Electron Concentration and Structural Transformation of Ni₂MnGa-Based Shape Memory Alloys

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In shape memory Ni₂MnGa based alloys, the structural transition temperature (T_i) increases with increasing valence electron concentration per atom (e/a). That is, when Ni or Mn atoms in Ni₂MnGa are replaced with a fourth element (X atom), the T_i increases with increasing atomic number of the X atom. To examine the experimental results, the electronic structures of these alloys were calculated for the cubic and monoclinic structures. The difference ΔE of total energies between the two structures was also calculated as a function of e/a . It was found that the features of T_i (e/a) are similar to those of ΔE (e/a). Their features are different in the lower and higher ranges than the boundary $e/a = 7.625$. The two features are characterized by two cases: a case that X atoms occupies Ni sites and the other case that X atoms occupy Mn sites. The characteristics mainly come from the difference of the density of states of X atoms at Ni and Mn sites.

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1. Introduction

The Heusler alloys Ni_{2+x}Mn_{1-x}Ga are ferromagnetic and have the shape memory property. The stoichiometric Ni₂MnGa ($x = 0$) transforms from a cubic (high temperature phase) to a tetragonal structure (low temperature phase).¹⁾ However, Ni_{2+x}Mn_{1-x}Ga ($x = 0.18$ and 0.19) and Ni₂(Pd_{0.16}Mn_{0.84})Ga transform from a cubic (high temperature phase) to a coexistent state of an orthorhombic and a monoclinic structure (low temperature phase).²⁾ The structural transition temperatures (T_i) and the Curie point (T_c) approach with increasing the Ni concentration and merge at the range of $x = 0.18$ – 0.2 of Ni_{2+x}Mn_{1-x}Ga.³⁾ Under these experimental results, it is reported by Ishida *et al.* that the tetragonal and orthorhombic structures may be metastable and the monoclinic structure is the most stable state among these structures for Ni_{2.17}Mn_{0.83}Ga and Ni₂(Pd_{0.17}Mn_{0.83})Ga.⁴⁾ This suggests that the coexistence states of the monoclinic and orthorhombic structures can appear at low temperature. The coexistent state corresponds to one observed by Inoue *et al.*²⁾

The valence electron concentration per atom (e/a) is an influential factor for the structural transition temperature. The relationship between T_i and e/a was examined for ternary alloys Ni–Mn–Ga and pseudo ternary alloys Ni–Mn–Ga–X. In ternary alloys Ni–Mn–Ga, the observed transition temperature T_i is 202 K for Ni₂MnGa ($e/a = 7.5$), 340 K for Ni_{2.18}Mn_{0.82}Ga ($e/a = 7.635$) and 350 K for Ni_{2.19}Mn_{0.81}Ga ($e/a = 7.6425$).^{1,2,5)} The variation of T_i (e/a) observed by Chernenko *et al.* and Tsuchiya *et al.* were represented by three straight lines with different slopes in the range of $e/a = 7.50$ – 7.80 .^{6,7)} On the other hand, in pseudo ternary alloys Ni–Mn–Ga–X with Co or Fe additions, the relationship T_i (e/a) seems to be also represented by a polygonal line at the boundary of $e/a \approx 7.625$.⁸⁾ That is, T_i (e/a) varies from 220 K to 317 K at the range of $e/a =$

7.57 – 7.63 for Ni_{2.20-z}Fe_zMn_{0.80}Ga, from 301 to 313 K at the range of $e/a = 7.5975$ – 7.6125 for Ni_{2.16-x}Co_xMn_{0.84}Ga and from 342 to 518 K at the range of $e/a = 7.64$ – 7.69 for Ni_{2.16}Mn_{0.84-y}Co_yGa.⁸⁾ The relation between T_i and e/a is represented by some curves. These interesting results suggest that T_i can be controlled by the concentration of the added element. In this paper, the electronic structures are calculated for pseudo ternary alloys Ni–Mn–Ga–X and ternary alloys Ni–Mn–Ga to investigate the relationship between T_i and e/a . And, the results will be compared with ones of experiments.

2. Crystal Structure and Method of Calculation

It was suggested that the tetragonal and orthorhombic structures may be metastable and the monoclinic structure is the most stable among four structures for Ni_{2.17}Mn_{0.83}Ga, as described in the previous section. In this paper, we pay attention to the cubic and monoclinic structures. The monoclinic structure has the lowest symmetry among four structures and the other structures also have the monoclinic symmetry. We treated the cubic structure as the monoclinic one with a unique angle of β shown in Fig. 1 to calculate under the same condition. The β angle of the monoclinic structure, which is equivalent to the cubic structure, is 71.565 degrees and one of the real monoclinic structure 98.461 degrees.⁴⁾ If the surface of this paper is assumed to be paralleled to a zx -plane, Mn and Ga atoms site on the $y = 0$ (or 1) and $1/2$ planes and Ni atoms on the $y = 1/4$ and $3/4$ planes in Fig. 1. Each of nickel, manganese and gallium in Ni₂MnGa has the four different atomic sites. For example, the four Mn atoms are distinguished by the symbols of Mn(1), Mn(2), Mn(3) and Mn(4) of which the sites are $1a$, $1f$, $2m$ and $2n$ sites in the unit cell with the P2/m symmetry of the tenth space group. The sites are the $1c$, $1b$, $2m$ and $2n$ sites for the Ni atoms and the $2j$, $2l$, $4o$ and $4o$ sites for Ga atoms. The twenty-four atoms in the unit cell are shown in Fig. 1. This unit cell corresponds to the observed monoclinic structure having the shuffling of 6 layers of (220)

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Fig. 1 Crystal structure of Ni₂MnGa. The constituent atoms on the $y = 0$ and $y = 1/4$ planes are shown in (a) and ones on $y = 1/2$ and $y = 3/4$ planes in (b). The cubic structure has the monoclinic symmetry except for the cubic symmetry. The unit cell with the monoclinic symmetry are shown, where the unique angle β is 71.565 degrees. The four types of constituent atoms are distinguished by the numbers. In Ni₂(Ni_{1/6}Mn_{5/6})Ga, the Mn(1) atoms in Ni₂MnGa are replaced with the Ni atoms. In the pseudo ternary alloys Ni–Mn–Ga–X, the Mn(2) or the Ni(1) atoms are replaced with the X atoms.

planes.²⁾

The alloy where a sixth of Mn atoms in stoichiometric Ni₂MnGa are replaced with Ni atoms is described as Ni_{2.17}Mn_{0.83}Ga in the previous papers.⁴⁾ In this paper, the alloy is described as Ni₂(Ni_{1/6}Mn_{5/6})Ga where the excess Ni atoms at the Mn(1) sites are described in parentheses with the Mn atoms. Here, we consider two cases where Ni or Mn atoms in Ni₂(Ni_{1/6}Mn_{5/6})Ga are replaced with X atoms. That is, X atoms are replaced with Ni atoms at the Ni(1) sites or Mn atoms at the Mn(2) sites. The former alloys are described as sys-N1 and the latter alloys as sys-M2 in this paper. The alloys in the sys-N1 and the sys-M2 are described as (Ni_{5/6}X_{1/6})₂(Ni_{1/6}Mn_{5/6})Ga and Ni₂(Ni_{1/6}Mn_{4/6}X_{1/6})Ga respectively. The environments of the constituent atoms are largely different in the cubic structure and the monoclinic structure.

When transition elements are chosen as the X atoms, (Ni_{5/6}X_{1/6})₂(Ni_{1/6}Mn_{5/6})Ga (sys-Ns1) is in the range of

$e/a = 7.5\text{--}7.625$ and Ni₂(Ni_{1/6}Mn_{4/6}X_{1/6})Ga (sys-M2) in the range of $e/a = 7.625\text{--}7.8$. The range of e/a for the sys-N1 and the sys-M2 correspond to the range of $e/a = 7.50\text{--}7.80$ of Tsuchiya *et al.*⁹⁾ When we cannot choose a real element as the X atom for the special value of e/a , we adopt an artificial atom. The artificial atom is described like Z27.5 where the number of 27.5 means the atomic number and the number of electrons. When we estimate the value of e/a , the numbers of valence electrons of Z27.5 and Z28.5 are assumed to be 9.5 and 10.5, respectively.

Band calculations were carried out self-consistently by the LMTO-ASA method.¹⁰⁾ The exchange correlation potential was treated within the framework of the local-spin-density (LSD) approximation.¹¹⁾

3. Results and Discussion

3.1 Density of states

3.1.1 Density of states in the sys-M2

We examine the local density of states (DOS) of the sys-N1 and the sys-M2 for the two structures, in order to examine the effect of substituting Ni(1) atoms or Mn(2) atoms for the X atoms. Then, we pay attention to the DOS of d-states of the X atom, because they are most different in the two systems. The X atom is strongly affected by the surrounding atoms, which are eight Ni atoms in the sys-M2 and four Ni atoms and four Ga atoms in the sys-N1. First of all, we pay attention to the local DOS of the X atom (X-DOS) in the sys-M2. The X-DOS the cubic structure is shown in Figs. 2(a) and (b) and those of the monoclinic structure in Figs. 2(c) and (d). The variation is seen in the X-DOS for X=Mn, Fe, Co and Ni atoms. The vertical line denotes the Fermi level. The X-DOS curves of the cubic structure have two large peaks. These two large peaks are the characteristic of the DOS of a bcc transition metal, because eight Ni atoms surround these atoms. The large valley of X atoms disappears and the occupied states generally move to the states with the lower energy, when the cubic structure changes to the monoclinic structure. This suggests that the energy of the monoclinic structure is lower than the cubic structure. The X-DOS curve in the minority spin states shifts from the higher energy region to the lower energy region beyond the Fermi level with increasing e/a , when the X atom changes from Mn to Ni in the order of Mn, Fe, Co and Ni. This is mainly due to the fact that the Coulomb potential becomes deeper with increasing the atomic number. On the other hand, the two large peaks of the majority spin exist under the Fermi level and shift to the higher energy region with increasing e/a , when the X atom is replaced with Fe, Co and Ni atom except for Mn in this order. This is a reason why the exchange split becomes small from X=Fe to Ni. That is, the split between the majority spin and the minority spin decreases with decreasing of the magnetic moment. The disappearance of the valley with a change from the cubic structure to the monoclinic structure brings a large difference in the occupancy of electrons. This difference tends to be larger with increasing number of valence electrons of the X atoms, that is, the electron concentration e/a . The difference also causes the energy difference between the two crystal structures.

Fig. 2 Local DOS of X atoms in the sys-M2. Four curves distinguish the cases of X=Mn, Fe, Co and Ni in $\text{Ni}_2(\text{Ni}_{1/6}\text{Mn}_{4/6}\text{X}_{1/6})\text{Ga}$, respectively. The DOS ((a) and (b)) of the cubic structure are shown in the left-hand side and those ((c) and (d)) of the monoclinic structure in the right-hand side. The upper ((a) and (c)) and the lower ((b) and (d)) are of the majority and the minority spin. The vertical line shows the Fermi level.

3.1.2 Density of states in the sys-N1

As described above, the circumstances of the X atom in the sys-N1 are different from those in the sys-M2. It is expected that the X-DOS is different between the two systems.

The X-DOS in the sys-N1 is compared for the cubic structure and the monoclinic structure in Fig. 3. In the cubic structure, the X-DOS of the sys-N1 has peaks in the large valley of the X-DOS in the sys-M2. In the monoclinic structure, the DOS of the sys-N1 roughly preserves the shape of the cubic structure, compared with the case of the sys-M2. Therefore, the molding of the DOS peaks with transforming from the cubic structure to the monoclinic structure is smaller in the sys-N1 than in the sys-M2. It is guessed that the energies difference (ΔE) between the two structures is smaller in the sys-N1 than the sys-M2.

Next, we examine the change of the DOS against e/a . In the cubic and the monoclinic structures, although the changes due to the difference of the X atom are seen in the majority spin as shown Figs. 3(a) and (c), the changes are extremely small, compared with those in the sys-M2 (in Figs. 2(a) and (c)). In the minority spin, the X-DOS shown in Figs. 3(b) and (d) is more occupied with increasing the atomic number as those in the sys-M2 (in Figs. 2(b) and (d)). Thus, the change of X-DOS due to the difference of X atoms is smaller, compared with those in the sys-M2. Therefore, the slope of ΔE (e/a) is expected to be small. The relation between the X-DOS and ΔE (e/a) will be described later in more detail.

3.2 Magnetic moment

The magnetic moment per atom for the cubic structure decreases like a straight line for the sys-N1 and like a sigmoid for the sys-M2 with increasing e/a as shown in Fig. 4. The magnetic moment per atom of the cubic is $2.87 \mu_B$ for X=Fe ($e/a = 7.667$), $1.57 \mu_B$ for X=Co ($e/a = 7.708$) of the sys-M2 and $1.21 \mu_B$ for X=Co ($e/a = 7.542$) of the sys-N1. The magnetic moment of Co for the sys-M2 is about 23 percent greater than Co in the sys-N1. This is due to the difference of the DOS of shapes of DOS curve between the sys-M2 and the sys-N1. The magnetic moment of Fe for the sys-M2 is about 30 percents greater than magnetic moment of bcc Fe.

3.3 Total energy and valence electron concentration

The difference (ΔE) of the total energies between the cubic and the monoclinic structure were calculated as a function of the valence electron concentration per atom (e/a). The total energies of $(\text{Ni}_{5/6}\text{X}_{1/6})_2(\text{Ni}_{1/6}\text{Mn}_{5/6})\text{Ga}$ (sys-N1) were calculated for X=Co, Z27.5 and Ni and those of $\text{Ni}_2(\text{Ni}_{1/6}\text{Mn}_{4/6}\text{X}_{1/6})\text{Ga}$ (sys-M2) for X=Mn, Fe, Co, Z27.5, Ni and Z28.5. Their values per unit cell are plotted by triangles for the sys-N1 in Fig. 5 and by circles for the sys-M2. The e/a range of the former is $e/a = 7.542\text{--}7.625$ and one of the latter $e/a = 7.625\text{--}7.77$. The case of X=Ni in the sys-N1 is equivalent to the case of X=Mn in the sys-M2 which corresponds to $e/a = 7.625$. The curve consists of a straight line and a parabolic line with a boundary of $e/a = 7.625$. The

Fig. 3 Local DOS of X atoms in the sys-N1. Three curves distinguish for the case of X=Co, Z27.5 and Ni in $(\text{Ni}_{5/6}\text{X}_{1/6})_2(\text{Ni}_{1/6}\text{Mn}_{5/6})\text{Ga}$, respectively. The DOS ((a) and (b)) of the cubic structure are shown in the left-hand side and those ((c) and (d)) of the monoclinic structure in the right-hand side. The upper ((a) and (c)) and the lower ((b) and (d)) are of the majority and the minority spin. The vertical line shows the Fermi level.

Fig. 4 Magnetic moment per atom of the X atom against the valence electron concentration (e/a) in the cubic structure. The open circles and the open triangles show the sys-M2 and the sys-N1, respectively. A open square shows the magnetic moment of the Mn atom in Ni_2MnGa .

difference ΔE increases linearly with increasing e/a in the range of the sys-N1. On the other hand, ΔE changes like a parabola with a top at X=Co, with increasing e/a in the range of the sys-M2. That is, the variation of ΔE is steeper for the sys-M2 than for the sys-N1.

Now, we examine relation between the difference ΔE and change of the X-DOS. As seen in Fig. 2 and Fig. 3, the X-DOS of the sys-N1 (X atoms at the Ni sites) and the sys-M2 (X atoms at the Mn sites) are fairly different in the cubic

Fig. 5 Difference (ΔE) of total energies between a cubic and a monoclinic structure and valence electron concentration (e/a). A straight line with the triangles and a parabolic line with the circles denote the sys-N1 and the sys-M2, respectively. A heavy broken line with the solid circles shows the line connecting ΔE for $\text{Ni}_2(\text{Mn})\text{Ga}$, $\text{Ni}_2(\text{Ni}_{1/6}\text{Mn}_{5/6})\text{Ga}$ and $\text{Ni}_2(\text{Ni}_{2/6}\text{Mn}_{4/6})\text{Ga}$. The vertical line shows $e/a = 7.625$. The case of X=Ni in the sys-N1 is equivalent to the case of X=Mn in the sys-M2 which corresponds to $e/a = 7.625$.

structure. When the cubic structure transforms to the monoclinic one, the change of the X-DOS is larger in the sys-M2 than in the sys-N1. Therefore, the structural transformation brings larger differences ΔE for the sys-M2, compared with

those of the sys-N1. Furthermore, we noticed that change of the X-DOS due to the difference of the X atom is larger for the sys-M2 than the sys-N1. These features correspond to the linear change and the parabolic change of the ΔE (e/a), respectively. Thus, the differences ΔE are reflected on the differences of the DOS curves due to different structures and different X atoms. The variation ΔE (e/a) is compared with the structural transition temperature T_t (e/a) in followings.

The Helmholtz free energy F is expressed as

$$F = U - TS,$$

where U is the internal energy, T is a temperature and S is the entropy. The differences of F , U and S between the cubic and monoclinic structures satisfy the equation

$$\Delta F = \Delta U - T_t \Delta S = 0$$

at the transition temperature T_t . Therefore, T_t can be estimated by $\Delta U/\Delta S$. However, we cannot calculate ΔS and the total energy does not include the temperature effects on the electronic structures and the lattice vibration energy. As generally speaking, it is very difficult to calculate T_t as well as the Curie temperature from the electronic structure. When we assume daringly $\Delta U = \Delta E$ and use the observed values of T_t , we can estimate very roughly the ΔS . For example, the values of ΔS for $e/a = 7.5\text{--}7.77$ are $\Delta S = 2.0\text{--}0.3\text{ J/gK}$, which decrease with increasing e/a . These values should be evaluated seriously because of the reasons described above.

In the followings, we compare T_t and ΔE . The heavy broken line in Fig. 5 corresponds to a line connecting three points of ternary alloys Ni–Mn–Ga: $\text{Ni}_2(\text{Mn})\text{Ga}$ ($e/a = 7.5$), $\text{Ni}_2(\text{Ni}_{1/6}\text{Mn}_{5/6})\text{Ga}$ ($e/a = 7.625$) and $\text{Ni}_2(\text{Ni}_{2/6}\text{Mn}_{4/6})\text{Ga}$ ($e/a = 7.75$). To examine the correspondence between ΔE and T_t , they are compared for the ternary alloys Ni–Mn–Ga and the pseudo ternary alloys Ni–Mn–Ga–X in Fig. 6.^{5,8,9)} Here, the values of T_t denotes a martensitic temperature. The values of T_t refer to the left axis and those of ΔE to the right axis. In the Fig. 6, the curves of ΔE are shown with the values of T_t so that the ΔE values of the case X=Ni in the sys-N1 and the case X=Mn in the sys-M2 are superposed on the values of T_t at $e/a = 7.625$ and 7.708 of the two cases. The values of T_t for ternary $\text{Ni}_{2+x}\text{Mn}_{1-x}\text{Ga}$ and $\text{Ni}_{2.18}\text{Mn}_{0.82}\text{Ga}$ are plotted by diamonds and cross, which were observed by Tsuchiya *et al.* and Inoue *et al.*, respectively.^{5,9)} These values distribute along the heavy broken line in Fig. 5. The T_t values of the pseudo ternary alloys Ni–Mn–Ga–X are also plotted in Figs. 6(b) and (c). In the lower range $e/a < 7.625$, their values distribute along the heavy line of ΔE (e/a) obtained for the sys-N1. That is, the heavy line of the sys-N1 corresponds to the data plotted by the solid squares for $(e/a, T_t) = (7.6125, 313\text{ K})$, $(7.605, 311\text{ K})$ and $(7.5975, 301\text{ K})$ of $\text{Ni}_{2.16-x}\text{Co}_x\text{Mn}_{0.84}\text{Ga}$ and the solid triangles for $(e/a, T_t) = (7.57, 220\text{ K})$, $(7.59, 266\text{ K})$, $(7.61, 292\text{ K})$ and $(7.63, 317\text{ K})$ of $\text{Ni}_{2.20}\text{Fe}_z\text{Mn}_{0.80-z}\text{Ga}$. Next, we pay attention to the data plotted in the higher range $e/a > 7.625$ which are shown in Fig. 6(c) by the solid circles for $(e/a, T_t) = (7.64, 342\text{ K})$, $(7.67, 429\text{ K})$, $(7.69, 518\text{ K})$ in $\text{Ni}_{2.16}\text{Mn}_{0.84-y}\text{Co}_y\text{Ga}$. They are along the heavy curve for the sys-M2. The correspondence between ΔE (e/a) and T_t (e/a) described above suggests that the X atoms prefer the Ni sites for the range $e/a < 7.625$ and the Mn sites for the range

Fig. 6 Comparison between transition temperature (T_t) and Difference (ΔE). The ΔE (e/a) curves drawn by a heavy line are compared with the experimental values (solid or open marks) of the T_t (e/a). In Fig. (a), the solid diamonds and cross and large square are of ternary alloys Ni–Mn–Ga, $\text{Ni}_{2.18}\text{Mn}_{0.82}\text{Ga}$ and Ni_2MnGa , respectively. In Figs. (b) and (c), the solid squares, triangles and circles, show the data of $\text{Ni}_{2.16-x}\text{Co}_x\text{Mn}_{0.84}\text{Ga}$, $\text{Ni}_{2.20}\text{Fe}_z\text{Mn}_{0.80-z}\text{Ga}$ and $\text{Ni}_{2.16}\text{Mn}_{0.84-y}\text{Co}_y\text{Ga}$, respectively. That is, Figs. (b) and (c) are for the sys-N1 and the sys-M2.

$e/a > 7.625$, when the constituent atoms of Ni_2MnGa are substituted for the X atoms. The value $e/a = 7.625$ seems to be the critical point for the structural transition temperature.

4. Conclusion

The electronic structures of $(\text{Ni}_{5/6}\text{X}_{1/6})_2(\text{Ni}_{1/6}\text{Mn}_{5/6})\text{Ga}$ (sys-N1) and $\text{Ni}_2(\text{Ni}_{1/6}\text{Mn}_{4/6}\text{X}_{1/6})\text{Ga}$ (sys-M2) were calculated for the cubic structure and the monoclinic one to examine the electron concentration dependence of the structural transition temperature $T_t(e/a)$. The difference of the total energies between the cubic structure and the monoclinic one is also calculated as a function of the concentration ΔE (e/a).

It was found that the features of T_t (e/a) and ΔE (e/a) are similar each other. That is, there is a good correspondence between T_t (e/a) and ΔE (e/a). Their curves consist of two parts with a boundary of $e/a = 7.625$ (Ni₂(Ni_{1/6}Mn_{5/6})Ga). In the range $e/a < 7.625$ (sys-N1), they increase linearly with increasing e/a and in the range $e/a > 7.625$ (sys-M2), they vary along a heavy line. Paying attention to the X atom which replaces the Mn or Ni atom in Ni₂(Ni_{1/6}Mn_{5/6})Ga, we can guess the variation of ΔE (e/a) from the local DOS of the X atom and the occupancy. The X atom occupies the Ni site in the range $e/a < 7.625$ (sys-N1) and the Mn site in the range $e/a > 7.625$. The change of the local DOS is larger for the X atom at the Mn site than the X atom at the Ni site, when the crystal structure changes between the cubic structure the monoclinic one. The changes reflect on the features of ΔE (e/a). Thus, the site of the X atom is an important factor in considering the structural transition temperature.

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