

Effect of Co substitution on magnetic properties of Ni–Mn–Sn magnetic shape memory alloys

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Abstract: The effect of Co substitution on magnetic properties of Ni–Mn–Sn shape memory alloy was revealed by first-principles calculations. Large magnetization difference in Ni–Mn–Sn alloy obtained by addition of Co arises from enhancement of magnetization of austenite due to change of Mn–Mn interaction from anti-ferromagnetism to ferromagnetism. Total energy difference between paramagnetic and ferromagnetic austenite plays an important role in magnetic transition of Ni–Co–Mn–Sn. The altered Mn 3d states due to Co substitution give rise to difference in magnetic properties.

Key words: ferromagnetic shape memory alloys; Ni–Mn–Sn; first-principles calculation; magnetic properties

1 Introduction

Off-stoichiometric Ni–Mn–Sn ferromagnetic shape memory alloys have attracted great interest due to the observations of magnetic field-induced reverse martensitic transformation [1–4]. The magnetization in martensite phase of these alloys is smaller than that in the austenite one. Ni–Mn–Sn alloys undergo martensitic transformation in a magnetically ordered state, and the interplay between the structure and magnetism gives rise to great interesting effects such as inverse magnetocaloric effect [5–8], giant strain due to field-induced reverse martensitic transformation [9,10], and giant magnetoresistivity [11,12]. These make Ni–Mn–Sn alloys good candidates for multifunctional application. A large magnetization difference between the austenite and martensite phases is of great importance to develop higher performance both in magnetoelastic properties and in magnetocaloric effect, due to the improved possibility of driving structural transformation by magnetic fields. The magnetic properties of the austenite and martensite phases in the Ni–Mn–Sn alloys have been intensively studied by many researchers [13–18]. It has been reported that the

substitution of Co for Ni in Ni–Mn–Sn alloys is an effective way to increase the difference in magnetization between austenite and martensite phases [15,16]. Recently, the magnetic properties of Ni–Mn–Sn and Ni–Co–Mn–Sn alloys have been studied by neutron powder diffractions and it is found that the ferromagnetic enhancement in Ni–Co–Mn–Sn occurs as result of the change in the magnetic structure due to the substitution of Co [16]. So far, although Co substitution has prominent effects on magnetic properties and magnetic field-induced reverse martensitic transformation, the mechanism for them is still unclear.

In this work, we revealed the effect of Co substitution on magnetic properties of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ from the electronic structure point of view by first-principles calculations. The results provide the theoretical data and directions for developing high-performance metamagnetic shape memory alloy in Ni–Mn-based Heusler alloys system.

2 Computational methods

First-principles calculations have been performed based on the density functional theory, using CASTEP code [19]. The interaction between ions and electrons is

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described by ultra-soft pseudo-potentials [20]. The spin-polarized generalized gradient approximation was used to describe the exchange correlation energy. The plane-wave cutoff energy was 400 eV and a (8, 8, 8) Monkhorst-Pack grid was employed to sample the Brillouin zone. For the cubic $L2_1$ structures of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0, 0.25, 0.5$), 16-atom unit cell is built with appropriate Sn atoms replaced by Mn atoms. In the case of Co substitution for Ni, the cubic structure of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0, 0.25, 0.5$; $y=0, 0.25, 0.5$) is built with appropriate Ni atoms replaced by Co atoms on the basis of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ structure.

3 Results and discussion

For the cubic phase of Ni_2MnSn , the magnetic interaction between Mn atoms is ferromagnetic. However, in the case of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ and the corresponding alloys with Co substitution for Ni, the origin of magnetic interaction is still open. Thus, we first calculated the equation of states of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ cubic phases, taking into account two situations that magnetic moment of excess Mn at the Sn sites (denoted as Mn_{Sn}) is parallel or anti-parallel to that of Mn at the Mn sites (denoted as Mn_{Mn}). For both situations, it is noted that, if starting with parallel or anti-parallel Mn–Mn magnetic coupling, the spin-polarized self-consistent calculations converge to the solutions without changing the initial magnetic orientation. Hereafter, the parallel and anti-parallel Mn–Mn magnetic interactions are denoted as P and AP states, respectively.

Figure 1 shows the curves of total energy E versus lattice constants for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0, 0.25, 0.5$; $y=0.25$) cubic phases. From Fig. 1(a), it is seen that around equilibrium lattice constant, the AP state of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25$) is more stable than its P state. The latter becomes more stable only if the lattice constant is expanded. This indicates that the magnetic moment of the Mn_{Sn} in $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ cubic phase is anti-ferromagnetically coupled to the magnetic moment of Mn_{Mn} . Thus, it is expected that with excess Mn substitution for Sn, the total magnetic moment decreases, which is agreement with the experiments [18]. However, in the similar Ni–Mn–In metamagnetic shape memory alloy, the magnetic moment per formula increases with increasing Mn content. Our previous studies show that this opposite concentration dependence is attributed to the different coupling conditions of magnetic moment [21]. In the case of Ni–Mn–In alloys, the Mn–Mn interaction between the Mn atoms at Mn and In sites is suggested to prefer the ferromagnetic coupling. In contrast to the case of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25$), when substitution of Co for Ni with $x=0.25$, the P state of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25, y=0.25$) is slightly more

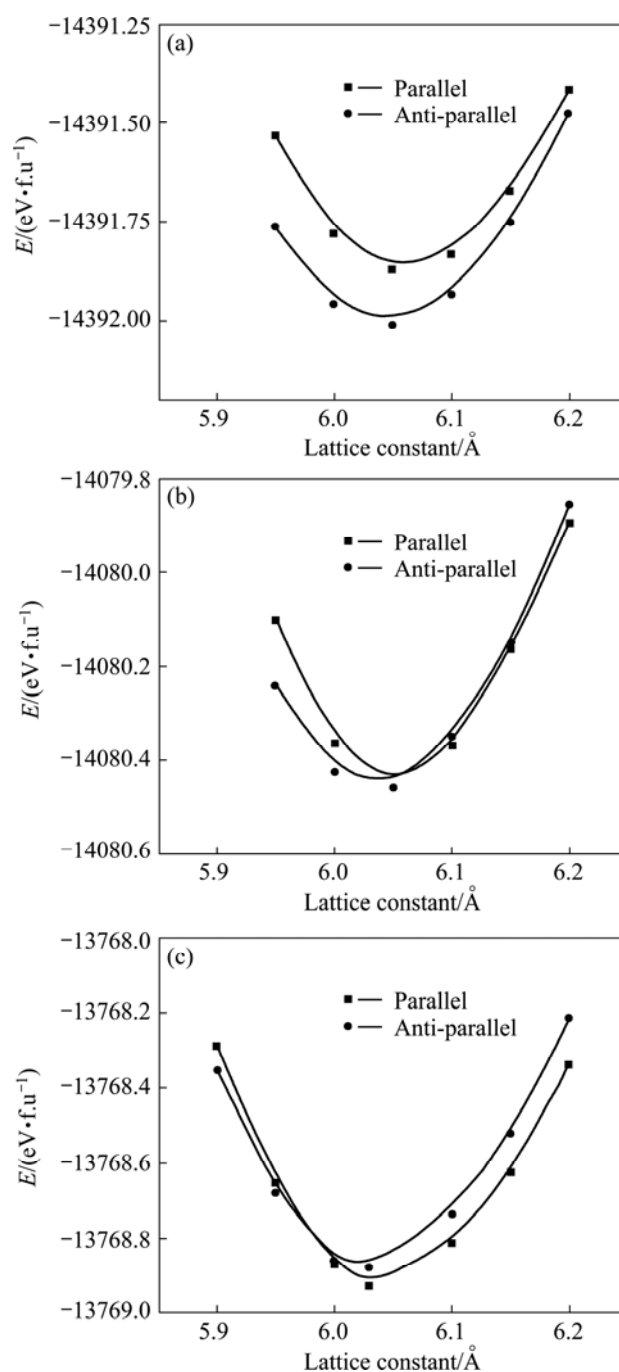


Fig. 1 Equation of states of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0, 0.25, 0.5$; $y=0.25$) cubic phases for both parallel and anti-parallel magnetic interactions: (a) $x=0$; (b) $x=0.25$; (c) $x=0.5$

stable than the AP state at equilibrium lattice constant, whereas the latter is more stable when the system is contracted, as shown in Fig. 1(b). However, the energy difference between two states is much small. Figure 1(c) shows that with the further substitution of Co for Ni ($x=0.5$), the P state of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.5, y=0.25$) obviously becomes more stable than the AP state at equilibrium lattice constant. Moreover, for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ with $y=0.5$, the effect of Co

substitution for Ni on magnetic interactions is similar to that with $y=0.25$. Therefore, it is suggested that for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ with $x>0.25$, the P state would be more stable than AP state. This suggests that Mn–Mn magnetic interaction in the cubic phases of Ni–Mn–Sn has been turned from anti-ferromagnetism to ferromagnetism by substitution Co for Ni.

The concentration dependences of the magnetic moment per formula unit for $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25$) cubic phases are shown in Fig. 2. It can be seen that the magnetic moment decreases with increasing Mn content (y) in the $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ alloys, while increases in the $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25$). This suggests that the magnetization of the high temperature cubic phase in $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ is enhanced by the substitution of Co for Ni. Furthermore, we have performed the geometrization for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$, and found that the cubic phase is energetically favorable for Ni_2MnSn . Interestingly, the cubic phase is unstable against the tetragonal distortion for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25, 0.5$) and undergoes the martensitic transformation to form tetragonal martensite. It should be noted that both in the martensite of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$, the magnetic moment of Mn_{Sn} is always anti-parallel to that of Mn_{Mn} . The anti-parallel arrangement of the Mn_{Sn} – Mn_{Mn} magnetic moment causes the decrease of total magnetization of martensite.

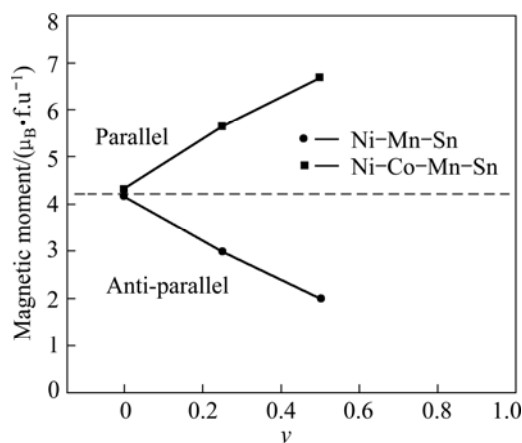


Fig. 2 Concentration dependence of magnetic moment per formula unit for $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25$)

It can be seen from Figs. 1 and 2 that the large magnetization difference in Ni–Mn–Sn obtained by addition of Co arises from substantial enhancement of the magnetization of the high-temperature cubic phase. This can be attributed to a change of magnetic structure caused by the substitution of Co for Ni, which turns the Mn–Mn interaction from anti-ferromagnetism to ferromagnetism. Therefore, the Co atoms work as a

ferromagnetic activator. Such a high magnetization difference provides a strong driving force for magnetic field-induced transformation, making this material a promising candidate for magnetic actuation applications. Actually, the ferromagnetic activation effect of Co has also been verified by our theoretical calculation in other Heusler alloys system such as Ni–Mn–Sb and Mn-rich Ni–Mn–Ga. Thus, the substitution of Co for Ni is a general way to enhance the magnetic field-induced transformation in Ni–Mn–X ($X=\text{Ga, Sn and Sb}$) alloys, which is very useful for the application and material design of metamagnetic shape memory alloy.

From the application point of view, the Curie temperature (T_c) is very important since it limits the operational temperature range of Ni–Mn–Sn-based alloys. In order to investigate the effect of Co substitution for Ni on T_c , the total energies of both ferromagnetic and paramagnetic cubic phases of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25$) alloys were calculated. It is found that the total energy of paramagnetic cubic phase is much higher than that of the ferromagnetic one at all the compositions studied, which is consistent with the fact that the paramagnetic cubic phase is the high-temperature phase. According to the Stoner theory, the total energy difference between the paramagnetic and the ferromagnetic state, ΔE , can give an estimation of T_c . The link between ΔE and T_c is given by $\Delta E = -k_b T_c \zeta$, where ζ represents the ratio of M to M_0 of the magnetic moment M at $T \neq 0$ K and the equilibrium magnetic moment M_0 at 0 K [22]. Our studies show that the total energy difference increases by about 140 meV when Ni is substituted by 6.25% Co (mole fraction; $x=0.25$) for $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ compared with $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$. Even the Stoner theory cannot be applied to describing high-temperature magnetic properties, T_c of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ alloys increases with the Co content, which is in fair agreement with the experimental observations [15]. The reason for increase of T_c should be attributed to the enhanced ferromagnetic exchange due to Co substitution for Ni.

To gain further insight into the origin of effect of Co substitution on magnetic properties in the Ni–Mn–Sn, the electronic structure of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25$) and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25, y=0.25$) was studied as an example. Figure 3(a) illustrates the density of states (DOS) for the cubic phase of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25$). Mn 3d states of majority and minority spin are split with respect to the Fermi level. This distribution makes Mn mostly responsible for the magnetization. Moreover, it can be noted that the magnetic moment of Mn_{Sn} is anti-parallel to that of Mn_{Mn} . Ni 3d states have similar distribution in the majority and minority spin, resulting in a rather small magnetization. Figure 3(b) shows the DOS for cubic phase of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25$,

$y=0.25$). The Mn_{Mn} 3d state is similar to that of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$. But, when the cubic $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ is doped by Co, Mn_{Sn} 3d state is altered. Mn_{Sn} 3d state of majority spin is mostly below the Fermi level, while that of minority spin is mostly above the Fermi level. Thus, the magnetic moment of Mn_{Sn} is parallel to that of Mn_{Mn} , giving rise to the enhancement of the total magnetic moment. This is attributed to that exchange interaction of Co–Mn is several times larger than that of Ni–Mn [15].

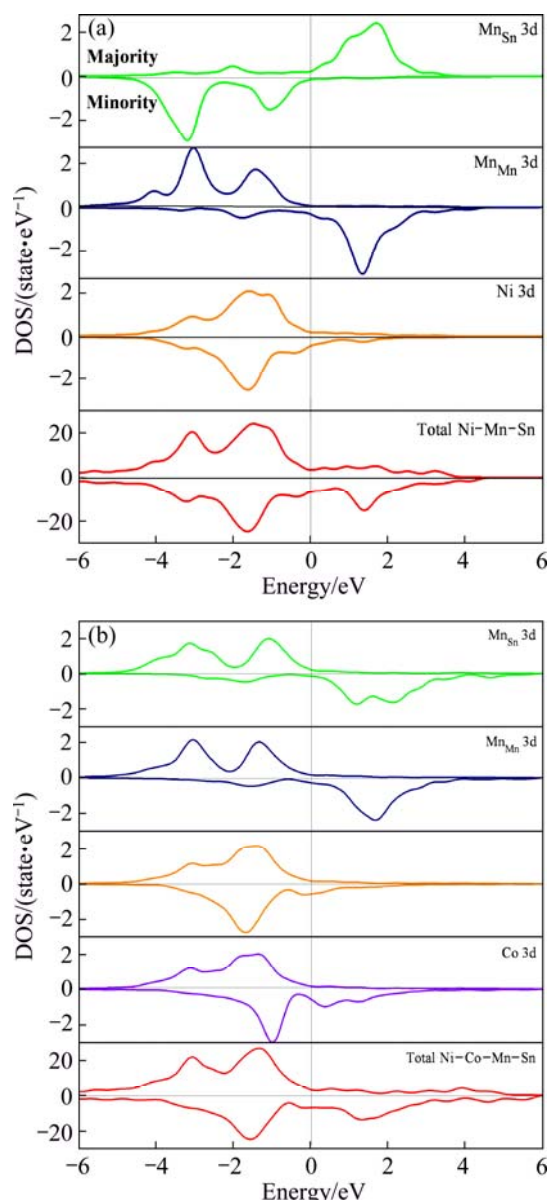


Fig. 3 DOS in cubic phases of $\text{Ni}_2\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($y=0.25$) (a) and $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ ($x=0.25, y=0.25$) (b) (The Fermi level is indicated by vertical line at 0)

4 Conclusions

1) The effect of Co substitution on magnetic properties of $\text{Ni}_{2-x}\text{Co}_x\text{Mn}_{1+y}\text{Sn}_{1-y}$ shape memory alloy is revealed by first-principles calculations. The large

magnetization difference in Ni–Mn–Sn obtained by addition of Co arises from substantial enhancement of the magnetization of the high-temperature cubic phase. This can be attributed to a change of magnetic structure caused by the substitution of Co for Ni, which turns the Mn–Mn interaction from anti-ferromagnetism to ferromagnetism.

2) The total energy difference between paramagnetic and ferromagnetic austenite indicates the increase in T_c with Co content.

3) The altered 3d state of Mn at the Sn site due to Co substitution plays an important role in establishing the magnetic properties.

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Co 掺杂对 Ni–Mn–Sn 铁磁形状记忆合金 磁性质的影响

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摘 要: 采用第一性原理计算揭示了 Co 掺杂对 Ni–Mn–Sn 形状记忆合金磁性质的影响。结果表明, 掺杂 Co 使 Ni–Mn–Sn 合金中两相饱和磁化强度差增大的原因在于其奥氏体的 Mn–Mn 磁交换作用由反铁磁性转变为铁磁性。奥氏体的顺磁态与铁磁态的能量差对 Ni–Co–Mn–Sn 的磁转变有重要影响。此外, Co 掺杂对磁性的影响与 Mn 3d 态的改变有关。

关键词: 磁性形状记忆合金; Ni–Mn–Sn; 第一性原理计算; 磁性质

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