Time-dependent nature and origin of displacive transformation

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Abstract

We have investigated athermal and isothermal martensitic transformations (typical displacive transformations) in Fe–Ni and Fe–Ni–Cr alloys under pulsed and static magnetic fields and hydrostatic pressures in order to understand the time-dependent nature of martensitic transformation, that is, the kinetics of martensitic transformation. Also, we have calculated electronic structures of B2 and $\zeta$ phases in AuCd by FLAPW and/or LAPW methods in order to understand the origin of B2–$\zeta$ transformation. The following results were obtained. (i) The two transformation processes are closely related to each other, that is, the athermal process changes to the isothermal process under a hydrostatic pressure and the isothermal process changes to the athermal one under a magnetic field. (ii) These findings of (i) can be explained by the phenomenological theory, which gives a unified explanation for the two transformation processes previously proposed by our group. (iii) The calculation of the generalized susceptibility, $\chi(q)$, for the B2 phase of AuCd shows that there exists a nesting vector of near $1/3(110)/2\pi/a$ as in the B2 phase of TiNi calculated previously. The density of states at the Fermi energy of the $\zeta$ phase is lower than that of the B2 phase, which is similar to the case of B2–R transformation in TiNi previously calculated. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Martensitic transformation is a typical first-order displacive transformation, which occurs in many Fe-, Cu-, and Ti-based alloys and ceramics. This transformation has been widely studied to understand its characteristics from physical, metallurgical, and crystallographical viewpoints. In addition, martensitic transformation has also been studied from a technological viewpoint, partly because fine martensite structures formed in quenched ferrous alloys and steels are effective for strengthening and toughening and are thus used as structural materials, and partly because the shape memory effect and the pseudoelasticity effect appear in relation to the thermoelastic martensitic transformation and these effects are useful for practical purposes as smart materials. One of the typical examples of smart materials use is shown in Fig. 1, where the flat ribbon TiNi shape memory actuator is used in the robotic hand and its related martensite morphology [1] is shown in Fig. 2. Thus, the martensitic transformation has recently been actively studied. According to the studies made so far, many aspects of martensitic transformations, such as transformation temperature, crystallography and morphology of the product martensites, have been almost clarified so far. However, the essential problems of the transformation, such as time-dependent nature and the origin of the martensitic transformation, which give important information to understand the nucleation and growth mechanism of martensitic transformation, have not been clarified yet. In the present paper, we will discuss the new results obtained by our group concerned with the time-dependent nature and origin of martensitic transformation in some ferrous alloys.

In the time-dependent nature of martensitic transformation, it is well known that martensitic transformations are classified into two groups with respect to the kinetics, athermal and isothermal ones. The former transformation has a well-defined transformation temperature, $M_s$, and occurs instantaneously at $M_s$, while the latter one does not have a definite $M_s$ temperature but occurs after some finite incubation time during isothermal holding [2]. Very few materials exhibit an isothermal transformation, and Fe–Ni–Mn and Fe–Ni–Cr alloys are considered to be typical such materials. Many studies on isothermal martensitic transformation in Fe–Ni–Mn and Fe–Ni–Cr alloys have been made so far [2–4]. According to the study by Kurdjumov...
and Maksimova [2], isothermal transformations are considered to be the general and athermal ones the special case, speculating that the incubation time necessary for an athermal transformation is undetectably short. However, this view has not been verified yet, and further investigation is needed. Thus, we investigated the influence of a magnetic field on the athermal and isothermal martensitic transformations in Fe–30.3Ni–0.5Cr (at.%) and Fe–24.0Ni–4.3Cr (at.%) alloys, respectively [5]. Among the results, some characteristic ones will be described here. The electrical resistivity measurements showed that the Fe–30.3Ni–0.5Cr (at.%) alloy has a clear transformation start temperature at 183 K, but the Fe–24.0Ni–4.3Cr (at.%) alloy does not. Then, the Fe–24.0Ni–4.3Cr (at.%) alloy was isothermally held at several temperatures between 4.2 and 293 K. A typical TTT (Time, Temperature, Transformation) diagram obtained is shown by the closed circles in Fig. 3. As seen in the figure, one should note that martensitic transformation occurs after some incubation time and the TTT diagram clearly forms a C-type curve whose nose temperature, at which the incubation time is shortest, is about 143 K. Then, we applied a pulsed magnetic field to these alloys. Fig. 4(a) is a typical $M(t)$–$H(t)$ curve for the Fe–30.3Ni–

![Fig. 1. The Robotic hand has been used with a flat ribbon TiNi-SMA actuator with elements with large surface area. They have enhanced the cooling rate and in the result the robotic finger motion has smoothed.](image1)

![Fig. 2. Optical micrograph of an intermediate state of the R-phase transformation in a Ti–48.2Ni–1.5Fe (at.%) alloy [1]. Regions indicated by P and R are the parent phase and the R-phase (martensite), respectively. The R-phase self-accommodates during the growth, and forms a herring bone pattern that is composed of four variants.](image2)

![Fig. 3. TTT diagram of the isothermal martensitic transformation in an Fe–24.0Ni–4.3Cr (at.%) alloy [5].](image3)

![Fig. 4. Magnetization vs magnetic field curves of: (a) Fe–30.3Ni–0.5Cr (at.%) alloy at 223 K; and (b) Fe–24.0Ni–4.3Cr (at.%) alloy at 4.2 K, the magnetization increases instantaneously at a critical magnetic field indicated by arrows [5].](image4)
alloy, as seen in (b), although no martensitic transformation was observed in the Fe–24.0Ni–4.3Cr (at.%) alloy down to 4.2 K in zero magnetic field, despite an isothermal holding longer than 8.64 × 10⁸ s. These results are the same as in the athermal and isothermal martensitic transformations in Fe–Ni–Mn alloys studied previously [7] and suggest that the isothermal martensitic transformation changes to an athermal one under a high magnetic field. This means that the two transformation processes are closely related to each other and that their differences are not intrinsic but the two transformation processes may be explained by one basic rule. Based on this finding, we constructed a phenomenological theory [8], which gives a unified explanation for the two transformation processes, making the following three assumptions. (1) Particles (atom, electron) must acquire a certain critical energy (potential barrier), \( \Delta \), before they can change the state from austenite to martensite. (2) The transition probability \( (Pe) \) from the austenitic state to martensitic state is proportional to the Boltzmann factor and is expressed as \( Pe = P_0 \exp(-\Delta/k_B T) \), where \( P_0 \) and \( k_B \) are constants. (3) In case of \( \Delta \neq 0 \), martensitic transformation does not start even if one particle is excited, but it does when some critical number of particles, \( n^* \), among excited particles, \( m \), make a cluster and are excited in some place in the austenite.

Based on these assumptions, the probability \( (P) \) of the occurrence of martensitic transformation [8] has been derived as

\[
P = \sum_{m(\geq n \geq n^*)}^{N} \sum_{n \geq n^*} f(N, m, n, n^*)(Pe)^m(1 - Pe)^{N-m},
\]

where \( N \) and \( n^* \) represent the total number of particles and a minimum number of particles in the cluster, which is able to make a martensitic transformation start, respectively, and \( m \) and \( n \) the number of excited particles and \( f(N, m, n, n^*) \) the possible number of clusters consisting of \( n \) particles within \( m \) excited particles. Supposing that the well-known ergodic hypothesis holds in the present analysis, the incubation time at which a martensitic transformation starts can be evaluated by the inverse of \( P, P^{-1} \). More details of the theory has been reported elsewhere [8].

Based on this theory, we could prove that in the materials, which exhibit the athermal transformations, isothermal holding at a temperature above \( M_s \) induces a martensitic transformation after some finite incubation time. We could also prove that in the materials, whose athermal martensitic transformation is suppressed by changing the content of the compositions, a martensitic transformation occurs isothermally after some finite incubation time. Moreover, we could prove that a hydrostatic pressure changes the transformation process from an athermal to an isothermal one. Further, we could prove that in the materials, which exhibit an isothermal martensitic transformation, a static magnetic field lowers the nose temperature and reduces the incubation time and a hydrostatic pressure raises the nose temperature and increases the incubation time. In fact, we found these predictions certainly realized in some ferrous alloys, such as Fe–Ni and Fe–Ni–Cr alloys. The results are presented and discussed based on the theory previously proposed [8].

We will also discuss the martensitic transformation of B2(CsC1)–\( \zeta' \) (trigonal) in Au–Cd alloys from the electronic structure point of view by referring to that of B2–R (trigonal) in Ti–Ni alloys studied previously [9–12] in order to obtain the information on the phase stability of those alloys. As is well known in Ti–Ni and Au–Cd alloys, some anomalies in physical properties of the parent phase prior to the martensitic transformation, so-called precursor phenomena, have been found, such as the appearance of streaks along 110 direction in X-ray and electron microscopy diffraction patterns [13,14], decrease in elastic constant \( c' = (c_{11} - c_{12})/2 \) [15,16] and TA 2 phonon softening near 1/3(110)2\( \pi/a \) [17,18] as temperature approaches their transformation temperatures. Considering these anomalies and the fact that B2–R and B2–\( \zeta' \) martensitic transformations are weakly first order transitions, we can speculate that these anomalies are related to the instability of electronic structures of the B2 phase in Ti–Ni and Au–Cd alloys, especially the nesting effect in Fermi surface. In fact, the existence of a nesting vector of near 1/3(110)2\( \pi/a \) was found in the band calculation of TiNi [9–12]. The typical result by our group [12] is shown in Fig. 5, where the nesting vector \( q_n \) is indicated with the solid arrow in the cross-section of the Fermi surface cut by a plane parallel to (001) of the B2 phase \( (k_z = 0) \) and the Fermi surface is constructed by the 7th and 8th bands. However, there is no such information in AuCd because any electronic structures of B2 and \( \zeta' \) phases in AuCd have not been calculated yet.

Another purpose of the present study, therefore, is to calculate the electronic structures of B2 and \( \zeta' \) phases in AuCd by Full-Potential Linearized Augmented Plane Wave (FLAPW) and/or LAPW methods to clarify the relation between the electronic structures of those phases and the
B2→\(\gamma'\) martensitic transformation. The results will be discussed in comparison with those of Ti–Ni alloys calculated previously [9–12].

2. Time-dependent nature of martensitic transformation

2.1. Experimental procedures

The specimens used in the present study are Fe-29.9, -31.7 and -32.3 at.% Ni and Fe–24.0Ni–4.3Cr (at.%) alloys. The alloys were produced by melting the component metals in a high frequency induction furnace under argon atmosphere and casting into a water-cooled iron mold. Details of the alloy production and sample preparation were the same as those in the previous studies [6,7]. Specimens for electrical resistivity measurements (2 mm × 5 mm × 0.5 mm) were cut from the ingot homogenized and finally solution-treated in a silica capsule filled with argon. Electrical resistivity measurements were made by holding the specimens at a temperature above \(M_s\), at zero external field for three kinds of Fe–Ni alloys. Also, electrical resistivity measurements during isothermal holding has been made in an Fe-32.6 at.% Ni, which does not show any athermal martensitic transformation even at 4.2 K, in order to confirm the occurrence of martensitic transformation after some incubation time. Moreover, electrical resistivity measurement under hydrostatic pressure and/or magnetic field were made by holding the specimen at temperatures between 77 and 220 K for Fe-31.7, -32.3 and -32.6 at.% Ni and Fe–24.0Ni–4.3Cr (at.%) alloys. The hydrostatic pressure was generated by a piston cylinder type of instrument (1.5 GPa), in which kerosene and transformer oil in a Teflon capsule were used as a liquid pressure medium. The magnetic fields used were static (10 MA/m) and/or pulsed high magnetic fields (30 MA/m).

2.2. Results

2.2.1. Isothermal holding at zero external field

Electrical resistivity measurements with the four-probe method have been made for Fe–Ni alloys in order to obtain their \(M_s\) temperatures. The cooling and heating rates are 0.05 K/s, which is usually employed in obtaining the \(M_s\) temperature. The \(M_s\) temperatures thus obtained are 212, 153 and 125 K for Fe-29.9, -31.7 and -32.3 at.% Ni alloys, respectively. Then, isothermal holding experiments of the alloys have been done by setting a temperature above respective \(M_s\), in order to confirm that a martensitic transformation induces after some finite incubation time. The typical result for the Fe-31.7 at.% Ni alloy is shown in Fig. 6. It is noted in the figure that martensitic transformation occurs instantaneously after a finite incubation time of 1020 s during isothermal holding. This experimental
phenomenon is in good agreement with the prediction based on the phenomenological theory, as mentioned before. Then, we obtained the incubation times of the alloys by varying holding temperature and the typical results are shown in Fig. 7 for Fe–Ni alloys. A characteristic feature in the figures is that the incubation time increases with increasing $D_T$ and decreases with increasing Ni content at a given $D_T$ for Fe–Ni alloys. The same incubation time has been observed in Cu–Al–Ni shape memory alloys [19] and metal sodium [20] exhibiting an athermal martensitic transformation. These results will be discussed later.

We also made electrical resistivity measurements during isothermal holding for the Fe-32.6 at.% Ni alloy, which does not show any athermal martensitic transformation even at 4.2 K, in order to confirm the occurrence of martensitic transformation after some incubation time. We found that martensitic transformation occurs instantaneously after a finite incubation time during isothermal holding at temperatures between 77 and 125 K and the $TTT$ diagram is a C type of curve with nose temperature of about 85 K, as shown in Fig. 8. Then, we applied a pulsed high magnetic field to the alloy at 4.2 K and the result is shown in Fig. 9, where the martensitic transformation occurs instantaneously under a critical magnetic field indicated with an arrow. The critical magnetic field has been obtained by varying some temperatures and the result is shown in Fig. 10. As known from the figure, the critical magnetic field increases with increasing temperature, which is the same as in the alloys previously examined exhibiting an athermal martensitic transformation [6]. The measured relation between the temperature and the critical magnetic field is in good agreement with the calculated one obtained by the equation previously derived [6], which is shown by the dotted line in the figure. This result shows that the isothermal process changes to the athermal process under high magnetic field.

2.2.2. Isothermal holding under hydrostatic pressure and magnetic field

We applied hydrostatic pressure to the Fe-29.9, Fe-31.7 and -32.3 at.% Ni alloys in order to confirm the relevance of the above predictions. In the experiment, a transformation temperature under pressure is obtained by electrical resistivity measurements. A typical result for the hydrostatic pressure dependence of $M_s$ in the Fe–Ni alloys is shown in Fig. 11. Note that the $M_s$ temperature decreases with increasing hydrostatic pressure, reaching values below 4.2 K under pressures of 0.9 and 0.5 GPa for Fe-31.7 and -32.3 at. %Ni, respectively. These measured relations between the transformation temperature and the hydrostatic pressure are in good agreement with the calculated ones obtained by the equation previously derived [21,22], which are shown by the dotted lines in the figures.

Then, isothermal holding experiments of the Fe-31.7 and Fe-32.3 at.% Ni alloys have been done by setting a temperature between 77 and 100 K under a pressure of 0.9 and 0.5 GPa, respectively, where an athermal martensitic transformation is not observed at any temperature, as mentioned above. We find that a martensitic transformation occurs after a finite incubation time, depending on the set temperature, and the results are shown in Fig. 12(a) and (b) for Fe-31.7 and Fe-32.3 at.% Ni alloys, respectively. Note in the figures that the $TTT$ diagram under pressure is a C type of curve for both the alloys. This means that a hydrostatic pressure changes the transformation process from an athermal to an isothermal one. Therefore, the prediction mentioned before is appropriate. These results will be discussed later.

We also made isothermal holding measurements of the Fe–24.0Ni–4.3Cr (at.%) alloy in a static magnetic field and in a hydrostatic pressure in order to produce $TTT$ diagrams in those fields. In these experiments, we applied magnetic fields lower than the critical one because magnetic fields
higher than the critical one induce martensitic transformation instantaneously, as shown in Fig. 4(b). The strengths of the static magnetic fields used in the present study were 3.2 and 5.6 MA/m, respectively, and whose values are lower than the critical magnetic fields previously obtained in the wide temperature range between 4.2 and 300 K [5]. The TTT diagrams obtained in these magnetic fields are shown by the solid triangles (3.2 MA/m) and solid squares (5.6 MA/m) in Fig. 13(a). The TTT diagram in zero magnetic field is also shown by the solid circles for comparison. Note in the figure that the TTT diagrams in static magnetic fields are C type of curves, whose nose temperatures and incubation times are lower and shorter, respectively, than those in the zero external magnetic field, being similar to those predicted by the constructed theory [8]. Another characteristic feature is that the shifts of nose temperature and incubation time increase with increasing magnetic field. Similar isothermal holding measurements have been done for the alloy under hydrostatic pressures, and the results are shown by the solid triangles (0.25 GPa) and solid squares (0.4 GPa) in Fig. 13(b), where the TTT diagram in zero hydrostatic pressure is also shown by solid circles. As known from the figure, the TTT diagrams of the isothermal martensitic transformation in: (a) Fe–24.0Ni–4.3Cr (at.%) alloy under static magnetic fields; and (b) that under hydrostatic pressures. The dotted lines represent the calculated TTT diagrams with the theory previously proposed [8].
diagrams under hydrostatic pressure also show C type of curves, and its nose temperature and incubation time are higher and longer, respectively, than those in zero external pressure, being also similar to those predicted by the theory [8]. Moreover, the shifts of nose temperature and incubation time increase with increasing hydrostatic pressure. Incidentally, the data for the incubation time at each set temperature shown in Fig. 13(a) and (b) are averaged ones for five measurements and the determination of the nose temperature has an error as much as \( \pm 5 \) K in the present experiment.

2.3. Discussion

We have shown that the incubation time required for the formation of martensites, which is obtained by setting a temperature above \( M_s \), increases with increasing \( \Delta T \) for Fe–Ni alloys. We now show that the above results can be explained by following the approximated equation, whose detailed derivation was already described in a previous paper [8]. The approximated equation for the incubation time, \( P^{-1} \), (\( P \) represent the probability of the occurrence of martensitic transformation) is expressed as

\[
P^{-1} = [A \exp(-m^* \Delta/k_B T) \exp(-B \exp(-\Delta/k_B T))]^{-1},
\]

where \( A \), \( m^* \) and \( B \) represent temperature-independent parameters and \( \Delta \) shows the potential barrier between the parent and the martensite phase.

Based on Eq. (2), we firstly make a least-square fit with the experimental relation between incubation time and \( \Delta T \) to obtain the fit parameters in Eq. (2), \( A \), \( m^* \) and \( B \). The fit parameters, for example, thus obtained by using the Fe-31.7 at.% Ni alloy are \( 6.46 \times 10^5, 800 \) and \( 150 \) for \( A \), \( m^* \) and \( B \), respectively, and the best fitted relation for the alloy is shown by a dotted line in Fig. 7. Then, the relations for Fe-29.9 and -32.3 at.% Ni alloys have been calculated on the basis of Eq. (2) using the same values of \( A \), \( m^* \) and \( B \). The results thus calculated are shown by the dotted lines in Fig. 7. Note in the figure that the calculated relations are in good agreement with the experimental ones: the incubation time required for the formation of martensite increases with increasing \( \Delta T \) and decreases with increasing Ni content at a given \( \Delta T \).
The same analysis has been made for the relation between temperature and incubation time for the Fe-32.6 at.% Ni alloy using the same parameters (A, m° and B) mentioned above. The result is shown in Fig. 8 by the dotted line, where the calculated relations are in good agreement with the experimental one.

We also made the same analysis for the relation between temperature and incubation time required for the occurrence of a martensitic transformation under hydrostatic pressure. In the calculation, the same parameters (A, m° and B) mentioned above are used and Δ under hydrostatic pressure of Fe–Ni alloys have been calculated using the difference in Gibbs chemical free energies between the parent and the martensitic states, ΔG(T), derived by Kaufman [23]. The detailed procedure of the calculation of Δ under hydrostatic pressure has been described in a previous paper [8]. The calculated relations for Fe-31.7 at.% Ni and Fe-32.3 at.% Ni alloys are shown in Fig. 12(a) and (b) by dotted lines. Note in the figure that the calculated relations are in good agreement with the experimental ones.

We also calculated the TTT diagrams of the Fe–24.0Ni–4.3Cr (at.%) alloy in static magnetic fields and hydrostatic pressures. In the calculation, Δ of the alloy under magnetic field and hydrostatic pressure have been calculated using ΔG(T) derived by Kaufman [23]. The detailed procedure of the calculation of Δ was described in the previous paper [8]. The results are shown with dotted lines in Fig. 13(a) and (b), where the TTT diagram under no external fields is also shown. It is noted from the figure that the C curves are reproduced well, also suggesting that the theory is quite appropriate.

From the above results, we conclude that the theory successfully explains the time-dependent nature of athermal and isothermal martensitic transformations in Fe–Ni and Fe–Ni–Cr alloys. Thus, we cannot intrinsically distinguish two different transformation processes. The theory previously derived is just a phenomenological one so there is need for a more exact expression to explain a martensitic transformation process.

By using the fit parameter, m°, (representing the number of particles in the cluster which is sufficient for a martensitic transformation to start) and the lattice parameter of the parent phase previously obtained [5,6], it is possible to evaluate the cluster size needed to induce a martensitic transformation in the present alloys. The size is estimated to be at most about 2 (nm)^3 for all the alloys in the present study, and is almost the same as that in the previous studies [19,24].

3. Origin of martensitic transformation

3.1. Procedure of band calculation

The energy band calculations of B2 and % in AuCd were performed by FLAPW and LAPW methods, respectively. In the calculation, we referred to the crystallographic data of B2 and % previously studied [25,26]. The energy-eigenvalues in the B2 and % phases were calculated for 165 and 302 k-points in the irreducible part of each Brillouin Zone, respectively. Self-consistency was considered to be achieved when the total energy variation from one iteration to the next iteration does not exceed 10^-5 Ry. The generalized susceptibility, χ(q), of B2 phases in AuCd and TiNi has been calculated by the analytical tetrahedron approximation and their electron concentration dependences have also been calculated by assuming the rigid band model in order to investigate the existence of the nesting vector.

3.2. Results and discussion

Fig. 14(a) and (b) show the density of states (DOS) of B2 and % phases in AuCd, respectively. For comparison, the total DOS of B2 and R phases in TiNi are also shown in Fig. 14(c) and (d), respectively, which were calculated previously by our group [12]. It is noted in (a) that the total DOS curve has two main peaks deeply below E_F; the left peak is mainly composed of Cd d-states and the right is composed of Au d-states and the total DOS at the Fermi energy D(E_F) is composed of mainly s- and p-states. On the contrary, in (c) of B2 phase in TiNi, the total DOS at the Fermi energy D(E_F) is composed of mainly d-states, which is different in (a) although the total DOS curve has two main peaks, as in (a): the left peak is mainly composed of Ni d-states and the right is of Ti d-states. It is also noted in the figure that the total DOS curve in (a) is quite similar to that in the % phase of AuCd, as shown in Fig. 14(b), and that in (c) is quite similar to that in the R phase of TiNi, as shown in Fig. 14(d). This similarity is due to the similarity of relative atom positions between the B2 and % and/or R phases. Another characteristic feature is that the total DOS at the Fermi energy of the % phase (1.18 Ry^-1 atom^-1) is lower than that (1.77 Ry^-1 atom^-1) of the B2 phase. This fact is consistent with our criteria previously proposed in the
Ti–Ni alloy system [9] that when we calculate the $D(E_F)$ of all the phases appearing in an alloy system, $D(E_F)$ at 0 K decreases in order from the high temperature phase to the low temperature phase.

We have also calculated the generalized susceptibility, $\chi(q)$, of the B2 phase of AuCd in order to investigate the existence of the nesting vector, especially the $\{110\}$ direction, because this direction is related to the precursor phenomena mentioned before [14,16,18]. The calculated result is shown in Fig. 15. As known from the figure, $\chi(q)$ has maximum around $1/3(110)2\pi/a(=q_n)$, as in the B2 phase of TiNi calculated previously [9–12], and $q_n$ is nearly the same as the vector observed by inelastic neutron scattering where the TA$_2$ phonon mode softens [25]. From the fact, we confirmed the existence of the nesting vector in the B2 phase of AuCd, as in the B2 phase of TiNi. In Fig. 16, we show the nesting vector $q_n$ indicated with the solid arrow in the cross-section of the Fermi surface cut by a plane parallel to (001) ($k_z = 0.4$) where the Fermi surface is constructed by the 11th and 12th bands and their holes are shown with shaded areas. It should be noted that the region connected by the nesting vector is only hole although the region connected by the nesting vector in the B2 phase of TiNi is only electron, as shown in Fig. 5. Then the electron concentration dependence of $\chi(q)$ for Au–Cd and Ti–Ni alloys have been calculated by the rigid band model in order to know their electron concentration ($e/a$) dependence of the nesting vector. The absolute value of the nesting vector obtained from the $\chi(q)$--$q$ curve described above is shown as a function of $e/a$ in Fig. 17(a) and (b) for Au–Cd and Ti–Ni alloys, respectively (the present result for TiNi is almost the same as that previously studied [9,10]). As known from the figures, the absolute value of the nesting vector decreases in AuCd, but increases in TiNi with increasing $e/a$. This difference can be explained, considering the difference in the region connected by the nesting vector between AuCd and TiNi mentioned above and the fact the hole region shrinks but the electron region expands with increasing with $e/a$. That is, the absolute value of the nesting vector in AuCd decreases because of the shrinkage of hole region and increases in TiNi because of the expansion of the electron region as $e/a$ increases.

In this way, we confirmed the existence of the nesting vector and its concentration dependence in Au–Cd alloys. This means that the B2 phase of AuCd is unstable at 0 K due to the nesting effect of the Fermi surface. Thus, we can speculate that when the electron–phonon interaction is large, the B2 phase comes to be incommensurate and finally commensurate ($\xi'$) as temperature approaches the transformation temperature of B2–$\xi'$ transformation. The same speculation holds in case of the B2–R transformation in TiNi. However, the electron–phonon interaction in AuCd

Fig. 16. Fermi surface of the B2 phase of AuCd cut by a plane parallel to (001) at $k_z = 0.4$.

Fig. 17. Electron concentration dependence of nesting vector: (a) B2–AuCd; (b) B2–TiNi.
has not been calculated yet, and will in the future be the problem to solve.

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