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First-Principles Study on the Crystal Structure and Martensitic Transformation of Ni_2MnZ (Z=Ti, V) Alloys

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Abstract: All-d-metal Heusler alloys have emerged as promising multifunctional materials. Based on first-principles methods, this paper investigates the crystal structure and martensitic transformation characteristics of Ni_2MnZ (Z=Ti, V) alloys. In the cubic phase, the FCC structure exhibits stability. When the c/a ratio ranges from 1.2 to 1.6, ΔEtot is negative and presents a local minimum, indicating the occurrence of martensitic transformation. It is concluded that the all-d-metal Heusler alloys Ni_2MnZ (Z=Ti, V) hold great potential in material design and applications. Further research can explore the influence of different alloy compositions on their microstructures to achieve broader application value.

Keywords: First-principles calculation; Martensitic transformation; Crystal structure; All-d-metal Heusler alloy

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1. Introduction

Heusler alloys occupy an important position in modern materials science due to their unique shape memory properties [1]. Ni-Mn-Ga alloy was the first ferromagnetic shape memory alloy discovered to possess both ferromagnetism and martensitic transformation characteristics, but it has limitations such as mechanical response constraints and low transformation temperature [2]. The emergence of all-d-metal Heusler alloys has effectively addressed these drawbacks. The research group led by Liu Enke from the Institute of Physics, Chinese Academy of Sciences, promoted the development of Ni-Mn-Ti-based Heusler alloys in 2015 [3–4]. Such alloys form stable chemical bonds through d-d electron hybridization instead of p-d hybridization, significantly improving the mechanical properties of the materials [5]. Ni_2MnZ (Z=Ti, V) alloys exhibit shape memory effect and excellent barocaloric effect [6]. Solid-state refrigeration technology based on martensitic transformation is characterized by high energy efficiency and environmental friendliness [7–8]. The general chemical formula of Heusler alloys is X_2YZ [9]. **Figure 1(a)** shows the $L2_1$ structure, where X atoms occupy (0.25, 0.25, 0.25) and (0.75, 0.75, 0.75), Y and Z atoms are located at (0.5, 0.5, 0.5) and (0, 0, 0), with a space group of Fm-3m. The XA structure has a space group of F-43m. When the Ni_2MnZ alloy in the $L2_1$ phase undergoes tetragonal deformation along the [110] crystal direction, it forms a BCT structure (**Figure 1(b)**), which can be further transformed into an FCC structure (**Figure 1(c)**) [10].

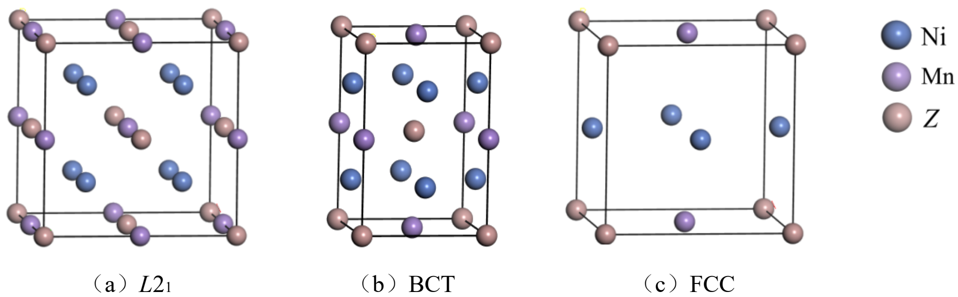

Figure 1. Crystal structures of Ni_2MnZ alloys: (a) $L2_1$; (b) BCT; (c) FCC

Calculation methods and parameter settings: In this paper, first-principles EMTO and CASTEP methods are used to calculate Ni_2MnZ (Z=Ti, V) alloys, combined with the Generalized Gradient Approximation (GGA) and Coherent Potential Approximation (CPA) methods. The EMTO wave function basis set includes s, p, d, and f orbitals, adopting the scalar relativistic approximation. The Brillouin zone is sampled by a 13×13×13 k-point grid. The valence electrons of the involved atoms are Ni-$3d^8 4s^2$, Mn-$3d^5 4s^2$, Ti-$3d^2 4s^2$, V-$3d^3 4s^2$, and Ga-$4s^2 4p^1$. In the CASTEP calculations, a cutoff energy of 500 eV and a convergence criterion of 10^{-6} eV are adopted.

2. Results and discussion

2.1. Cubic lattice structure

This section calculates the variation of electronic total energy (E_{tot}) with radius for Ni_2MnZ (Z=Ti, V, and Ga) alloys in three structures: $L2_1$, XA, and FCC (**Figure 2**). The calculation results show that for the Ni_2MnGa alloy, compared with the XA and FCC structures, the E_{tot} under the $L2_1$ structure is relatively lower, indicating that the $L2_1$ structure is more stable. In the Ni_2MnZ (Z=Ti, V) alloys, the E_{tot} of the FCC structure is relatively lower than that of the XA and $L2_1$ structures, indicating that the Ni_2MnZ (Z=Ti, V) alloys tend to be stable in the FCC structure [11].

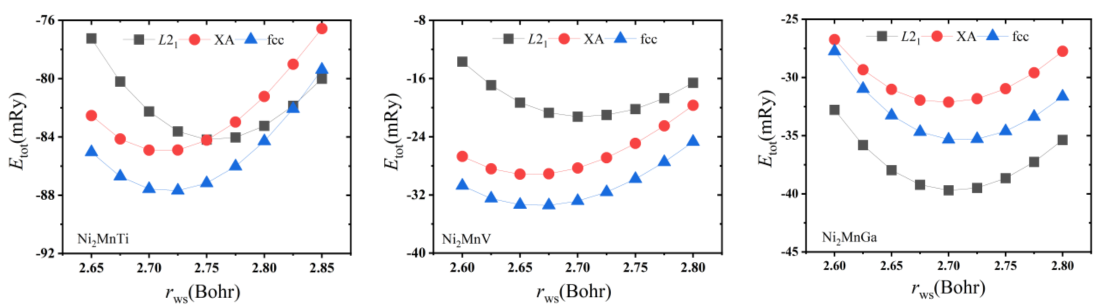

Figure 2. Variation of Etot with rws for $L2_1$-, XA-, and FCC-Ni_2MnZ (Z=Ti, V, and Ga) alloys

2.2. Tetragonal lattice deformation and martensitic transformation

Figure 3 shows that, based on the $L2_1$ cubic phase (c/a=1), when the c/a ratio of $L2_1$-Ni_2MnZ (Z=Ti, V) alloys ranges from 1.2 to 1.6, ΔE_{tot} is negative and presents a local minimum, indicating that both can undergo martensitic transformation. However, the Δ_{Etot} of the XA-Ni_2MnV alloy remains above the cubic phase when $c/a \neq 1$, lacking the conditions for martensitic transformation [12]. The Ni_2MnZ (Z=Ti, V) alloys exhibit excellent mechanical stability and significant volume change characteristics during the entire phase transformation process. The lattice volume change can be effectively induced by adjusting hydrostatic pressure, resulting in a large barocaloric effect [13]. The volume change rate of all-d-metal Heusler alloys during phase transformation can reach 3%–5%, which can produce a more significant barocaloric effect and magnetocaloric effect [14–15]. Through the synergistic effect of magnetic field and hydrostatic pressure, the martensitic transformation temperature and entropy change value of the alloy system can be precisely regulated.

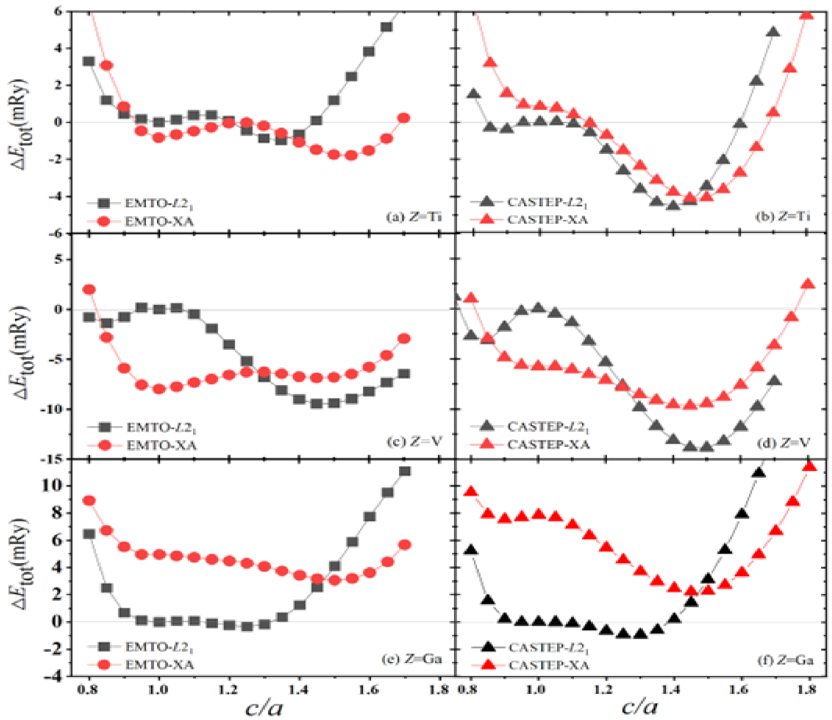

Figure 3. Variation of Δ^{Etot} with *c/a* for $L2_1$- and XA-Ni_2MnZ (Z=Ti, V, and Ga) alloys

3. Conclusions

In this paper, first-principles EMTO and CASTEP methods are used to study the cubic lattice structure and tetragonal lattice deformation of Ni_2MnZ (Z=Ti, V) alloys. The conclusions are as follows:

(1) Under the cubic lattice, the Ni_2MnGa alloy has a stable $L2_1$ structure; while the Ni_2MnZ (Z=Ti, V) alloys have a lower E^{tot} in the FCC structure, indicating that the alloys have a stable FCC structure. This reveals the influence of all-d-metal element substitution on crystal stability.

(2) Except for the XA-Ni_2MnV alloy, other alloys can undergo martensitic transformation. When the *c/a* ratio is in the range of 1.2–1.6, the alloy system has the lowest energy, corresponding to the most stable martensitic phase. Martensitic transformation can be induced by adjusting pressure, generating a barocaloric effect.

(3) The all-d-metal Heusler alloys Ni_2MnZ (Z=Ti, V) have potential in material design, providing a theoretical basis for their optimal design, and showing excellent performance in fields such as solid-state refrigeration and intelligent sensing.

Disclosure statement

The authors declare no conflict of interest.

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