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Possible martensitic transformation and ferrimagnetic properties in Heusler alloy Mn_2NiSn

Ying-Ni Duan [a,*], Xiao-Xi Fan [a], Abdugheni Kutluk [a], Xiu-Juan Du [b], Zheng-Wei Zhang [c], Yu-Ling Song [d]

[a] Department of Medical Engineering and Technology, Xinjiang Medical University, Urumqi 830011, Xinjiang, PR China
[b] School of Applied Science, Taiyuan University of Science and Technology, Taiyuan 030024, Shanxi, PR China
[c] Chemistry and Chemical Engineering Laboratory, The Xinjiang Technical Institute of Physics & Chemistry, Chinese Academy of Sciences, Urumqi 830011, Xinjiang, PR China
[d] College of Physics and Electronic Engineering, Nanyang Normal University, Nanyang 473061, Henan, PR China

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ABSTRACT

The electronic structure and magnetic properties of Hg_2CuTi-type Mn_2NiSn have been studied by performing the first-principle calculations. It is found that the phase transformation from the cubic to the tetragonal structure reduces the total energy, indicating that the martensitic phase is more stable and the phase transition from austenite to martensite may happen at low temperature for Hg_2CuTi-type Mn_2NiSn. Concerning the magnetism of Hg_2CuTi-type Mn_2NiSn, both austenitic and martensitic phases are suggested to be ferrimagnets. Furthermore, martensitic transformation decreases the magnetic moment per formula unit compared with austenitic phase. The results are helpful to accelerate the use of Mn_2NiSn alloys in the series for magnetic shape memory applications.

1. Introduction

Recently, researches on ferromagnetic shape memory alloys (FSMAs) have attracted considerable attention for their potential applications in many technical fields like magnetic actuator or magnetocaloric materials. The first FSMA is Ni_2MnGa, which is a Heusler alloy and large magnetic field-induced strain (MFIS) has been observed in it [1–4]. However, the problems in using Ni_2MnGa as a commercial magnetic field induced actuator are its brittleness and that the MFIS is highly dependent on the crystal quality. To overcome these problems, current research efforts are directed toward search for new FSMAs [5]. Ni–Fe–Ga could have been an alternative but it exhibits only 0.02% reversible MFIS at 100 K. However, addition of Co in Ni–Fe–Ga increases the MFIS to 0.7% at 300 K [6]. From density functional theory and experimental studies, the results showed Ga_2MnNi to be a FSMA at room temperature (T_C=330 K) with high martensitic start temperature (T_M =780 K) [7]. In nonstoichiometric Ni–Mn–Ga compositions, evidence of reversible martensites that are also ferromagnetic has been reported [8,9]. The martensitic transformation can be induced by external magnetic filed [10–12]. Accompanied with this, many interesting physical properties have been observed. So, exploring new FSMAs and investigating their properties can be a quite meaningful work.

Till now, research on the fully stoichiometric Mn_2NiX is rather limited and experimental information on phase stability and magnetic property of Mn_2NiAl and Mn_2NiIn are not yet available. The results from first-principles calculations in these systems have started to come up only recently [13–21]. So it is necessary to make a systematic analysis on the trends in the structural and magnetic properties in these systems based upon their electronic structures for two reasons: (1) to ascertain the usefulness of the alloys in the series for magnetic shape memory applications that is whether martensitic transformation can be realized around room temperature and the other key parameter like the magnetization is substantial; (2) to ascertain the role of the electronic structure in interpreting the similarities and the differences among the members in the series with regard to their properties related to magnetic shape memory effects.

In this work, the magnetic and electronic properties of Mn_2NiSn alloys with cubic and tetragonal phases are investigated by using the first-principle. Also, the possibility of martensite transformation behavior in the alloy is predicted. These results can

* Corresponding author.
E-mail address: duanyingni@163.com (Y.-N. Duan).

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help to discover and prepare new FSMAs. The rest of the paper is organized as follows: The computational methods and model are summarized in Section 2, and the calculated results as well as the corresponding discussions are presented in Section 3. Finally, in Section 4, we propose some conclusive remarks.

2. Computational methods and model

In this paper, the calculations are performed using the Vienna *ab-initio* simulation package (VASP) based on the density function theory (DFT) [22–24]. The electron-ionic core interaction is represented by the projector augmented wave (PAW) potentials [25] which are more accurate than the ultra-soft pseudopotentials. To treat electron exchange and correlation, we choose the Perdew–Burke–Ernzerhof (PBE) [26] formulation of the generalized gradient approximation (GGA). A conjugate-gradient algorithm is used to relax the ions into their ground states, and the energies and the forces on each ion are converged within 1.0×10^{-4} eV/atom and 0.02 eV/Å, respectively. The cutoff energy for the plane-waves is chosen to be 450 eV. A $9\times9\times9$ Monkhorst-Pack grid for *k*-point sampling is adopted for Brillouin zone integration, together with a Gaussian smearing broadening of 0.2 eV.

The Heusler alloys represent a class of ternary intermetallic compounds with the general formula X_2YZ where X and Y are transition metal elements and Z is a main group element [27]. Usually, the Heusler structure can be looked as four interpenetrating face-centered-cubic (fcc) lattices and has four unique crystal sites namely A (0,0,0), B (1/4,1/4,1/4), C (1/2,1/2,1/2), D (3/4,3/4,3/4) in Wyckoff coordinates, as shown in Fig. 1. It is found that the site preference of the X and Y atoms is strongly influenced by the number of their valence electrons [28]. The Y atom will occupy B site (Cu_2MnAl-type structure) or C site (Hg_2CuTi-type structure), which rests with its less or more valence electrons compared with X atom. For alloy Mn_2NiSn the two Mn atoms occupy the A (0,0,0) and B (1/4,1/4,1/4) sites, and residual Ni and Sn atoms enter the C (1/2,1/2,1/2) and D (3/4,3/4,3/4) sites respectively, which is known as the Hg_2CuTi-type of the structure [29–32]. This structure is different from the Cu_2MnAl-type structure in which the two Mn atoms occupy the A (0,0,0) and C (1/2,1/2,1/2) sites equally and leave the B (1/4,1/4,1/4) site to Ni.

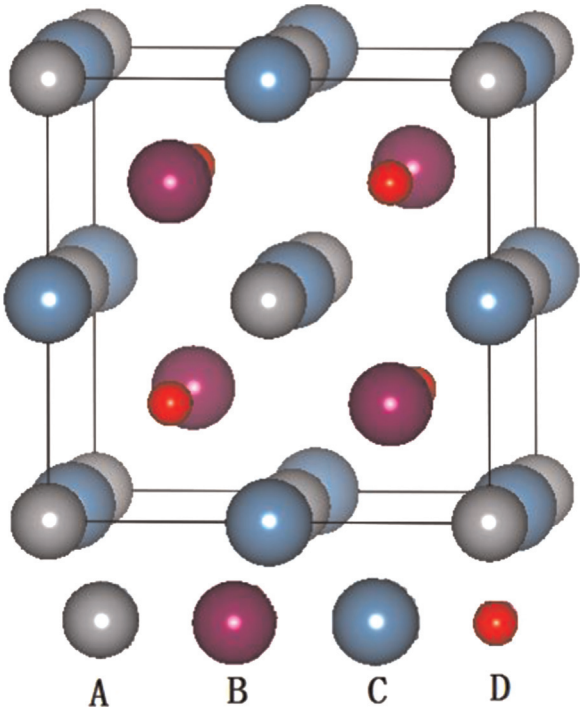

Fig. 1. Crystal structure of Heusler alloy. The unit cell has four crystal sites as the basis: A (0,0,0), B (1/4,1/4,1/4), C (1/2,1/2,1/2) and D (3/4,3/4,3/4) in Wyckoff coordinates.

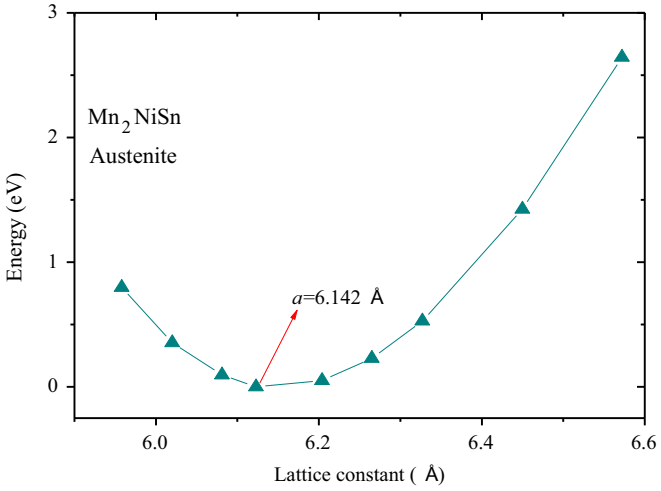

Fig. 2. Calculated total energy as a function of the lattice constant for Mn_2NiSn with the Hg_2CuTi-type structure in ferrimagnetic state. The minimum total energy at equilibrium lattice constant is chosen as zero.

Table 1
The calculated lattice constants *a*, *b*, *c* and atomic magnetic moments for austenitic and martensitic Mn_2NiSn.

Compounds	*a* (Å)	*b* (Å)	*c* (Å)	*c*/*a*	$M_{Mn(A)}$ (μ_B)	$M_{Mn(B)}$ (μ_B)	M_{Ni} (μ_B)
Mn_2NiSn austenite	6.142	6.142	6.142	1.000	−2.981	3.400	0.111
Mn_2NiSn martensite	5.813	5.813	6.859	1.180	−3.045	3.335	0.033

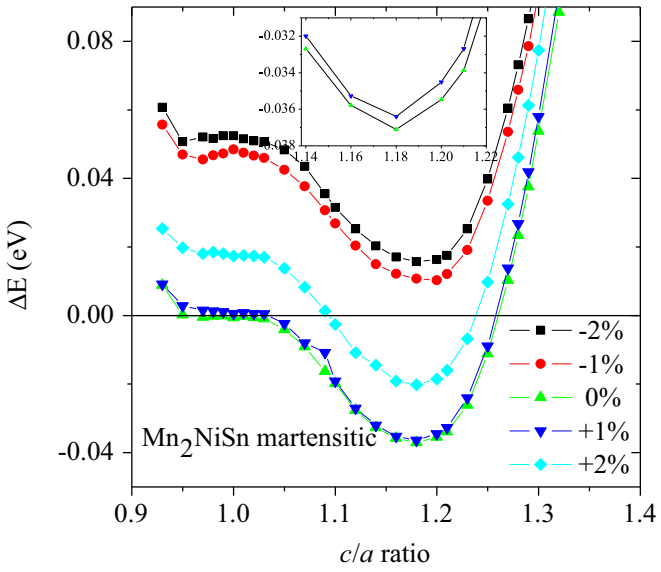

Fig. 3. Total energy as a function of the *c*/*a* ratio for the Hg_2CuTi-type Mn_2NiSn with martensitic phase. The total energy of the cubic austenitic phase (*c*/*a*=1) is chosen as zero.

3. Results and discussion

To determine the lattice constant the austenitic Mn_2NiSn alloy,