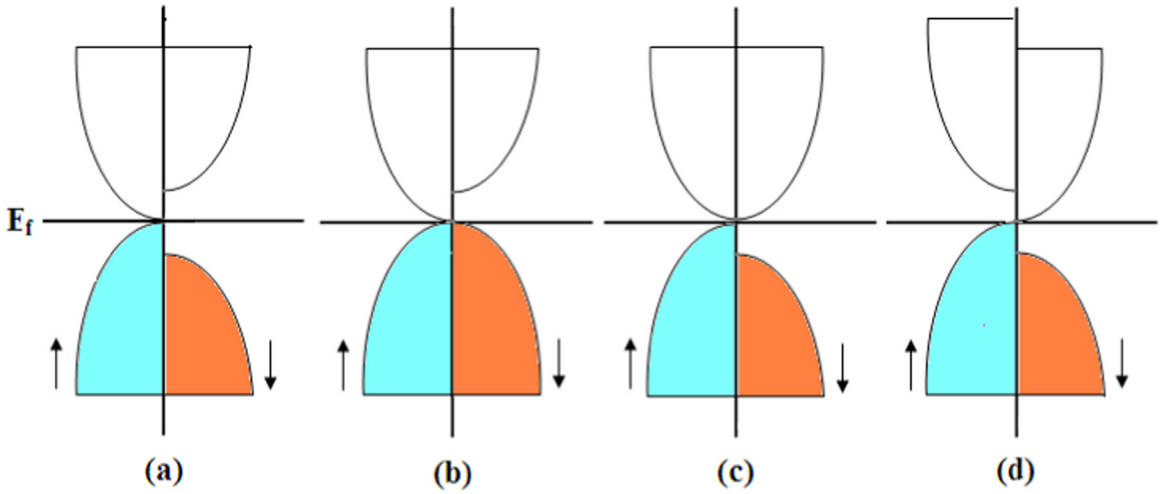

Fig. 1. Density-of-states (DOS) scheme of the four possible band structure configurations with spin gapless features: (a)–(d). Filled areas represent occupied states, and the arrows indicate majority (↑) spin and minority (↓) spin.

2. Computational details

Our calculation used the CASTEP code based on the pseudopotential method with a plane-wave basis set [15,16]. We adopt the generalized gradient approximation (GGA) in the Perdew–Bueke–Ernzerhof scheme for the electronic exchange-correlation functional [17,18]. The interactions between the valence electrons and the atomic core were described by the ultrasoft pseudopotential [19]. A plane-wave basis set cut-off energy of 400 eV and a mesh of $12 \times 12 \times 12$ k-points were employed to ensure good convergence. The calculations continue until the energy deviation is less than 1×10^{-6} eV/atom. By performing the geometry optimization calculation, we obtained the equilibrium lattice constants.

3. Results and discussion

Quaternary Heusler compound has the chemical formula X-Y-M-Z, where the X, Y and M are transition metal atoms. The structural prototype of the quaternary Heusler compounds is the LiMgPdSb [20], with the space group of $F\bar{4}3m$. There are three possible different types of atom arrangement in the quaternary Heusler compound X-Y-M-Z: typeI(XMYZ) X (0,0,0), Y (1/4,1/4,1/4), M (1/2,1/2,1/2) and Z (3/4,3/4,3/4); typeII(YMXZ) X (1/4,1/4,1/4), Y (0,0,0), M (1/2,1/2,1/2) and Z (3/4,3/4,3/4); type III (YXMZ) X (1/2,1/2,1/2), Y (0,0,0), M (1/4,1/4,1/4) and Z (3/4,3/4,3/4). In order to determine the equilibrium structure of the quaternary Heusler compounds Cr-Mn-Ni-Al studied, we firstly perform geometry optimization for Cr-Mn-Ni-Al in their respective three different configurations by calculating the total energy as a function of volumes, the optimized results are shown in Fig. 2. For all the Cr-Mn-Ni-Al, the structure of type II AAC (MnNiCrAl) is the most stable one among the three configurations due to the lowest energy and type III AAC (MnNiCrAl) is the highest one. This indicates that this quaternary Heusler compound with a 1:1:1:1 stoichiometry prefers crystallizing in the type II AAC (MnNiCrAl) structure. The type I (CrNiMnAl) structure is the metastable state, and it is possible to transform from type II (MnNiCrAl) to type I (CrNiMnAl) structure under an external driving force. The obtained equilibrium lattice parameters of CrNiMnAl, MnNiCrAl and MnCrNiAl are 5.665 Å, 5.638 Å and 5.660 Å, respectively.

The band structures of the three nonequivalent structures were calculated with the optimized lattice parameter. The calculated results are shown in Figs. 3–5. From Fig. 3, it can be seen that the

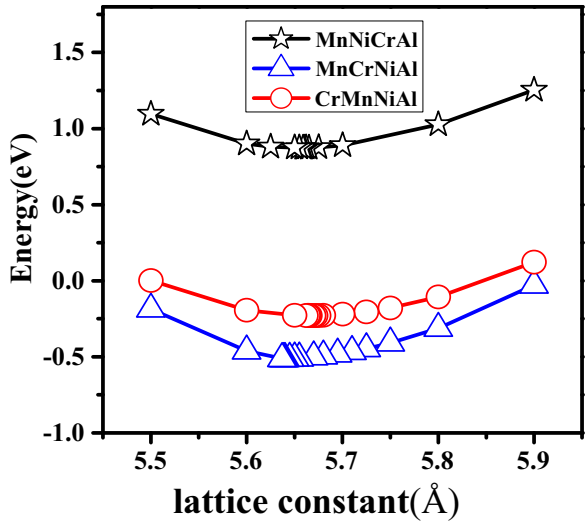

Fig. 2. (Color online) The optimization curves of lattice parameter for MnCrNiAl (five-pointed star line), MnNiCrAl (hollow triangle line), CrNiMnAl (hollow round line) compounds. The total energy is a relative value.

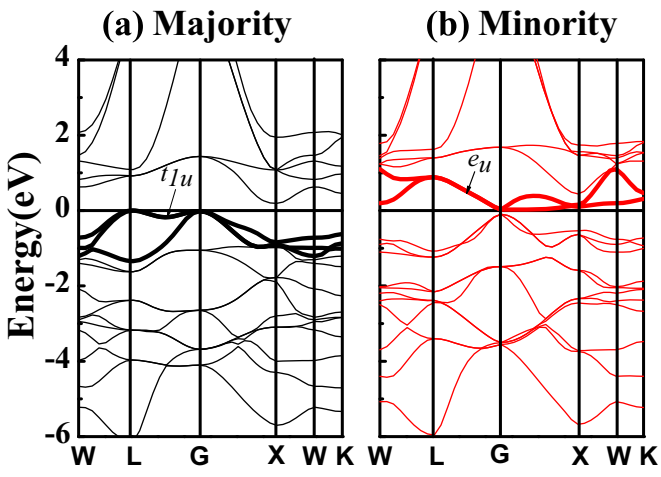

Fig. 3. (Color online) Part of the band structure and density of states (DOS) of CrNiMnAl (a) majority spin (the bold lines are used to emphasize the top of the valence band in majority spin and the bottom of the conduction band in minority spin), (b) minority spin.