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## On a possible mechanism for R-phase formation in TiNi

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**Abstract.** The multi-atom per unit cell average  $t$ -matrix approximation is used to study evolution of the  $\text{Ti}(\text{Ni}_{1-x}\text{Fe}_x)$  and  $\text{Ti}(\text{Ni}_{1-x}\text{Pd}_x)$  Fermi surfaces, as the concentration  $x$  is increased. The possible relation of the Fermi surface peculiarities with the B2-R martensitic transformation in these alloys is discussed. It is theoretically shown that the appearance of the charge-density wave with wavevector  $Q_1 = \frac{1}{2}\pi(1, 1, 1)$  in the presence of a rhombic distortion can be caused by softening of the phonon mode with wavevector  $Q_2 = \frac{1}{2}\pi(1, 1, 0)$ . On this basis a new microscopic mechanism for the R-phase formation in TiNi is proposed.

### 1. Introduction

Depending upon the composition and method of preparation of a sample, different sequences of structural martensitic transformations (MTs) are observed in the intermetallic compound TiNi [1, 2]. In particular, for a nickel content of more than 50%, showing some second-order characteristics, the transition from the B2 to the rhombohedral R-phase takes place [2]. Substitution of Fe or Pd for Ni enhances the stability of the high-temperature phase towards the B2-R transformation [3, 4].

Unfortunately, numerous experimental studies on TiNi have not resulted in a clear interpretation for the rhombohedral phase structure. A model [5] in which this phase is treated as due to lattice waves of the type  $\frac{1}{2}\langle 111 \rangle \langle 111 \rangle$  and  $\frac{1}{2}\langle 110 \rangle \langle 1\bar{1}0 \rangle$  seems to be most adequate. In this case, the rhombohedral deformation is apparently small [6]. The validity of the above-mentioned model is supported by the B2-phase vibration spectrum of TiNi, according to [7]; the transverse acoustic ( $T_{2A}$ ) branch along the  $\Gamma M$  direction indicates a sharp minimum at  $Q = Q_2 = \frac{1}{2}\pi(1, 1, 0)$ . Its depth increases as the system reaches the starting temperature  $M_s$  of the martensitic transformation. There is also a softening of the longitudinal acoustic (LA) mode along the  $\Gamma R$  direction at the point  $\frac{1}{2}\pi(1, 1, 1)$  [8]; however, here it manifests itself less clearly than at the point  $\frac{1}{2}\pi(1, 1, 0)$ . Also two elastic moduli,  $C'$  and  $C_{44}$ , are softened as well [9, 10]. It is essential that their dependences on temperature are very different [10]. Indeed, the former is small far from the point of the B2-R MT while the latter decreases rapidly near  $M_s$  only, i.e. the R-phase seems to be formed when a rhombic deformation has already occurred (in separate domains of the initial B2-phase at least).

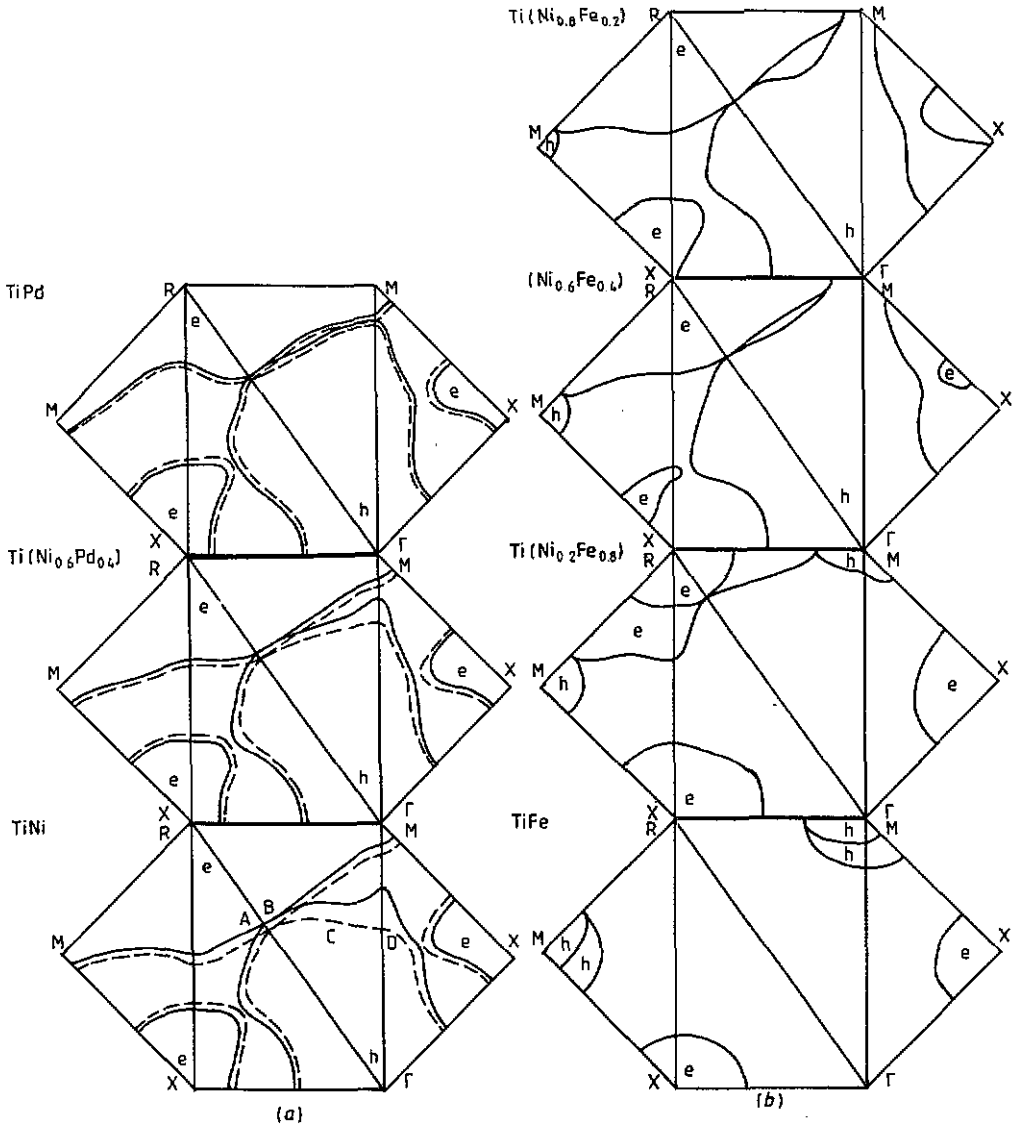
There is good reason to think that the B2–R MT in TiNi is electronic in origin and mainly connected with the electronic subsystem instability towards onset of charge-density waves (CDWs) with certain wavevectors. Indeed, according to [11], a number of electronic characteristics of the compound in question (electroresistance, optics, etc) have undergone qualitative alterations before the structural distortion occurs. Thus one or two superstructures (with  $Q_1 = \frac{2}{3}\pi(1, 1, 1)$  or (and)  $Q_2 = \frac{2}{3}\pi(1, 1, 0)$ ), characterizing the R-phase, can be due to the CDWs while the waves of atomic displacements with these wavevectors (one or two) either have small amplitudes or are completely absent.

Attempts to associate instability of the B2-phase in TiNi with its electronic structure peculiarities and thus to establish a microscopic mechanism of the B2–R transformation have been undertaken in a few theoretical investigations [12–15]. For example in [12], where the Fermi surface (FS) cuts in TiNi were calculated, occurrence of the superstructure with the wavevector  $Q_1$  is thought to be related to the FS flat parts perpendicular to the  $\Gamma R$  direction and passing approximately through the point  $\frac{2}{3}\pi(1, 1, 1)$ . Utilization of the TiNi electronic structure obtained in [12] for the study of vibration modes of this compound [13] has made it possible to describe the behaviour of the phonon branch along the  $\Gamma R$  direction. However, the softening of the phonon mode at the point  $Q_2$  in the  $\Gamma M$  direction [7, 8] has not been reproduced. There is another theoretical study [14] in which the FS flat parts mentioned above were also found. On the basis of results obtained in [14] an electronic theory of the B2–R transition, treating the B2-phase instability in TiNi as due to this peculiarity of the electronic spectrum, was proposed. It enables one to describe the polarization of the static wave of atomic displacements with wavevector  $Q_1$  in the low-temperature phase of TiNi. However, more accurate self-consistent calculations [15] showed bad nesting of the FS parts perpendicular to the  $\Gamma R$  direction as well as a small magnitude of the electron–phonon coupling constant for the corresponding electronic transitions. In [15], instability of the B2-phase towards the R-phase was associated with the fact that the contact between electronic and hole sheets in the  $\Gamma M$  direction disappeared with the temperature change of the lattice parameter. However, such an approach is not appropriate for describing the B2–R MT as it does not make it possible to explain the loss of translation symmetry. Up to now, the presence of the nesting FS parts to be spanned by  $Q_2$  as well as the origin of the superstructure with this wavevector have not been discussed at all in the literature.

Thus, although an electronic origin of the B2–R MT in TiNi is at present taken for granted, its mechanism has not been actually found. In our opinion this is so because previously attempts were made to account for the onset of the only lattice wave  $\frac{2}{3}\langle 111 \rangle \langle 111 \rangle$ . Contrary to this view we assume that, in order to understand the character of the MT in TiNi, the occurrence of all possible waves of atomic displacements as well as all types of deformation observed should be considered. In just such a manner, by studying the FS evolution in  $Ti(Ni_{1-x}Fe_x)$  and  $Ti(Ni_{1-x}Pd_x)$ , as the concentration  $x$  is increased, we shall attempt to establish a microscopic mechanism for the R-phase formation in TiNi.

## 2. Fermi surfaces

The FS cuts of the B2-phase of  $Ti(Ni_{1-x}Fe_x)$  and  $Ti(Ni_{1-x}Pd_x)$  calculated similarly to [16, 17] in the multi-atom per unit cell average  $\mathbf{k}$ -matrix approximation are represented



**Figure 1.** Fermi surface cuts for the B2-phase of (a)  $\text{Ti}(\text{Ni}_{1-x}\text{Pd}_x)$  and (b)  $\text{Ti}(\text{Ni}_{1-x}\text{Fe}_x)$ . Two isoenergetic surfaces corresponding to an upper (---) and a lower (—) boundary of the Fermi level localization range (0.005 Ryd) are represented for  $\text{Ti}(\text{Ni}_{1-x}\text{Pd}_x)$ . Damping of electronic states is not shown.

in figure 1. As the concentration of the third component increases, the evolution of the FS in those systems goes in completely different directions. As the number of valence electrons of Fe is smaller than that of Ni, upon substitution of iron for nickel, the Fermi level is rapidly moved downwards and, as a result, the FS topology changes. In this system the FS is altered so quickly (see figure 1(b)) that those peculiarities which lead to the B2-R MT at low  $x$  can hardly be seen. Analysis of the FS evolution in  $\text{Ti}(\text{Ni}_{1-x}\text{Pd}_x)$  turns out to be more useful and informative. This is so because palladium is isoelectronic to nickel;

with increasing concentration, the location of the Fermi level remains unchanged and the FS undergoes only rather small alterations which, nevertheless, suppress the B2-R MT as quickly as in  $\text{Ti}(\text{Ni}_{1-x}\text{Fe}_x)$ .

Among the FS changes pointed out, those in the vicinity of the  $\Gamma\text{M}$  direction are most marked. The electrons which are situated here are characterized by a small value of the Fermi velocity [17]. This leads to an indefiniteness in the FS position; therefore two isoenergetic surfaces are represented in figure 1(a). They correspond to an upper (broken curves) and a lower (full curves) boundary of the Fermi level localization range the magnitude of which is of the order of the step in energy (0.005 Ryd). As follows from the calculation carried out, in TiNi the distance from the point of intersection of the FS sheet with the  $\Gamma\text{M}$  direction to the point  $\Gamma$  is approximately equal to two thirds of the  $\Gamma\text{M}$  segment length. Moreover, in the vicinity of the  $\Gamma\text{M}$  direction, the FS has flat areas which are here manifested rather distinctly, their presence being confirmed by other workers [12, 14]. We do relate the instability of the high-temperature phase of TiNi towards the R-phase formation to this peculiarity of the electronic spectrum of the compound.

Indeed, as can be easily seen from figure 1(a), as the concentration of Pd is increased, a distortion of the flat areas CD to be spanned by the wavevector  $\mathbf{Q}_2$  takes place. On the contrary, intersecting the  $\Gamma\text{R}$  direction at the point  $\frac{1}{2}\pi(1, 1, 1)$  the flat area AB, which is small at low  $x$ , increases. Also the point of intersection remains almost unchanged, in going from TiNi to TiPd. Substitution of Pd for Ni would seem to enhance a Peierls instability of the B2-phase towards the lattice wave  $\frac{1}{2}\langle 111 \rangle \langle 111 \rangle$ ; however, this does not happen. Such behaviour of the system can only be explained by the fact that destruction of the flat areas CD spanned by the vector  $\mathbf{Q}_2$  prevents the formation of both the superstructure with this wavevector and that with the wavevector  $\mathbf{Q}_1 \neq \mathbf{Q}_2$ . Thus, both superstructures defining the R-phase seem to be due to one and the same peculiarity of the TiNi electronic spectrum: the FS flat parts perpendicular to the  $\Gamma\text{M}$  direction. At the same time the FS flat parts in the  $\Gamma\text{R}$  direction are able to cause no structural distortion.

To establish how far such a viewpoint is true, a study should be made of whether the soft mode  $\mathbf{Q}_2$  can lead to formation of the superstructure with the wavevector  $\mathbf{Q}_1$ . To this end, using the results in this section, we shall formulate a microscopic model for the B2-R MT in TiNi.

### 3. Model

To derive a microscopic model for the B2-R MT in TiNi all the main FS peculiarities which lead to instability of the high-temperature phase should be taken into consideration. In our opinion, they are as follows (see figure 1).

(i) There are large nesting (flat) parts CD perpendicular to the  $\Gamma\text{M}$  direction and spanned by the vector  $\mathbf{Q}_2$ . From our point of view, it is the presence of these areas that results in softening of the phonon mode at the point  $\frac{1}{2}\pi(1, 1, 0)$  and the lattice wave  $\frac{1}{2}\langle 110 \rangle \langle 1\bar{1}0 \rangle$ .

(ii) There are flat parts AB in the  $\Gamma\text{R}$  direction which pass through the points  $\frac{1}{2}\pi(1, 1, 1)$ . They are small in the sense that here the density  $N_{\text{AB}}$  of electronic states is smaller than the density  $N_{\text{CD}}$  of electronic states in the areas CD. It is more important for our treatment that, for the matrix elements  $g_{\text{AB}(\text{CD})}$  of the coupling of the electrons in AB (CD) via the  $\mathbf{Q}_1$  ( $\mathbf{Q}_2$ ) phonons, the correlation  $g_{\text{AB}} \ll g_{\text{CD}}$  seems to be valid [15].

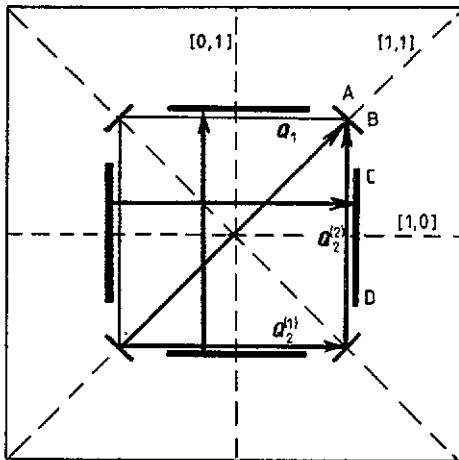


Figure 2. Two-dimensional model for the B2-phase Fermi surface of TiNi.

The following fact should be noted. If the areas CD are extended, they pass just through the point of intersection of the areas AB and the  $\Gamma R$  direction.

(iii) The areas AB are formed by doubly degenerate electronic states, having such a symmetry ( $\Lambda_3$ ) that homogeneous rhombic deformation removes their degeneration.

In the present work we are not going to carry out a quantitative study of the B2-R MT but shall attempt to establish its mechanism only. Therefore, to simplify calculations, one can confine oneself to derivation of a two-dimensional model (figure 2) and also consider the occurrence of a superstructure with a double, but not a triple, period. In essence, this means that we deal with two soft phonon modes (with  $Q_2^{(1)} = \pi(1, 0)$  and  $Q_2^{(2)} = \pi(0, 1)$ ) instead of six modes. Moreover, the rhombic deformation is replaced by a tetragonal deformation which is its analogy within the two-dimensional model. The simplifications assumed are not a matter of principle because all the FS peculiarities discussed above are as before taken into account. Going over to the two-dimensional model we shall retain the notation used before.

The model Hamiltonian  $H$  will be applied to the description of the B2-R transformation:

$$H = H_c + H_{ph} + H_{e-ph} + H_{e-def}. \quad (1)$$

Electron-electron interaction is not included in (1). This is associated with the fact that, within the mean-field approximation used below, this interaction leads to only a renormalization of the effective electron-phonon coupling constant and, hence, will not be able to influence the character of the final results.

The Hamiltonian  $H_c$  in (1) corresponds to an itinerant-electron system:

$$H_c = \sum_{\alpha} \sum_{k \in CD} [\varepsilon(k) - \mu] a_{k,\alpha}^{\dagger} a_{k,\alpha} + \sum_{\alpha} \sum_{k \in AB} \sum_i \tilde{\varepsilon}(k) a_{k,\alpha i}^{\dagger} a_{k,\alpha i} \quad (2)$$

where  $\varepsilon(k)$ ,  $\tilde{\varepsilon}(k)$  and  $a_{k,\alpha}^{\dagger}$  ( $a_{k,\alpha}$ ) are the energies and creation (annihilation) operators for itinerant electrons,  $k$  is the quasi-momentum,  $\alpha$  is the spin index, and  $\mu$  is the chemical potential which defines a shift in the Fermi level upon a change in occupation of electronic bands. If the bands are treated as rigid, then at  $\mu \neq 0$  the vector spanning the FS flat areas does not coincide with the wavevector of a superstructure, the difference between those

vectors increasing as  $\mu$  is increased. Thus, within our model, the chemical potential takes account of the FS nesting destruction with increasing concentration. The index  $i = 1, 2$  in the second term of Hamiltonian  $H_c$  stands for the rows of two-dimensional representation by which the electronic states forming the AB segments are transformed. For simplicity, we shall suppose that the electronic energies satisfy the conditions

$$\varepsilon(k + Q_2) = -\varepsilon(k) \quad \tilde{\varepsilon}(k + Q_1) = -\tilde{\varepsilon}(k). \quad (3)$$

The first equality is based on the results of our FS calculation. The second equality is asserted by the fact that the AB parts are small enough and, therefore, may be treated as straight.

The Hamiltonians  $H_{ph}$  and  $H_{e-ph}$  represent bare phonons and the electron-phonon interaction. In writing them we take into consideration only the unstable phonon modes responsible for formation of structural distortion. Then  $H_{ph}$  and  $H_{e-ph}$  can be presented as

$$H_{ph} = \omega_0(Q_2)(b_{Q_2^{(1)}}^+ b_{Q_2^{(1)}} + b_{Q_2^{(2)}}^+ b_{Q_2^{(2)}}) \quad (4)$$

$$H_{e-ph} = \sum_{\alpha} \sum_{k \in CD} g_{CD}(u_2^{(1)} a_{k+Q_2^{(1)},\alpha}^+ + u_2^{(2)} a_{k+Q_2^{(2)},\alpha}^+) a_{k,\alpha} \\ + \sum_{\alpha} \sum_{k \in AB} \sum_i \tilde{g}_{CD}(u_2^{(1)} a_{k+Q_2^{(1)},\alpha i}^+ + u_2^{(2)} a_{k+Q_2^{(2)},\alpha i}^+) a_{k,\alpha i} + CC \quad (5)$$

where  $u_2^{(1),(2)} = [2\omega_0(Q_2)]^{-1/2} (b_{Q_2^{(1),(2)}} + b_{-Q_2^{(1),(2)}}^+)$  is the operator of displacement;  $\omega_0(Q_2)$  and  $b_{Q_2^{(1),(2)}}^+$  ( $b_{Q_2^{(1),(2)}}$ ) are the frequency and creation (annihilation) operators for bare phonons with  $Q_2^{(1)}$  and  $Q_2^{(2)}$ ;  $g_{CD}$  and  $\tilde{g}_{CD}$  are the electron-phonon coupling constants which can be believed to be real. The Hamiltonians (4) and (5) were written within the high-density approximation [18]. Since  $g_{AB} \ll g_{CD}$  the interaction between itinerant electrons at the segments AB and bare phonons with the wavevector  $Q_1$  is not essential for formation of superstructure with  $Q_1$ . To emphasize this fact we have not included it into (5), i.e.  $g_{AB}$  has been assumed to be equal to zero.

Writing down the Hamiltonian  $H_{e-def}$ , which represents the interaction between itinerant electrons and the deformation potential, we proceed from the fact that there is a strong softening of the elastic modulus  $C'$  in the B2-phase of TiNi above  $M_s$ . This asserts that, above  $M_s$ , a rhombic deformation  $e$  (a tetragonal deformation in the framework of the two-dimensional model of the MT) is likely to have already occurred in this compound. It is a splitting of the doubly degenerate electronic band in the  $\Gamma R$  direction due to this deformation that is described by  $H_{e-def}$ :

$$H_{e-def} = g_e \sum_{\alpha} \sum_{k \in AB} e a_{k,\alpha 2}^+ a_{k,\alpha 1} + CC. \quad (6)$$

Here, the electron-deformation coupling constant  $g_e$  is real when  $g_{CD}$  and  $\tilde{g}_{CD}$  are real too.

#### 4. CDW with $Q_1 = \frac{2}{3}\pi(1, 1, 1)$ induced by the soft-phonon mode with $Q_2 = \frac{2}{3}\pi(1, 1, 0)$

In order to describe the ground state of the system studied, we shall make use of the Green functions (GFS)

$$G_{ij,\alpha}(k, k'; \tau) = -i \langle T a_{k,\alpha i}(\tau) a_{k',\alpha j}^{\dagger}(0) \rangle. \quad (7)$$

In carrying out a calculation, we shall confine ourselves to the mean-field approximation. The formalism of the GF method for this case is well known [18, 19]. Namely,

the set of equations for the GF and the equations of self-consistency for the order parameters  $\Delta_2^{(1),(2)} = g_{CD} \langle u_2^{(1),(2)} \rangle$  can be easily obtained from the equation of motion for the operators  $a_{k,\alpha i}$ ,  $a_{k,\alpha i}^\dagger$  and  $b_{Q_2^{(1),(2)}}$ ,  $b_{Q_2^{(1),(2)}}^\dagger$ . In doing so, one has to distinguish between two cases.

(i) The momentum  $k$  is in the vicinity of the FS parts CD. Then the GFs are defined by the following set of equations of the second order:

$$\begin{pmatrix} \omega + \mu - \varepsilon(k) & -\Delta_2^{(1),(2)} \\ -\Delta_2^{(1),(2)} & \omega + \mu + \varepsilon(k) \end{pmatrix} \begin{pmatrix} G_\alpha(k, k; \omega) \\ G_\alpha(k, k + Q_2^{(1),(2)}; \omega) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (8)$$

The band indices of the GF are omitted since the electronic states near CD are not degenerate.

(ii) The momentum  $k$  is in the vicinity of the FS parts AB. There is then the following set of equations of the eighth order in this case:

$$\begin{pmatrix} \hat{\mathbf{A}} & \hat{\mathbf{B}} \\ \hat{\mathbf{B}} & \hat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} \hat{\mathbf{G}}_{11} \\ \hat{\mathbf{G}}_{12} \end{pmatrix} = \begin{pmatrix} \hat{\mathbf{I}} \\ \hat{\mathbf{0}} \end{pmatrix} \quad (9)$$

Here, the four-dimensional matrices  $\hat{\mathbf{A}}$  and  $\hat{\mathbf{B}}$  and the column matrices  $\hat{\mathbf{G}}_{11}$ ,  $\hat{\mathbf{G}}_{12}$ ,  $\hat{\mathbf{I}}$  and  $\hat{\mathbf{0}}$  have the forms

$$\hat{\mathbf{A}} = \begin{pmatrix} \omega - \varepsilon(k) & -\Delta_2^{(1)} & -\Delta_2^{(2)} & 0 \\ -\Delta_2^{(1)} & \omega - \varepsilon(k + Q_2^{(1)}) & 0 & -\Delta_2^{(2)} \\ -\Delta_2^{(2)} & 0 & \omega - \varepsilon(k + Q_2^{(2)}) & -\Delta_2^{(1)} \\ 0 & -\Delta_2^{(2)} & -\Delta_2^{(1)} & \omega - \varepsilon(k + Q_1) \end{pmatrix}$$

$$\hat{\mathbf{G}}_{1i} = \begin{pmatrix} G_{li,\alpha}(k, k; \omega) \\ G_{li,\alpha}(k, k + Q_2^{(1)}; \omega) \\ G_{li,\alpha}(k, k + Q_2^{(2)}; \omega) \\ G_{li,\alpha}(k, k + Q_1; \omega) \end{pmatrix} \quad \mathbf{I} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{0} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

( $i = 1, 2$ )

and  $\hat{\mathbf{B}} = -\sigma \hat{\mathbf{I}}$ , where  $\hat{\mathbf{I}}$  is the unit matrix ( $\sigma = g_e e$ ). In writing (9), we have assumed that  $\tilde{g}_{CD} = g_{CD}$ . The parameters in (9) satisfy the equations

$$\Delta_2^{(1),(2)} = \frac{2g_{CD}^2}{\omega_0^2(Q_2)} \left( \sum_{k \in CD} + \sum_{k \in AB} \right) \text{Im} \left( \int \frac{d\omega}{2\pi} G_\alpha(k, k + Q_2^{(1),(2)}; \omega) \right). \quad (10)$$

Obviously, the second term on the right of (10) is much smaller than the first term. Therefore, it can be neglected; then  $\Delta_2^{(1),(2)}$  are defined by the well known formula [19]

$$\Delta_2^{(1),(2)} = [(\Delta_0 - 2\mu)\Delta_0]^{1/2} \equiv \Delta_2 \quad (11)$$

where  $\Delta_0 = 2\omega_D \exp(-1/g_{\text{eff}})$ ,  $g_{\text{eff}} \approx 4g_{CD}^2 N_{CD} / \omega_0^2(Q_2)$ .

As follows from (9), in spite of the fact that  $g_{AB} = 0$ , at  $\Delta_2^{(1),(2)} \neq 0$  the intraband GFs  $G_{ii,\alpha}(k, k + Q_i; \omega)$  are not equal to zero. Besides, if  $\sigma \neq 0$ , then the interband GFs  $G_{ij \neq i,\alpha}(k, k + Q_1; \omega) \neq 0$  as well. This asserts that the CDW with wavevector  $Q_1$  can appear in the system in question. In order to be convinced that this is really so, let us show that the CDW amplitude  $\rho_1^{(0)}$  is not equal to zero.



The CDW is connected with anomalous GFS according to the formula [20]

$$\rho_1 = -i \sum_{\alpha} \sum_{ij} \sum_{k \in AB} \Psi_{ik}^*(r) \Psi_{jk+Q_1}(r) G_{ij,\alpha}(k, k + Q_1) + cc. \tag{12}$$

Then  $\rho_1^{(0)}$  is obviously equal to

$$\rho_1^{(0)} = -4i \sum_{ij} \sum_{k \in AB} \int \frac{d\omega}{2\pi} G_{ij,\alpha}(k, k + Q_1; \omega) \tag{13}$$

where the GFS are found from the set (9). Substituting them into (13), one can be convinced that  $\rho_1^{(0)} \neq 0$ , only the interband GFS making a contribution to the CDW amplitude. Omitting the cumbersome intermediate calculations, we write the final result

$$\begin{aligned} \rho_1^{(0)} = & \frac{\Delta_2^2}{8\pi^2 V_F^2} \int_{\sigma}^{V_F \bar{k}} dx \int_0^{\sigma} dy \frac{1}{\sqrt{\xi^2 + \Delta_2^2} \sqrt{\eta^2 + \Delta_2^2}} \left[ \frac{1}{\varphi_{\xi}^{(+)} + \varphi_{\eta}^{(-)}} \right. \\ & \times \left( \frac{F(|\varphi_{\xi}^{(-)} + \varphi_{\eta}^{(-)} + \sigma|)}{|\varphi_{\xi}^{(-)} + \varphi_{\eta}^{(-)} + \sigma| \varphi_{\xi}^{(-)} \varphi_{\eta}^{(-)}} - \frac{F(\varphi_{\xi}^{(+)} + \varphi_{\eta}^{(+)} - \sigma)}{(\varphi_{\xi}^{(+)} + \varphi_{\eta}^{(+)} - \sigma) \varphi_{\xi}^{(+)} \varphi_{\eta}^{(+)}} \right) \\ & + \frac{1}{|\varphi_{\xi}^{(+)} - \varphi_{\eta}^{(+)}|} \left( \frac{F(|\varphi_{\xi}^{(+)} - \varphi_{\eta}^{(+)}| - \sigma)}{|\varphi_{\xi}^{(+)} - \varphi_{\eta}^{(+)}| - \sigma |f_1(\xi, \eta)} \right. \\ & \left. \left. - \frac{F(|\varphi_{\xi}^{(+)} - \varphi_{\eta}^{(+)}| + \sigma)}{(|\varphi_{\xi}^{(+)} - \varphi_{\eta}^{(+)}| + \sigma) f_2(\xi, \eta)} \right) \right]. \tag{14} \end{aligned}$$

Here

$$f_i = \theta(|\xi| - |\eta|) \begin{cases} \varphi_{\xi}^{(-)} \varphi_{\eta}^{(+)} \\ \varphi_{\xi}^{(+)} \varphi_{\eta}^{(-)} \end{cases} + \theta(|\eta| - |\xi|) \begin{cases} \varphi_{\xi}^{(+)} \varphi_{\eta}^{(-)} \\ \varphi_{\xi}^{(-)} \varphi_{\eta}^{(+)} \end{cases} \quad \begin{cases} i = 1 \\ i = 2 \end{cases}$$

$$\begin{aligned} F(z) = & (z^2 - x^2)(z^2 + y^2) + 2z^2(z^2 - y^2) - \sigma^2(2z^2 - x^2 - y^2) \\ & - 4z^2 \Delta_2^2 + 4\sigma^2 \Delta_2^2 - \sigma^4 \end{aligned}$$

$$\varphi_{\beta}^{(\pm)} = \sqrt{\beta^2 + \Delta_2^2} \pm \sigma$$

$$\xi = \frac{1}{2}(x + y) \quad \eta = \frac{1}{2}(x - y)$$

$$\theta(x) = \begin{cases} 1 & \text{at } x \geq 0 \\ 0 & \text{at } x < 0 \end{cases}$$

$\bar{k}$  is half of the segment AB and  $V_F$  is the Fermi velocity of the electrons in the areas AB.

One cannot calculate the integrals in (13) analytically. However, it is not necessary to do this since we are only interested in the possibility of formation of the superstructure with the wavevector  $Q_1$  in the softening of the  $Q_2 (\neq Q_1)$  phonon mode. As follows from analysis of equality (14), at  $\Delta_2 \neq 0$  a rhombic deformation  $e$  splitting the doubly degenerate electronic band  $\Lambda_3$  in the  $\Gamma R$  direction leads to onset of the CDW with  $Q_1$ . For example, at  $\sigma \ll \Delta_2$  this can be evidently shown. Assuming that  $V_F \bar{k} \geq \sigma$ , one finds from (14) that

$$\rho_1^{(0)} \approx 2\sigma(V_F \bar{k} - \sigma)/\pi^2 V_F^2 + o(\sigma/\Delta_2). \tag{15}$$

## 5. Discussion

Proceeding from the results of the investigation carried out above we consider that the R-phase formation in TiNi is related to softening of the short-wave and long-wave phonon modes in the  $\Gamma M$  direction. As our and other calculations of the FS show, softening of the phonon mode at  $Q_2 = \frac{2}{3}\pi(1, 1, 0)$  and, therefore, occurrence of the superstructure with this wavevector can be treated as a Peierls instability of the high-temperature phase due to the nesting flat areas to be spanned by  $Q_2$ . As for softening of the long-wave mode, i.e. the appearance of a rhombic deformation, this results from the anomalous behaviour of the elastic modulus  $C'$  above the temperature  $M_s$ . (In the present work this effect was phenomenologically introduced into the model of the MT under consideration.)

As was shown, in TiNi the occurrence of the lattice wave  $\frac{2}{3}(110)(1\bar{1}0)$  in the presence of the rhombic deformation can lead to onset of the CDW with the wavevector  $\frac{2}{3}\pi(1, 1, 1)$ . In our opinion, the superstructure with  $Q_1 = \frac{2}{3}\pi(1, 1, 1)$  is mainly caused by this CDW. This is so because the presence of the FS flat parts perpendicular to the  $\Gamma R$  direction and spanned by the vector  $Q_1$  is not able to lead to any structural distortion by itself since the interaction  $g_{AB}$  between the electrons in these parts and the  $Q_1$  phonons is sufficiently small [15].

Treating the superstructure with the wavevector  $Q_1$  as due to onset of the CDW, one can account for the experimentally observed anomalous behaviour of the electronic properties of TiNi [7, 8, 11] when the temperature is close to  $M_s$ . Also it is becoming clear why softening of the phonon branch in the  $\Gamma R$  direction manifests itself less distinctly than that in the  $\Gamma M$  direction. Of course, even a weak anomaly of the vibration spectrum shows that, in addition to the CDW with  $Q = Q_1$ , there is also a periodic lattice distortion with the same wavevector. However, in the case under study, atomic displacements are likely to be negligible and secondary in origin since they themselves are induced by the CDW. As for rhombohedral deformation, this phenomenon is not treated within the proposed model for the B2-R MT.

As a result, we arrive at a conclusion that the B2-R MT in TiNi is a Peierls type by nature; however, its mechanism is rather unusual. Firstly, this MT occurs in presence of a rhombic deformation which results in a splitting of the band  $\Lambda_3$  in the  $\Gamma R$  direction. Secondly, it is realized in a system with a particular FS which has nesting areas spanned by both vector  $Q_1$  and vector  $Q_2$ . Therefore, the B2-phase instability towards the lattice wave  $\frac{2}{3}(110)(1\bar{1}0)$  leads to the occurrence of the superstructure with wavevector  $\frac{2}{3}\pi(1, 1, 1)$  and, thus, ensures formation of the whole R-phase.

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