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2) The experimental data obtained at temperatures $T = 2.02$ and 2.55 K were analyzed only in the one-Gaussian approximations, inasmuch as the measurements were made with lower statistical accuracy.

3) The temperature dependence of $\langle E_k \rangle$ was calculated also in Ref. 19.

[1]L. D. Landau, Zh. Eksp. Teor. Fiz. **11**, 592 (1941).
[2]D. R. Tilley and J. Tilley, Superfluidity and Superconductivity, Halsted, 1975.
[3]R. Cowley and A. D. B. Woods, Phys. Rev. Lett. **21**, 787 (1969).
[4]O. Harling, Phys. Rev. A **3**, 1073 (1971).
[5]H. A. Mook, R. Sherm, and M. K. Vilkinson, Phys. Rev. A **6**, 2268 (1972); L. J. Rodrigues, H. A. Gersch, and H. A. Mook, Phys. Rev. A **9**, 2085 (1974).
[6]L. Aleksandrov, V. A. Zagrebnov, Zh. A. Kozlov, V. A. Parfenov, and V. B. Priezzhev, Zh. Eksp. Teor. Fiz. **68**, 1825 (1975) [Sov. Phys. JETP **41**, 915 (1975)].
[7]J. Gavoret and P. Nozieres, Ann. Phys. (Paris) **28**, 349 (1964).
[8]P. Hohenberg and P. Platzman, Phys. Rev. **152**, 199 (1966).
[9]R. A. Ferrell, N. Nenyhard, and H. Schmidt, Ann. Phys. (N.Y.) **47**, 595 (1968).
[10]W. P. Francis, G. V. Chester, and L. Reatto, Phys. Rev. A **1**, 86 (1970).
[11]R. Puff and J. Tenn, Phys. Rev. A **1**, 125 (197).
[12]G. J. Hyland, G. Rowlands, and F. W. Comming, Phys. Lett. A **31**, 465 (1970).
[13]V. A. Zagrebnov and V. B. Priezzhev, JINR R17-3634, Dubna, 1976.
[14]H. A. Mook, Phys. Rev. Lett. **32**, 1167 (1974).
[15]H. W. Jackson, Phys. Rev. A **10**, 278 (1974).
[16]E. Andronikashvili, J. Phys. USSR **10**, 201 (1964).
[17]E. B. Dokukin, Zh. A. Kozlov, V. A. Parfenov, and A. V. Puchkov, Pis'ma Zh. Eksp. Teor. Fiz. **23**, 459 (1976)], Preprint FEN-710, Obninski, 1976.
[18]V. V. Galikov, Zh. A. Kozlov, L. K. Kul'kin, L. B. Pikel'ner, V. T. Rudenko, and E. I. Sharapov, JINR R3-5736, Dubna, 1971.
[19]A. G. Gibbs and O. Harling, Phys. Lett. A **36**, 203 (1971); Phys. Rev. A **3**, 1713 (1971).
[20]N. N. Borolyubov, Izbrannye trudy, Vol. 2, Naukova Dumka, 1970.
[21]G. J. Hyland and G. Rowlands, Phys. Lett. A **62**, 154 (1977).

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Microscopic mechanism of martensitic transformation in the Fe–Ni system

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A martensitic transformation is assumed to be due to phonon generation by narrow-band electrons. The threshold population inversion and amplitude of the generated vibrations are found in the single-mode approximation. Two basically different ways of population inversion are considered. In both cases flat constant-energy parts of the electron spectra of the transforming phases are of fundamental importance. An analysis of the electron spectra with the aim of revealing such parts is made for the specific examples of the fcc and bcc modifications of iron. It is pointed out that different martensitic transformations can occur for the same type of flat parts of constant-energy surfaces.

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§1. INTRODUCTION. POPULATION INVERSION. RESONATOR

A martensitic transformation is a diffusionless change in the lattice structure occurring in steels, many transition metals, and their alloys with pronounced features of first-order phase transitions.[1] For example, in the case of the Fe–Ni system (0–34% Ni) in which cooling (forward transformation, beginning at a temperature M_s) or heating (reverse transformation) produces fcc → bcc ($\gamma \to \alpha$) or bcc → fcc ($\alpha \to \gamma$) changes in the lattice,[1)] the relative change in volume amounts to 2.4%. This significant change suggests that longitudinal displacement waves play a leading role in the transformation. In an earlier paper[2] we suggested a mechanism of generation of longitudinal acoustic waves by electrons in narrow energy bands in the presence of a temperature gradient ∇T. The aim of the present paper is to give a description of a martensitic transformation in the theoretical framework developed for lasers (see the lectures of Haken and Weidlich in Ref. 3). The idea of describing a martensitic transformation in the phonon maser model without specifying the mechanism of its action was put forward earlier by Kayser.[4]

A necessary condition for stimulated emission is a

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population inversion of the states in the emitting system. As shown in Ref. 2, the maximum population inversion is obtained for electron states with antiparallel quasimomenta directed along and against ∇T: $\mathbf{p} \uparrow\!\uparrow \nabla T$ and $\mathbf{p}' \uparrow\!\downarrow \nabla T$. For simplicity, we shall assume that $\nabla T \neq 0$ only in one direction and we shall consider solely phonon generation (specifically, generation of acoustic longitudinal phonons) by electron transitions between the states with maximum population inversion in one of the narrow bands intersected by the Fermi level μ. We shall use $f_{\mathbf{p}}$ for the nonequilibrium distribution function of electrons of energy $\varepsilon_{\mathbf{p}}$, when the inversion condition is of the form

$$\sigma^0 = f_{\mathbf{p}'} - f_{\mathbf{p}} > 0, \qquad (1)$$

provided the following laws of conversion are obeyed:[2)]

$$\varepsilon_{\mathbf{p}'} - \varepsilon_{\mathbf{p}} - \omega_{\mathbf{q}} = 0, \quad \mathbf{p}' - \mathbf{p} - \mathbf{q} = 0, \mathbf{Q}, \qquad (2)$$

where $\omega_{\mathbf{q}}$ is the energy of a phonon with a quasimomentum $\mathbf{q}$; in the second expression in Eq. (2) the zero value and the reciprocal lattice vector $\mathbf{Q}$ correspond to the normal and umklapp (U) scattering processes, respectively.

We shall introduce $\Lambda_{\mathbf{p}}$ for the mean free path of electrons assuming that $\Lambda_{\mathbf{p}} \approx -\Lambda_{\mathbf{p}'} \approx \Lambda$; then, in the linear approximation in respect of the parameters

$$\eta_1 = \Lambda \nabla T |\varepsilon_{\mathbf{p}} - \mu|^{-1}, \quad \eta_2 = \omega_{\mathbf{q}} |\varepsilon_{\mathbf{p}} - \mu|^{-1}$$

the condition (1) subject to (2) can be conveniently written in the form

$$\sigma^0 = f_{\mathbf{p}'} - f_{\mathbf{p}} \approx y \left| \frac{\partial f^0}{\partial y} \right| (2y\eta_1 - \eta_2). \qquad (1')$$

Here, $y = |\varepsilon_{\mathbf{p}} - \mu| T^{-1}$; $f^0(e^y + 1)^{-1}$ is the equilibrium Fermi function; introduction of the modulus $|\varepsilon_{\mathbf{p}} - \mu|$ makes it possible to use Eq. (1′) for electron transitions above and below the Fermi level.[2]

It should be pointed out that for given values of $\omega_{\mathbf{q}}$ (and, consequently, for given $|\varepsilon_{\mathbf{p}} - \mu|$) and ∇T, the function $y^2|\partial f^0/\partial y|$ depends nonmonotonically on y reaching a maximum of ≈ 0.44 at $y = y_m \approx 2.4$, i.e., there is an optimum generation temperature $T_m = y_m |\varepsilon_{\mathbf{p}} - \mu|$ at which $\sigma^0 = \sigma^0_{\max}$. At $T = T_m$, the condition (1′) is satisfied for phonon energies

$$0 < \omega_{\mathbf{q}} < 2y_m \Lambda \nabla T, \qquad (3)$$

where the upper limit is given by the condition $\sigma^0 = 0$.

However, we shall show in §2 that the condition (1) applies only to the generation of phonons with infinite lifetime. In reality, the population difference σ^0 should exceed a threshold value σ^{th}, which limits the upper limit of the interval (3). In accordance with the concept of soft phonon modes,[5] in a first-order structural transition the energy $\omega_{\mathbf{q}}$ of a specific phonon mode has (at the transition point) a value which decreases with the degree of supercooling (or overheating) relative to the phase equilibrium temperature T_0, defined by the equality of the free energies of the phases $F_\gamma(T_0) = F_\alpha(T_0)$. At the temperature T_c corresponding to the absolute loss of the stability by a phase ($T_c > T_0$ for the α phase and $T_c < T_0$ for the γ phase) the frequency is $\omega_{\mathbf{q}} = \omega_{\mathbf{q}}(T_c) = 0$. Bearing in mind the possibility of strong supercooling, we shall retain the zero lower limit for the frequencies (3), and we shall assume that it applies to wavelengths $\lambda < \lambda_{\max} < \infty$.

The upper limit $\lambda = \lambda_{\max}$ can be estimated by assuming that phonon generation occurs at one of the natural modes of a resonator formed by a regular system of defects. For example, in the case of a material with an ideal bulk structure, these may be the parallel boundaries of a sample, whereas in a polycrystalline material these might be grain or subgrain boundaries. If the resonator is formed by two parallel plane boundaries (an analog of the Fabry–Perot resonator) separated by a distance D, the wavelengths λ of the natural modes satisfy the condition

$$D = m\lambda/2, \quad m = 1, 2, 3\ldots, \qquad (4)$$

and hence we have $\lambda_{\max} = 2D$. However, the condition (4) presupposes specular reflection by the boundaries, which is valid in the $\lambda \ll D$ case for elastic waves,[6] i.e., $\lambda_{\max}$ is at least an order of magnitude less than D.

In the case of nonparallel grain boundaries (which is more typical), a resonator may be formed by a dislocation network. The appearance of additional (apart from the lattice constants) periodicity parameter in the form of edges of a network cell l_i ($i = 1, 2, 3$) results in selection of the modes satisfying $2l_i = m\lambda$. Since for grains which are not too small we have $l_i \ll D$, we may assume that $\lambda_{\max} < 0.1D$ applies once again.

§2. THRESHOLD POPULATION DIFFERENCE AND AMPLITUDE OF GENERATED DISPLACEMENTS

For simplicity, we shall consider single-mode generation and then the Hamiltonian of the problem can be regarded, as in Ref. 3, as the sum $\mathscr{H} = \mathscr{H}_1 + \mathscr{H}_2$, where

$$\mathscr{H}_1 = \omega_{\mathbf{q}} b_{\mathbf{q}}^+ b_{\mathbf{q}} + \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} a_{\mathbf{p}}^+ a_{\mathbf{p}} + \sum_{\mathbf{p}} (W_{\mathbf{q}}^* b_{\mathbf{q}} a_{\mathbf{p}+\mathbf{q}}^+ a_{\mathbf{p}} + W_{\mathbf{q}} b_{\mathbf{q}}^+ a_{\mathbf{p}}^+ a_{\mathbf{p}+\mathbf{q}}) \qquad (5)$$

is the Hamiltonian of the electron–phonon system in the case of a single phonon mode; $b_{\mathbf{q}}, b_{\mathbf{q}}^+$ and $a_{\mathbf{p}}, a_{\mathbf{p}}^+$ are the phonon and electron annihilation and creation operators; $W_{\mathbf{q}}$ is the matrix element of the electron–phonon interaction; the Hamiltonian $\mathscr{H}_2$ describes the action of thermal reservoirs. An approximate expression for $W_{\mathbf{q}}$ is obtained in the tight-binding approximation by retaining only linear (in respect of atomic displacements) terms in the expansion of a resonance integral G, whose value is of the order of the electron band width.[7] For values of q which are small compared with $q_{\max}$, we find that on the Brillouin zone boundary in the case of normal and U processes we have

$$W_{\mathbf{q}} \approx iG\mathbf{e}_{\mathbf{q}}\mathbf{q}/(2MN\omega_{\mathbf{q}})^{1/2}, \qquad (6)$$

where M is the atomic mass; N is the number of atoms; $\mathbf{e}_{\mathbf{q}}$ is the phonon polarization vector.

In the Heisenberg representation, we obtain the following equations of motion for any operator x:

$$\frac{\partial x}{\partial t} \equiv \dot{x} = i[\mathscr{H}, x] = i[\mathscr{H}_1, x] + i[\mathscr{H}_2, x] \equiv \dot{x}_1 + \dot{x}_2. \qquad (7)$$

Applying the commutation

$$[b_p^+, b_q] = \delta_{q,p}, \quad [b_q^+, b_p^+] = [b_q, b_p] = 0$$

and anticommutation

$$[a_p^+, a_q]_+ = \delta_{q,p}, \quad [a_p^+, a_q^+]_+ = [a_p, a_q]_+ = 0,$$

relationships, we find from Eqs. (7) and (5) that the following expressions describe the phonon field operators b_q^+, electron polarization operators $d_{p,q}^+ = a_{p+q}^+ a_p$, and the population difference $\sigma_{q,p} = a_{p+q}^+ a_{p+q} - a_p^+ a_p$:

$$\left.\begin{aligned} \dot{b}_q^+ &= (i\omega_q - \varkappa_q) b_q^+ + i\sum_p W_q^* d_{p,q}, \\ \dot{d}_{p,q}^+ &= (i\omega_{p,q} - \Gamma_q) d_{p,q}^+ - iW_q b_q^+ \sigma_{p,q}, \\ \dot{\sigma}_{p,q} &= (\sigma_{p,q}^0 - \sigma_{p,q}) t_\sigma^{-1} + 2iW_q d_{p,q} b_q^+ - 2iW_q^* d_{p,q}^+ b_q, \\ \dot{b}_q &= (\dot{b}_q^+), \quad \dot{d}_{p,q} = (\dot{d}_{p,q}^+)^+, \quad \omega_{p,q} = \varepsilon_{p+q} - \varepsilon_p. \end{aligned}\right\} \tag{8}$$

The system (8) is derived ignoring the fluctuating action of thermal reservoirs because we are interested only in the average values of the operators and we shall allow phenomenologically for the dissipative action[3] by introducing the relaxation times t_σ of electron populations, phonon damping $\varkappa_q$, and electron damping Γ_q. The index q of Γ_q shows that this damping is exhibited by a pair of electron states such that the transition between them results in the emission of a phonon with a quasimomentum q, i.e., $\Gamma_q \approx \Gamma_{p+q} \approx \Gamma_p$.

In the generation (stimulated emission) regime the number of quanta of the emitted mode becomes macroscopic and the operators b_q^+ and b_q are described satisfactorily by the c-number functions of time. Hence, it is clear that in the generation regime the equations of the system (8) averaged by the density matrix of the system are identical with the classical expressions if all the operators are replaced with their average values. Such a replacement will be assumed to be made and the notation used earlier for the operators will now apply to their averages. The oscillatory time dependence can be eliminated by adopting the quantities

$$\left.\begin{aligned} \tilde{b}_q^+ &= \exp[-i\Omega_q t] b_q^+, \quad \tilde{b}_q = \exp[i\Omega_q t] b_q, \\ \tilde{d}_{p,q}^+ &= \exp[-i\Omega_q t] d_{p,q}^+, \quad \tilde{d}_{p,q} = \exp[i\Omega_q t] d_{p,q} \end{aligned}\right\} \tag{9}$$

and considering the case of exact resonance,

$$\Omega_q = \omega_q = \varepsilon_{p+q} - \varepsilon_p = \omega_{p,q}. \tag{10}$$

Under steady-state conditions, we find that the system (8) subject to Eqs. (9) and (10) yields the following system of nonlinear algebraic equations:

$$\left.\begin{aligned} \varkappa_q \tilde{b}_q^+ - iW_q \sum_p \tilde{d}_{p,q}^+ = 0, \quad \Gamma_q \tilde{d}_{p,q}^+ + iW_q \tilde{b}_q^+ \sigma_{p,q} = 0, \\ \Gamma_q \tilde{d}_{p,q} - iW_q^* \tilde{b}_q \sigma_{p,q} = 0, \\ (\sigma_{p,q}^0 - \sigma_{p,q}) t_\sigma^{-1} + 2iW_q \tilde{d}_{p,q} \tilde{b}_q^+ - 2iW_q^* \tilde{d}_{p,q}^+ \tilde{b}_q = 0, \end{aligned}\right\} \tag{8$'$}$$

where the initial value $\sigma_{p,q}^0$ is given by Eqs. (1) and (1′).

The steady-state value of the population difference σ corresponding to the compensation of the gain by the losses is the threshold value σ^{th}. Assuming the existence of the solution $\tilde{b}_q^+ \neq 0$, we find from the first two equations of the system (8′) that

$$\sum_p \sigma_{p,q}^{th} = \Gamma_q \varkappa_q / |W_q|^2. \tag{11}$$

It follows from Eq. (11) that σ^{th} decreases when Γ_q^{-1} (the quasiparticle lifetime), q^{-1}, the electron–phonon interaction, or the number of inverted states with the quasimomentum p is increased. This number is large if the constant-energy electron surfaces have flat regions perpendicular to the quasimomentum q of the generated phonons. The reason for the formation of such regions (because of the equality $\varepsilon_p = \varepsilon_{-p}$, they always appear in pairs) may be the anisotropy of the spatial distribution of electrons.[8] For example, in the case of a strong overlap of the spatial wave functions of electrons along one axis (z), nearly flat regions are perpendicular to the quasimomentum in the direction z. If the generation involves the U processes with electron transitions between states of quasimomenta close to the limiting values, then large flat parts of the constant-energy surface may appear only parallel to the flat parts of the Brillouin zone.

In the presence of flat constant-energy regions, we have

$$\sum_p \sigma_{p,q}^{th} \approx \sigma_q^{th} n_q, \quad \sigma_q^{th} = \Gamma_q \varkappa_q / n_q |W_q|^2, \tag{11$'$}$$

where σ_q^{th} is the threshold population difference between any pair of electron states associated with the flat regions such that the transition between these states results in the emission of a phonon with a quasimomentum q; n_q is the number of such pairs.

Using the last three expressions in the system (8′) to express $\tilde{d}_{p,q}^+$ in terms of $\tilde{b}_q^+$ and $\tilde{b}_q$ and substituting the result in the first equation in the system (8′), we obtain with the aid of Eq. (11′)

$$\tilde{b}_q^+ [\sigma_q^0 / \sigma_q^{th} (1 + 4t_\sigma |W_q|^2 \Gamma_q^{-1} \tilde{b}_q \tilde{b}_q^+) - 1] = 0. \tag{12}$$

Equation (12) has two solutions

$$\tilde{b}_q^+ = 0 \quad \text{for} \quad \sigma_q^0 < \sigma_q^{th}, \tag{13}$$

$$\tilde{b}_q^+ \tilde{b}_q = \frac{\Gamma_q}{4t_\sigma |W_q|^2} \left(\frac{\sigma_q^0}{\sigma_q^{th}} - 1 \right) \quad \text{for} \quad \sigma_q^0 > \sigma_q^{th}, \tag{14}$$

showing that the amplitude of the displacements

$$u_q = (2/MN\omega_q)^{1/2} \tilde{b}_q \tag{15}$$

vanishes below the generation threshold and is finite above this threshold, which indicates that displacements are classical. In fact, it is clear from Eqs. (14) and (6) that for $\sigma_q^0 > \sigma_q^{th}$ the number of phonons $\tilde{b}_q + b_q \equiv b_q^2 \sim |W_q|^{-2} \sim N$ becomes macroscopic and, therefore, the energy of the mode in question is comparable with the total energy of all other noncoherent phonons.

§3. DISCUSSION OF RESULTS IN THE CASE OF A POPULATION INVERSION DUE TO ΔT

A martensitic transformation may begin in regions whose local temperature T is lower (to be specific, we shall consider only the forward transformation) than the phase equilibrium temperature T_0 and that the generation condition $\sigma_q^0 > \sigma_q^{th}$ is satisfied.

The population inversion σ_q^0 can be found if we know ∇T and ω_q. In estimating ∇T, we must distinguish two situations. Firstly, ∇T can be created by strong cooling of the surface of the sample. Then, $(\nabla T)_{max}$ on the surface can be estimated from[9] $\nabla T = \chi\theta^{-1}\Delta T$, where χ is the heat transfer coefficient, θ is the thermal conductivity, and ΔT is the difference between the temperature of the surface of the sample and the cooling medium. For example, in the case of quenching of steel in water, we can assume that $\Delta T \approx 10^2-10^3$ °K, $\theta \approx 5\times 10^6$ erg.sec^{-1}.cm^{-1}.°K^{-1}, $\chi = \chi_{max} \approx 5\times 10^7$ erg.sec^{-1}.cm^{-2}.°K^{-1} under bubble boiling conditions and we than obtain $\nabla T \approx 10^3-10^4$ °K/cm.

Secondly, if $T < T_0$, then ∇T appears as a result of the usual fluctuation-induced nucleation of a new phase. In fact, under thermodynamic instability conditions the heat evolved increases the temperature of a sample and this reflects the tendency of the system to approach the equilibrium temperature T_0, so that a temperature difference ΔT appears between a nucleus and the old phase and this difference increases with the supercooling $T_0 - T$ ($T_0 - T \approx 200$ °K for Fe–Ni and Fe–C systems[1]). Clearly, $\Delta T = 0$ applies when $T = T_0$ because the specific heat becomes infinite. The value of ΔT can be deduced from the change in the temperature of the sample if a considerable amount of martensite forms in a short time. This occurs in Fe–30% Ni alloys where up to 25% of all the martensite appears simultaneously[1] and the rise of the temperature of the sample reaches tens of degrees. Therefore, we find that $\Delta T = 10-100$ °K. Since over distances of the order of the mean free path Λ the local temperature is, by definition, the same, it follows that for ∇T near a martensite nucleus is $\nabla T \approx \Delta T(10\Lambda)^{-1}$, i.e., $\nabla\Lambda \sim 10^{-6}-10^{-7}$ cm the maximum values of ∇T may reach 10^7-10^8 °K/cm.

The wavelengths of the displacements responsible for a martensitic transformation can be deduced most conveniently from the influence of temperature on the phonon dispersion law right up to the temperature M_s throughout the full range of wave vectors. However, the available data are far from complete. For example, in the case of the Fe–30% Ni system this influence has been investigated in the short-wavelength range[10] by the method of inelastic neutron scattering and at relatively long wavelengths[11,12] by measuring the velocity of sound at 10^7 Hz; however, the wide intermediate range has not been studied. It is characteristic that in the long-wavelength range, lowering of T from 500 °K to $M_s = 248$ °K results in "softening" of the elastic moduli c_{11} by about 21% and of the moduli c_L by 12%. Although this is evidence of lattice instability, it does not include the possibility of even stronger softening in the intermediate range.

Direct information on the wavelength λ can be deduced from metallographic investigations by assuming the validity of the mechanism of formation of an elementary martensite platelet,[13] according to which the thickness of the platelet should be of the order of $\lambda/2$. In the Fe–Ni and Fe–C systems the platelet thickness is within the range $(0.25-2.25)\times 10^{-4}$ cm (Ref. 1), which corresponds to wavelengths between three and four orders of magnitude greater than the minimum value $\lambda_{max} \approx 2a \approx 10^{-7}$ cm. If the softening does not alter the order of magnitude of the frequencies, a martensitic transformation generates phonons of frequencies $\omega_q \approx 10^9-10^{10}$ rad/sec.

It follows from Eq. (1′) that even in the case of weak softening the value of $\sigma_q^0 > 0$ for ∇T associated with the fluctuation-induced nucleation may reach 0.1 when the temperature is optimal for phonon generation ($\varepsilon_p - \mu \approx 2.4T$) and fairly low ($T\,10-10^2$ °K).

The existence of flat constant-energy surfaces in the electron spectrum is of fundamental importance. The electron spectra are usually calculated for several symmetric directions of the reciprocal lattice and along lines joining the points of intersection of these directions with the boundaries of the first Brillouin zone. Continuing our discussion of the fcc–bcc transformation for illustrative purposes, we recall that the boundaries of the Brillouin zone of the fcc lattice are hexagons and squares perpendicular to the three- and fourfold symmetry axes and that the centers and vertices of these boundaries are denoted by the pairs of points (L, W) and (X, W). Calculations of the energy band structure of the fcc modification of Ni (Ref. 14) showed that the energies of the branch X_5W_1' and of a considerable part of the branch L_3W_1' differ slightly from the values at the points X_5 and L_3. This provides an argument in favor of the existence of constant-energy flat regions parallel to the Brillouin zone boundaries whose areas are comparable with the areas of these boundaries (faces). Calculations of the energy band spectrum of the fcc modification of Fe (Ref. 15) give the same picture as for Ni along the symmetry directions and, although the calculations for the X_5W_1' and L_3W_1' directions are not given, we may expect the existence of similar flat constant-energy regions.

According to Wood,[15] the difference between the energies at the points X_5 and L_3 is 0.02 Ry and the Fermi level (measured from the Fermi level of the paramagnetic bcc modification of Fe) lies below the energy of the point L_3 and the difference is the same. A martensitic transformation of the fcc form of Fe begins at $M_s \approx 1000$ °K, which is close to the optimal temperature of generation of phonons by electron states of energies close to that of the point L_3. The constant-energy region parallel to the square face may play an important role either when the Fermi level rises significantly (for example, in Cu–Ni alloys) or when magnetic ordering precedes a martensitic transformation so that the exchange splitting reduces the energy of electrons with spins of one of the orientations (Fe–Ni system, with 30–34% Ni). Moreover, there is a flat constant-energy surface of smaller area and parallel to the square face; the energy is close to that of the point X_2, which is practically identical with the energy at the point L_3. Thus, in the simplest single-mode case described by the Hamiltonian (5) we may expect, under the conditions assumed above, generation of phonons with wave vectors along the fourfold and threefold axes because of the umklapp processes. Clearly, the gradient ∇T which appears in the course of fluctuation-induced nucleation is more likely to be isotropic than unidirectional, as assumed initially in order to identify the electron states with the maximum population inversion. However, the real reason for the selection of specific electron states is the anisotropy of the electron energy spectrum.

In estimating the value of σ_q^{th} we must bear in mind that the finite width Γ_q (for $\Gamma_q > \omega_q$) of the electron energy levels makes it possible to describe the maximum number of the electron states n_q without conflict with the laws of conservation of energy and quasimomentum:

$$(n_q)_{max} \approx 2qS\delta^{-1}, \quad N\delta \approx (2\pi/a)^3 \sim q_{max}^3.$$

Here, δ is the volume in the reciprical space per unit quasimomentum; the factor of 2 allows for the two spin orientations; S is the area of one of a packet of flat constant-energy regions parallel to a Brillouin zone face and separated from it by no more than a quasimomentum **q** of an emitted phonon, which ensures electron transfer from a volume Sq of states with quasimomenta $\mathbf{p}' \upuparrows \nabla T$ to the same volume with $\mathbf{p}' \uparrow\downarrow \nabla T$. Assuming that $\Gamma_q \approx \omega_q$, $\varkappa_q \approx (10^{-1}-10^{-2})\omega_q$, $n_q \approx (n_q)_{max}$, $S \approx 10^{16}$ cm^{-2}, $M \approx 10^{-22}$ g, $q \approx 10^{-3}\, q_{max}$, $G \lesssim 10^{15}$ rad/sec, we find that in the absence of softening Eqs. (11′)[3)] and (6) give $\sigma_q^{th} \approx 10^{-2}-10^{-1}$ for $\omega_q \approx 10^{10}$ rad/sec. Lowering of the frequency to 10^9 rad/sec for a constant **q** (lattice softening) gives $\sigma_q^{th} \approx 10^{-4}-10^{-3}$ and the generation condition $\sigma_q^0 > \sigma_q^{th}$ is easily satisfied. This estimate is clearly illustrative and does not allow us to draw definite conclusions because the values of Γ_q, χ_q, W_q, and ω_q are not know exactly at the transition point M_s.

§4. MECHANISM OF PHONON GENERATION IN γ–α ELECTRON TRANSITIONS

The above mechanism of a martensitic transformation presupposes establishment of a population inversion between states belonging to a phase of given symmetry. However, there is another possibility of phonon generation because of electron transitions between states belonging to phases of different symmetry. In fact, in the range $T < T_0$ the temperature dependence of the electron energy spectrum may give rise to a situation when the energy of at least one of the electron bands of the γ phase is close to the energy of an electron band of the α phase. Clearly, this case is ideal from the point of view of a population inversion because the electron levels of the γ phase are filled and the potential levels of the α phase are empty. Then, the initial inversion σ^0 is identical with the Fermi function for the γ-phase electrons. The conclusions relating to the threshold inversion σ^{th} in §2 are completely general. In particular, it is clear that generation of phonons of one frequency is effective if electron transitions occur between extensive flat parts of the constant-energy surfaces of the γ and α phases.

The Brillouin zone of the bcc phase is a dodecahedron; the center and two types of vertices of rhombic faces are denoted by the points N, P, and H. The calculation of the energy band structure of electrons in the bcc phase of Fe (Ref. 15) shows that the smallest change in the energy along the NP direction is exhibited by the N_4P_3 branch and that the energy at the point N_4 is identical with the energy at the point L_3 of the γ phase. Moreover, the energy remains constant between P_3 and the point F_3, which is approximately half-way between P_3 and $H_{25'}$. However, in the direction from N to H the energy of the N_4H_{15} band varies rapidly. This means that there is a constant-energy surface of area more than half the area of the Brillouin zone face (four times the area of the triangle NF_3H). It follows that the conditions necessary for phonon generation exist in the case of γ–α electron transitions.

The genetic link between the flat regions of the constant-energy surfaces of the γ and α phases which are parallel to the $\{111\}_\gamma$ and $\{110\}_\alpha$ planes, respectively, can be understood if we bear in mind that the fcc lattice can be regarded as the body-centered tetragonal (bct) and that the $\{111\}_\gamma$ planes expressed in the bct coordinates are described by $\{110\}$ (see Fig. 52 in Ref. 1). Moreover, experimental evidence shows that in the coexisting γ and α phases these planes are always parallel[1] (this ensures the smoothest change in the electron density) and, therefore, in the single-mode approximation we can expect generation of phonons with wave vectors along the threefold axis of the γ phase.

It should be noted that in the case of generation of two and three modes we can expect electron transitions accompanied by a change in the momentum along a threefold axis to produce two or three phonons with wave vectors along the perpendicular twofold and fourfold axes or along three fourfold axes. Such phonon combinations correspond to the Bain deformation[13] which causes a transformation from the fcc to the bcc lattice.

Generation of longitudinal displacement waves along a threefold axis is important in transformations modeled by shear or sliding of the $\{111\}_\gamma$ planes parallel to one another. Such shear or sliding may occur if at a given moment a longitudinal mode expands the lattice and acts as the driving force of shear modes. This transformation mechanism is most effective at low stacking-fault energies (Fe–Mn systems) and may result in the γ–α (fcc–bcc) structural changes in the lattice in accordance with the Kurdyumov–Sachs crystal-geometry scheme[1] or in γ–α (fcc–hcp) and γ–ε' transformations.

We shall not compare in detail the mechanisms of phonon generation as a result of γ–γ and γ–α electron transitions but we shall stress that the second case differs from the first because it admits the possibility of vanishingly narrow electron levels ($\Gamma \to 0$) at a fixed frequency ω_q without a reduction in the number of the electron states participating in the generation process. Therefore, in the case of generation by γ–α transitions the threshold inversion may be considerably less, in agreement with Eq. (11). In general, separate and combined action of both generation mechanisms is possible.

§ 5. CONCLUSIONS

Although the proposed martensitic transformation mechanism may occur in any first-order structural transitions in conducting systems, it should play a leading role only in reconstructive transformations without the imposed limitation (in contrast to distortional transformations) that the symmetries of the old and new phases be in subordinate relationship. This limitation gives a clear description of a distortional transformation (analogous to second-order transitions (as the result of freezing of a soft mode which lowers the symmetry of the high-temperature phase. It is, therefore, no accident that distortional transformations have less pronounced characteristics of first-order transitions that are almost of second order.

However, in the case of reconstructive transformations, which usually have clear characteristics of first-order transitions and which include, for example, the diffusionless fcc–bcc, fcc–hcp, and hcp–bcc transitions, we cannot apply the existing theory of soft modes. Hence, it follows naturally that a transformation can be described in a different way and in this description a new phase appears as a result of propagation of generated waves in a crystal.[13] Naturally, the two approaches share the common concept of lattice instability within whose framework any structural transition is associated with the Bose condensation of some phonon modes.

At present the theory of distortional martensitic transformations in conducting systems is developed furthest for the A-15 compounds[16] (see also Ref. 17). The relationship between a martensitic transformation and a singularity of the density of electron states is the main assumption of the theory which makes it possible to explain the anomalous properties in the case of a singularity near the bottom of the d band[18] and near its top.[19,20] The general nature of this assumption is reflected also in the maser model of a martensitic transformation because the efficiency of generation (stimulated emission) is governed by the presence of flat regions of constant-energy surfaces which give rise, according to Weger,[8] to the strongest density-of-states singularities.

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1) We shall use γ and α for the high- and low-temperature phases.

2) We shall employ a system of units in which the Planck $\hbar$ and Boltzmann k constants obey $\hbar = k = 1$.

3) In substituting these quantities the denominator of Eq. (11′) should be multiplied by $\hbar$.

[1] G. V. Kurdyumov, L. M. Utevskiĭ, and R. I. Éntin, Prevrashcheniya v zheleze i stali (Transformations in Iron and Steel), Nauka, M., 1977, Chap. 3.

[2] M. P. Kashchenko and R. I. Mints, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 433 (1977) [JETP Lett. **26**, 309 (1977)].

[3] F. T. Arecchi, M. O. Scully, H. Haken, and W. Weidlich, Quantum Fluctuations of Laser Radiation (Russ. Transl.), Mir, M., 1974.

[4] U. Kayser, J. Phys. F **2**, L60 (1972).

[5] R. Blinc and R. Žeks, Soft Modes in Ferroelectrics and Antiferroelectrics, North-Holland, Amsterdam, 1974 (Russ. Transl., Mir, M., 1975).

[6] W. P. Mason and H. J. McSkimin, J. Appl. Phys. **19**, 940 (1948).

[7] L. N. Bulaevskiĭ, Usp. Fiz. Nauk **115**, 263 (1975) [Sov. Phys. Usp. **18**, 131 (1975)].

[8] M. Weger, Rev. Mod. Phys. **36**, 175 (1964).

[9] A. V. Lykov, Teoriya teploprovodnosti (Theory of Heat Conduction), Vysshaya shkola, M., 1967, p. 28.

[10] E. D. Hallman and B. N. Brockhouse, Can. J. Phys. **47**, 1117 (1969).

[11] K. Salama and C. A. Alers, J. Appl. Phys. **39**, 4857 (1968).

[12] G. Hausch and H. Warlimont, Acta Metall. **21**, 401 (1973).

[13] M. P. Kashchenko and R. I. Mints, Fiz. Tverd. Tela (Leningrad) **19**, 329 (1977) [Sov. Phys. Solid State **19**, 189 (1977)].

[14] E. I. Zornberg, Phys. Rev. B **1**, 244 (1970).

[15] J. H. Wood, Phys. Rev. **126**, 517 (1962).

[16] L. R. Testardi, M. Weger, and I. B. Goldberg, Superconducting Compounds with the β-Tungsten Structure (Russ. Transl.), Mir, M., 1977.

[17] S. V. Vonsovskiĭ, Yu. A. Izyumov, and É. Z. Kurmaev, Sverkhprovodimost' perekhovnykh metallov, ikh splabob i soedineniĭ (Superconductivity of Transition Metals, Their Alloys, and Compounds), Nauka, M., 1977, Chap. 5.

[18] J. Labbe and J. Friedel, J. Phys. Radium **27**, 153 (1966).

[19] L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **65**, 1658 (1973) [Sov. Phys. JETP **38**, 830 (1974)].

[20] L. P. Gor'kov and O. N. Dorokhov, J. Low Temp. Phys. **22**, 1 (1976).

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