Structural instability at line defects

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The singularities of a displacive phase transition at a system of line defects in a crystal are investigated. The case of large supercriticality of the unrenormalized spectrum of the local phonons is considered. This makes it possible to apply perturbation theory in terms of the small anharmonicity. The criteria for the validity of the perturbation theory used by Vinokur and Kravchenko [JETP Lett. **29**, 572 (1977)] and of the method used in the present paper are obtained. The temperatures of the transitions to the commensurate and incommensurate phases are calculated and the influence of quantum effects are analyzed. The effect of impurities on the conditions for observing the predicted transition is considered.

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A preceding paper[1] dealt with the feasibility of a displacive transition at line defects. It was shown that if the perturbation produced by the defect in the force-constant matrix of the initial crystal is large enough, then an instability $[\omega_0^2(q^*)=0, q^*\neq 0]$ arises in the spectrum of the phonons localized at the defect, meaning in fact the feasibility of a structural transition at the defect line. Such a transition will take place if the crystal contains a large enough system of defects parallel to one another [since a transition is at a single defect (in a one dimensional system) is impossible.[2]].

To estimate the transition temperature we used a scheme borrowed from the theory of phase transitions in ferroelectrics[3] and based on a consistent allowance for the anharmonic corrections to the spectrum of the localized phonons. The transition temperature is then estimated at[1]

$$t_c\sim\Delta_0^2c^{1/2}/\alpha. \tag{1}$$

Here

$$t=T/\Theta,\quad \Delta_0{}^2=-\Omega_0{}^2(Q^*)=-\omega_0{}^2(q^*)/\omega_D>0,\quad Q=q/q_0,$$

$\Theta=\hbar s q_0=\hbar\omega_D$ is the Debye temperature, $\alpha=\Theta/Ms^2$, M is the mass of the atom, s is the speed of sound, c is the dimensionless density of the line defects (the atomic density of the atoms belonging to the defect lines), and q_0 is the maximum value of the wave vector. The calculation was made under the assumption that $\Delta_0\ll 1$. It should be noted that this assumption is natural in the theory of ferroelectrics, inasmuch as in the three-dimensional problem the temperature $t_{c0}\sim\Delta_0^2/\alpha$, and if $\Delta_0\sim 1$, then t_c turns out to be higher than the melting temperature. In our case, however, when t_c is estimated from formula (1) and its smallness is ensured by the smallness of the density c, the condition $\Delta_0\ll 1$ is not necessary. On the contrary, it is more natural to assume that $\Delta_0\sim 1$ is possible under real conditions.

A large value of Δ_0 can no longer be offset by small anharmonic corrections. To consider the transition in this case it is convenient to use the method developed by Efetov and Larkin,[4] in which perturbation theory in small anharmonicities is not used. This method[4] is applicable, however, only when the fluctuations of the modulus of the order parameter can be neglected and the fluctuating quantity is the phase. To estimate the fluctuations of the modulus, we compare T_c with the free energy per unit cell at the instant of the three-dimensional transition.

The expansion of the free energy near $q=q^*$ can be written in the form

$$F\approx -M\omega_0{}^2|\psi_q|^2+\frac{Ms^2}{a^4}|\psi_q|^4, \tag{2}$$

where ψ is the order parameter (the average displacement) and a is the interatomic distance. The average displacement is determined by minimizing F:

$$\bar{\psi}_q{}^2=\omega_0{}^2a^4/2s^2\sim\Delta_0{}^2a^2 \tag{3}$$

and the free energy

$$F_{min}\sim -M\omega_0{}^4a^4/s^2\sim -Ms^2\Delta_0{}^4. \tag{4}$$

Comparing $F_{\min}$ with T_c from (1), we have

$$|F_{min}|/T_c\sim\Delta_0{}^2/c^{1/2}. \tag{5}$$

At $\Delta_0^2/c^{1/2}\ll 1$ the modulus of the order parameter does not have time to become fixed (the fluctuations of the modulus are large) and the method of Efetov and Larkin[4] is not applicable. The use of perturbation theory is then justified, just as was done in Ref. 1, since $\Delta_0^2\ll c^{1/2}<1$.

If, however, $\Delta_0^2/c^{1/2}\gg 1$, the modulus of the order parameter is frozen at temperatures $\sim T^*\sim|F_{\min}|\gg T_c$. In this case a transition will take place when the correlations of the phases at the different defects suppress the one-dimensional fluctuations. In other words, the increment to the free energy $F[\varphi]$ due to the interaction of different defects should be of the order of the energy of the phase fluctuations at the given defect at temperatures $\sim T_c$, i.e.,

$$T_c\sim W\left(\frac{\Phi}{a}\right)^2\frac{r_c}{a},$$

where W is the energy of the interaction of the fluctuations at the different defects, and r_c is the one-dimensional correlation radius. The temperature T_c obtained from this estimate is much less than $|F_{\min}|$, thus justifying the assumption that the fluctuations of the modulus of ψ are small.

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The foregoing estimate shows that T_c depends substantially on the temperature behavior of the correlation radius r_c. It is known that if the transition is into a phase commensurate with the initial lattice, then r_c depends on the temperature exponentially, and if the transition is into a incommensurate phase, the dependence follows a power law. It is clear that at $\Delta_0^2/c^{1/2} \ll 1$, when the modulus of the order parameter is not fixed at the instant of the transition, then t_c is independent of the type of the produced structure.

CALCULATION OF THE TRANSITION TEMPERATURE

The one-dimensional-system free energy connected with the fluctuations of the phase of the order parameter is of the form

$$F=\int\frac{dx}{a}\left\{\frac{1}{2}M\psi_0^2\left(\frac{\partial\varphi}{\partial\tau}\right)^2+\frac{1}{2}M\psi_0^2s^2\xi^2(\nabla\varphi-\varkappa_0)^2\right.$$
$$\left.+BMs^2\left(\frac{\psi_0}{a}\right)^m(1-\cos m\varphi)\right\}, \tag{6}$$

where $\psi=\psi_0\exp(i\varphi+iq_0xn/m), s\xi\approx(\partial\omega/\partial q)_{q\approx q^*}$ is the phason velocity, and $\varkappa_0=q^*-q_0n/m$ is the incommensurability vector. The last term in (6) is the commensurability energy that takes into account the invariance of the system to a shift by m lattice periods; B is a number of the order of unity. If the system is noncommensurate, then $m\to\infty$ and the commensurability energy vanishes ($\psi_0/a<1$). The quantity $\psi_0=|\bar\psi_q|$ is determined by Eq. (3).

We obtain now the free-energy increment produced by the interaction of the defects. We consider for this purpose, for example, a crystal containing a regular (quadratic in the section perpendicular to the lines) lattice of parallel line defects. It is easy to write down Dyson's equation for the lattice Green's functions:

$$G_q^d(\mathbf{n}_i-\mathbf{n}_j;\,\omega)=G_q^0(\mathbf{n}_i-\mathbf{n}_j;\,\omega)+U_q\sum_{\mathbf{n}_k}G_q^0(\mathbf{n}_i-\mathbf{n}_k;\,\omega)G_q^d(\mathbf{n}_k-\mathbf{n}_j;\,\omega),$$

where q is the wave vector along the defects, U_q is the Fourier component of the local perturbation introduced by an individual defect,[1] and $\mathbf{n}_i$ (the lattice indices) are the coordinates of the defect atoms in a plane perpendicular to the defect; the superscript d indicates that one considers Green's functions with lattice indices that describe the defect atoms,

$$G_q^0(\mathbf{n}_\perp,\omega)=\frac{1}{N_\perp}\sum_{q_\perp}\frac{\exp(i\mathbf{q}_\perp\mathbf{n}_\perp)}{\omega^2-\omega^2(q)}$$

is the Fourier component [with respect to $(n_\parallel)$ of the Green's function of a defect-free crystal.

Carrying our a Fourier transformation over the defect lattice, we easily obtain the following expression for the defect Green's function:

$$G_q^d(\mathbf{n}_\perp=0;\,\omega)=\frac{1}{N_\perp}\sum_g\sum_\varkappa\frac{G^0_{q,\varkappa+g}}{1-U_qG_q^0(0,\omega)+cU_q/[\omega^2(q,\varkappa)-\omega^2]},$$

where g are the defect-reciprocal-lattice vectors ($g_\alpha=\pi k_\alpha/L_d$, L_d is the distance between the nearest line defects, k_α are integers, α is the coordinate index), $\varkappa=\pi k_\alpha/L_{\text{cr}}$ (L_{cr} is the dimension of the crystal in the plane perpendicular to the defects), and $\varkappa_{\max}=\pi/L_d$. Carrying out the summation, we easily obtain an expression for $G_q^d(0,\omega)$ and the increment to the dispersion law of the local phonons (in dimensionless units):

$$\Delta\Omega^2=-c\left[\left|\frac{dG_q^0(0,\Omega_0^2)}{d\Omega_0^2}\right|(\Omega^2(Q)-\Omega^2)\right]^{-1}, \tag{7}$$

where Ω_0 is the dispersion law of a single defect.

The free energy of a defect passing through the origin takes in this case the form

$$F=F_0-\sum_{ll'}\sum_{\mathbf{n}_\perp}W(\mathbf{n}_\perp,l-l')\psi_{\mathbf{n}_\perp l}\psi_{0l'}, \tag{8}$$

$$W(\mathbf{n}_\perp,l)=\frac{1}{N}\sum_q W_q(\mathbf{n}_\perp)e^{iql},$$

$$W_q=\frac{1}{2}M\omega_D^2c\frac{G_q^0(\mathbf{n}_\perp,\Omega_0^2)}{|dG_q^0(0,\Omega_0^2)/d\Omega_0^2|}, \tag{9}$$

where the index l numbers the sites along the defect, and $\mathbf{n}_\perp$ lies in the plane perpendicular to the defects. The same result can be easily obtained by calculating the corrections to the spectrum of the local vibrations of the given defect in a crystal containing a system of randomly distributed defects[1,6] and averaging next the increment to the free energy over all the defect configurations.

We write down, following Ref. 4, the self-consistency equation for $\langle\psi\rangle$:

$$\langle\psi(0,l_0;\,\tau_0)\rangle=\frac{1}{Z}\int D\varphi\psi(0,l_0;\,\tau_0)\exp\left[-\int_0^\beta d\tau F_0(\tau)\right.$$
$$\left.+\int_0^\beta d\tau\sum_{\mathbf{n}_\perp ll'}W(\mathbf{n}_\perp,l-l')\langle\psi(\mathbf{n}_\perp,l';\,0)\psi^*(0,l;\,\tau)\rangle\right]. \tag{10}$$

Assuming the fluctuations of ψ to be small, we expand in the small interaction W and, putting $l_0=0$ and $\tau_0=0$, obtain

$$\langle\psi(0,0)\rangle=\frac{1}{Z}\int D\varphi\psi(0,0)\exp\left(-\int_0^\beta F_0d\tau\right)\cdot$$
$$\times\int_0^\beta d\tau\sum_{ll'}W(l-l')\langle\psi(l',0)\rangle\psi^*(l,\tau)$$
$$=\int_0^\beta d\tau\sum_{ll'}W(l-l')\langle\psi(0,0)\psi^*(l,\tau)\rangle_0\langle\psi(l',0)\rangle, \tag{11}$$

where

$$W(l-l')=\sum_{\mathbf{n}_\perp}W(\mathbf{n}_\perp,l-l'). \tag{12}$$

Here $\langle\ldots\rangle_0$ denotes averaging with a purely one-dimensional free energy F_0.

Taking the Fourier transform with respect to q along the defects

$$\langle\psi(0,0)\rangle=\frac{1}{N}\sum_q\bar\Psi_q \tag{13}$$

and taking (12) and (9) into account, we obtain ($\Omega_0^2(Q^*)\ll\Omega^2(Q^*,0)\sim1$, $|G'_{Q^*}(\Omega_0^2)|\sim1$):

$$\frac{1}{N}\sum_q\bar\Psi_q=\frac{c}{N}\sum_{l,q}\int_0^\beta d\tau M\omega_D^2e^{iql}\langle\psi(0,0)\psi^*(l,\tau)\rangle_0\bar\Psi_q. \tag{14}$$

Since the instability point is $q=q^*$, it follows that $\bar\psi_q=\psi_{q^*}\delta_{qq^*}$. We obtain thus the known relation that determines the transition temperature:

$$1=\int_0^\beta d\tau \sum_l cM\omega_D^2 \exp(iq^* l)\langle\psi(0,0)\psi^*(l,\tau)\rangle_0. \tag{15}$$

The correlation functions of one-dimensional systems were calculated in Refs. 7 and 8. It is convenient to consider separately the transitions into the commensurate and incommensurate phases.

TEMPERATURE OF TRANSITION INTO THE INCOMMENSURATE PHASE

1. *Classical region.* In this region we can neglect the dependence of $\overline{\psi}$ on the imaginary time τ. We have[7,8]

$$\langle\psi(0)\psi^*(l)\rangle=\psi_0^2\langle\exp[i\varphi(0)-i\varphi(l)]\rangle_0\exp\left(-i\frac{2\pi l}{a}\frac{n}{m}\right), \tag{16}$$
$$\langle\exp[i\varphi(0)-i\varphi(l)]\rangle_0=\exp(-|l|/r_c-i\varkappa l),$$

where $\varkappa$ is a certain function of $\varkappa_0=q^*-2\pi n/am$. In the case of a noncommensurate structure[8] $\varkappa\approx\varkappa_0$. Summing over l in (15), we get

$$1=c\frac{M\omega_D^2\psi_0^2}{T}\frac{r_c}{a},\quad r_c=\frac{2Ms^2\xi^2\psi_0^2}{aT}, \tag{17}$$

whence

$$t_c\sim\Delta_0^2c^{1/2}/\alpha, \tag{18}$$

which, as expected, coincides with (1).

2. *Quantum region.* The quantum effects become significant at temperatures

$$T\ll s\xi q/2\pi\sim\xi\omega_D/2\pi. \tag{19}$$

Writing

$$\varphi(x,\tau)=\varphi_0(x)+\sum_{n\neq0}\varphi(\omega_n)e^{-i\omega_n\tau}\equiv\varphi_0+\varphi_1 \tag{20}$$

(we have replaced the lattice index l along the defect by the coordinate x), we easily obtain

$$\langle\ldots\rangle_0\equiv K(x,\tau)=\exp\left\{-\frac{T}{2aM\Delta_0^2L}\sum_{q,\omega_n\neq0}\frac{1-\cos(qx-\omega_n\tau)}{\omega_n^2+u^2q^2}\right\}K_0(x), \tag{21}$$

where $u-\xi s, \omega_n=2\pi T, K_0(d)$ is the classical correlation function, and L is the length of the defect.

Taking into account the cutoff in q $(q<\omega_D/s)$, we get

$$K(x,\tau)=\left(\frac{\omega_D}{2T}\right)^{-\sigma}\exp\left\{-\frac{\sigma}{2}\ln\left[(1-e^{-2\pi Tx/u})^2\right.\right.$$
$$\left.\left.\times\cos^2(\pi T\tau)+(1+e^{-2\pi Tx/u})^2\sin^2(\pi T\tau)\right]\right\}K_0(x), \tag{22}$$

$\sigma=\alpha/4\xi\Delta_0^2$. Integrating with respect to τ, we obtain for

$$K(x)=T\int_0^\beta d\tau K(x,\tau)$$

the expression

$$K(x)=\left(\frac{\omega_D}{2T}\right)^{-\sigma}F\left(\frac{\sigma}{2},\frac{\sigma}{2},1,e^{-4\pi Tx/u}\right)K_0(x). \tag{23}$$

Taking into account the smallness of σ $(\sigma\ll1)$, we easily verify that both at $4\pi Tx/u\ll1$ and at $4\pi Tx/u\gg1$ the hypergeometric function $F\approx1$. This circumstance enables us to assume the following interpolation formula for $K(x)$:

$$K(x)\approx\left(\frac{\omega_D}{2T}\right)^{-\sigma}K_0(x). \tag{24}$$

In view of the smallness of σ the quantum corrections lower the transition insignificantly.

TEMPERATURE OF TRANSITION INTO THE COMMENSURATE PHASE

In the transition into the commensurate phase, the free energy $F[\varphi]$ of a one-dimensional system is given by Eq. (6). It is known that the nonlinearity connected with the commensurability energy leads to a specific behavior of the system at low temperatures. The destruction of the long-range order in such one-dimensional systems is the result of breakup into regions of finite length (domains) with almost constant values of the phase. The domains are separated by rather narrow domain walls in which the phase changes by $\sim\pi$. These domain walls are solitons, whose dynamics is described by a sine-Gordon equation derived in standard fashion from (6).

1. *Classical region.* In this case the quantity $\varkappa$ is exponentially small and $q^*\approx2\pi n/am$, since $\varkappa_0$ is also small. In this case[8]

$$\frac{a}{r_c}\approx\frac{4m}{\sqrt{\pi}}\left(1-\cos^2\frac{2\pi}{m}\right)\Omega_p^{3/2}\left[\frac{\Delta_0^2}{\alpha t}\frac{\xi}{(aq_0)^2}\right]^{1/2}$$
$$\times\exp\left\{-\frac{2^{3/2}}{m}\frac{\xi}{(aq_0)^2}\frac{\Delta_0^2}{\alpha t}\left[\frac{aq_0}{B\sqrt{2}}\Omega_p-\frac{\pi}{8^{1/2}}a\varkappa_0\xi\right]\right\}, \tag{25}$$

where

$$\Omega_p=\frac{\omega_p}{\omega_D}\frac{\sqrt{2}}{aq_0}B\left(\frac{\Delta_0}{aq_0}\right)^{m/2-1}\sim\Delta_0^{m/2-1}$$

is the dimensionless pinning frequency.

We estimate the transition temperature for $m=2$. Substituting (25) in (17), we obtain

$$1\sim\frac{c}{\Omega_p^2}z^{1/2}e^z,\quad z=\frac{2\xi}{\pi}\frac{\Delta_0^2}{\alpha t}\frac{aq_0}{B}\Omega_p,$$

and hence, with logarithmic accuracy,

$$t_c\sim\frac{4aq_0\Omega_p}{B}\frac{\Delta_0^2}{\alpha}\left\{\ln\left[\frac{\Omega_p^2}{c}\left(\ln\frac{\Omega_p^2}{c}\right)^{-1/2}\right]\right\}^{-1}. \tag{26}$$

At $c\sim10^{-8}$

$$t_c\sim\frac{\Delta_0^2}{\alpha\ln(1/c)}\sim5\Delta_0^2$$

(we have taken it into account that $\Omega_p\sim1$ at $m=2$).

2. *Quantum region.* If the defect density c is not too large, $c<\Omega_p^2\exp(-\Delta_0^2/\alpha)$, then the transition temperature obtained from (26) turns out to be in the quantum region:

$$t_c\sim\Delta_0^2/\alpha\ln(\Omega_p^2/c).$$

In this case the foregoing analysis is not valid and to obtain a correct estimate of t_c we must take quantum effects into account. Nonetheless, the result (26) remains practically unchanged if $\omega_p\ll\omega_D$ and the transition temperature is not too low, so that the condition $\omega_D\gg T_c\gg\omega_p$ is satisfied. In fact, by using the representation (20) for φ we can, integrating with respect to $\varphi_1(x,\tau)$ leave out (at $T\gg\omega_p$) the nonlinear term of the free energy (6), after which we obtain for the correlation function formula (24) [where $K_0(x)$ is, naturally, the correlation function of the classical commensurate system]. Just as in the transition into the noncommensurate phase, the quantum corrections cause t_c to decrease slightly.

The situation is different if $T_c < \omega_p$ (particular interest attaches in this connection to the case $m=2$, when $\omega_p \sim \omega_D$). In the low temperature region, $T < \omega_p$, the term proportional to $1-\cos m\varphi$ in the free energy can no longer be neglected when integrating with respect to φ_1, and to obtain the correlation function we must consider the quantum statistics of the nonlinear system.

The argument of the exponential in (19) is the effective action of the phase connected with the fluctuations, and the quantity F_0 in (6) is none other than the effective Lagrangian, which depends on the imaginary time τ. By making the substitutions

$$\frac{x}{a} \to x, \quad s\xi q_0 \tau \to \tau, \quad \frac{\xi \Delta_0^2}{(\pi\alpha)^{1/2}} \varphi \to \varphi$$

we can reduce the Lagrangian (6) to the standard form

$$\mathscr{L} = -\frac{\omega_D}{2} \int dx \left\{ \left(\frac{\partial\varphi}{\partial\tau} \right)^2 + \left(\frac{\partial\varphi}{\partial x} \right)^2 + \frac{2\mu}{g^2} (1 - \cos g\varphi) \right\} \tag{27}$$

with a coupling constant $g^2 = (\alpha/\Delta_0^2)(\pi M/\xi)$ and with an effective mass $\mu = \Omega_p/\xi$.

The quantum statistics of a system with a Lagrangian (27) was constructed in the papers of Maki and Takayama.[9] Using the results of these papers, we easily obtain the correlation function

$$K(x) \approx \exp\left\{ \frac{\alpha}{4\xi\Delta_0^2} \mathscr{K}_0 \left(\frac{|x|}{r_p} \right) \right\} \exp(-4n_s|x|),$$

where n_s is the density of the domain walls (solitons) that disturb the long-range order in the one-dimensional system, and $\mathscr{K}_0$ is a MacDonald function. The pinning radius $r_p = \xi s/\omega_p$ ($\sim a$) is quite small.

For the soliton density we have[9]

$$n_s = (E_s^{(0)} T/2\pi)^{1/2} \exp(-E_s^{(0)}/T), \quad T \ll \mu,$$
$$n_s = \mu (E_s/2\pi T)^{1/2} \exp(-E_s/T), \quad T \gg \mu,$$

where the soliton energy is

$$E_s = 8\mu/g^2, \quad E_s^{(0)} = E_s(T=0) \approx E_s$$

accurate to $o(g^2)$. Returning to the initial notation, we have

$$n_s = \frac{1}{a} \left(\frac{2\Omega_p\xi}{\pi^2} \frac{\Delta_0^2 t}{\alpha} \right)^{1/2} \exp\left(-\frac{4\Omega_p\xi}{\pi} \frac{\Delta_0^2}{\alpha t} \right) \times \begin{cases} 1, & t \ll \Omega_p \\ \Omega_p/\xi t, & t \gg \Omega_p \end{cases}. \tag{29}$$

At $T < \omega_p \lesssim \omega_D$, the quantum effects lead to an effective increase of the soliton energy and consequently to a decrease of their density compared with the classical value at the same temperature. As seen from (28), the correlation radius is simply a quantity inversely proportional to the soliton density: $r_c = a(4n_s)^{-1}$. Substituting this expression in (17) we obtain for t_c the estimate ($t_c < \Omega_p$)

$$1 \sim c \frac{4\Delta_0^2}{\alpha t_c} \left(\frac{\alpha}{t_c \Delta_0^2} \frac{\pi^2}{2\Omega_p \xi} \right)^{1/2} \exp\left(\frac{4\Omega_p\xi}{\pi} \frac{\Delta_0^2}{\alpha t_c} \right), \tag{30}$$

whence we obtain at $\xi \sim 1$ and $\Omega_p \sim 1$, with logarithmic accuracy,

$$t_c \sim \frac{\Delta_0^2}{\alpha} \left\{ \ln\left[\frac{1}{c} \left(\ln\frac{1}{c} \right)^{-1/2} \frac{\Delta_0^2}{\alpha \ln(1/c)} \right] \right\}^{-1}. \tag{31}$$

The transition temperature is somewhat higher than would be obtained by using the classical value for n_s, since, as already noted, we land in the quantum region if $\Delta_0^2/\alpha \ln(1/c) < 1$. If, for example, we assume $\Delta_0^2 \sim 0.1$, then t_c lies in the quantum region at $c < 10^{-6}$.

EFFECT OF IMPURITIES

The considered structural transition leads to the onset of an additional peak in the structure factor of a crystal with line defects at a wave-vector value $q = q^*$. However, the impurities inevitably present in the crystal (in particular, those located on the defect lines themselves), scatter the local phonons and, by breaking down the correlation of the phases, destroy the long-range order. In the presence of impurities, the sharp peaks in the structure factor become smeared out and the conditions for observing the phase transition become worse.

The effect of impurities on the structure transition in a one-dimensional system was considered in a number of papers.[10-13] We assume that all the impurities the constitute local (single-site) perturbations of the force constants are located on defect lines. The perturbation of the mass can be disregarded, since it enters in the equations of motion only together with the frequency, and we are considering a situation $\omega \approx 0$. The interaction of the phonons with the impurities leads to the appearance in the free energy of an additional term

$$\sim V M \psi_0^2 s^2 \cos(2q^* x + \varphi(x)),$$

where V is a dimensionless quantity that characterizes the change of the force constants by the impurities: $V \approx \Delta\Phi/\Phi$. We introduce also the dimensionless impurity density $n_i = a/l$, where l is the average distance between the impurities on the defect line, and analyze separately the transitions into commensurate and incommensurate structures.

1. *Transition into an incommensurate phase*. The free energy of a system of defects can be approximately written in the form

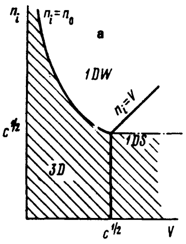
$$F[\varphi] \sim Ms^2 \frac{\psi_0^2}{a^2} \int dx \int \frac{d\mathbf{r}_\perp}{d^2} \left\{ a \left(\frac{\partial\varphi}{\partial x} \right)^2 + c \frac{d^2}{a^2} (\nabla_\perp \varphi)^2 \right\} + \sum_i V \cos(2q^* x + \varphi) \delta(\mathbf{r} - \mathbf{r}_i), \tag{32}$$

$\mathbf{r} = (x, \mathbf{r}_\perp)$, where the last term in the braces is the energy of the impurities and d is the average distance between defects.

The characteristic phase-change distances L_x and $L_\perp$ can be obtained by minimizing the free energy. If $L_\perp \gg d$, we are dealing with the three-dimensional situation considered in Ref. 11. At $L_\perp < d$, each defect must be considered independently (from the point of view of the influence of the impurities), as was done in Ref. 12. It is easy to show that in the three-dimensional region

$$L_x \sim L_\perp = L_{EL} \sim ac/n_i V^2 \tag{33}$$

in accord with the results of Efetov and Larkin.[11]



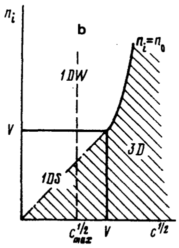


FIG. 1.

In the one-dimensional region it is necessary to consider separately the cases of weak ($V \ll n_i$) and strong ($V \gg n_i$) pinning. In the case of weak pinning each impurity changes the phase little, and[12]

$$L_s = L_{LF} \sim a V^{-2/3} n_i^{-1/3}. \tag{34}$$

In the case of strong pinning, the characteristic distance is simply the average distance between the impurities

$$L_s \sim a/n_i. \tag{35}$$

The foregoing situation are lucidly represented in the form of the phase diagram of our system on a plane with coordinates (n_i, V) and $(n_i, c^{1/2})$ (Fig. 1). The boundary between the three-dimensional (3D) region and the one-dimensional region with weak pinning (1SW) is the curve $n_i = n_0 \equiv c^{3/2} V^{-2}$. The regions 1DW and the one-dimensional region with strong pinning border on the line $n_i = V$, and finally the boundary between the regions 1DS and 3D is the line $c^{1/2} = V$.

The possibility of observing a structural transition in the presence of impurities is determined by the relation between the temperature correlation radius $r_c(T)$ near $T = T_c$ and the impurity characteristic length. In the absence of impurities, at $T = T_c$, the system becomes three-dimensional and, with decreasing temperature, $r_c(T)$ increases abruptly to infinity—a phase transition takes place. On going into the incommensurate phase, $r_c(T_c) \sim a/c^{1/2}$. If we are in the 3D region in this case, then

$$r_c(T_c)/L_{EL} \sim n_i/n_0 \ll 1$$

and $r_c(T)$ increases rapidly at $T < T_c$ to a value $r_c = L_{EL}$ and then remains constant with further lowering of the temperature. In this case, a phase transition can be observed: rather sharp peaks are present in the structure factor at $q = q^*$.

The situation is similar also in the 1DS region when the condition $n_i \ll c^{1/2}$ [i.e., $r_c(T_c) \ll L_s$] is satisfied. In the 1DW region, on the other hand, we have

$$r_c(T_c)/L_{LF} \sim (n_0/n_i)^{1/3} \gg 1.$$

There will be no abrupt increase of r_c, i.e., the transition becomes washed out by the impurities and is not observed. The phase-diagram (Fig. 1) region in which a structural transition is observable is shown shaded. We note that since the characteristic values of the potential V are $V \lesssim 1$, and $c \ll 1$, it appears that under real conditions only part of the diagram can be realized, the one located to the left of the vertical line $c^{1/2} = c^{1/2}_{\max}$ (Fig. 1b).

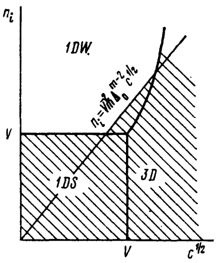


FIG. 2.

2. *Transition to the commensurate phase*. In this case there is added to the free energy (32) a term $a^{-1}\Delta_0^{m-2}(1-\cos m\varphi)$ in the braces under the integral sign. It is easy to obtain the conditions under which the influence of the impurities can be regarded as a small perturbation against the background of the commensurability energy:

$$\begin{gathered} n_i \ll c\Delta_0^{m/2-1} V^{-2} \quad (3D), \\ V \ll \Omega_p \Delta_0^2 \quad (1DS), \\ n_i \ll c^{1/2} V^{-2} m \Delta_0^{m-2} \quad (1DW). \end{gathered} \tag{36}$$

The condition (36) in the 1DS region denotes merely that the impurity energy is small compared with soliton-formation energy. If $\Omega_p \sim 1$, this condition is satisfied for the small perturbations caused by the impurities $V \ll 1$, and then the impurities do not destroy the long-range order in the 1DS region. At small V we have $mV^{-2}\Delta_0^{m-2} > 1$ and a small corner, cut off from this region by the line $n_i = (m\Delta_0^{m-2}/V^2)c^{1/2}$ appears in the 1DW region; a phase transition can be observed in this corner, too (Fig. 2). On the other hand, in the region 3D the condition (36) is practically always satisfied. Thus, on going into the commensurate phase and at $V \ll \Omega_p \Delta_0^2$ the region of existence of a well pronounced transition takes the form shown (shaded) in Fig. 2. When the conditions (36) are not satisfied in the 1D regions, the perturbation is the pinning energy, and the possibility of observing the transition is described by the diagrams of Fig. 1.

CONCLUSION

The line-defect model investigated by us can be used to describe, for example, long chains of foreign atoms that have penetrated into a crystal. A suitable object for the realization of the considered effect can apparently be also a system of straight dislocations. There are grounds for assuming that in the immediate vicinity of the dislocation core the elastic moduli of the crystal become greatly softened. Within the framework of the lattice model used by us, this softening can be described as a decrease in the values of the force constants directly on the dislocation line.

The phonon-spectrum distortions that arise in such a model should lead to definite singularities in the behavior of the critical characteristics of crystals with dislocations. The earlier calculation of the contribution of the local phonons to the dislocations electric resistivity of metals and to the relaxation of the dislocation spin system[1,14] lead to results that make it possible to explain qualitatively the available experimental data (the agreement with experiment improves if it is assumed that the local phonon spectrum has a dip at $q = q^* \neq 0$). This circumstance can be regarded as an additional argument favoring the use of our model to describe a system of dislocations.

If a deformed material is investigated by x-ray structure analysis method, then the postulated effect should manifest itself in the form of an additional maximum of the structure factor. With decreasing temperature, the line intensity should increase, and the width decrease. As the transition point T_c is approached, this intensity increases sharply. If the dislocations are parallel to one another, then the proposed structure produces on the Laue pattern a maximum in a plane perpendicular to the dislocations. On the other hand, if the dislocations are randomly oriented, then with respect to the resultant superstructure the sample is a polycrystal. One should search for new reflections on the corresponding Debye–Scherer diagram. As shown above, impurities on dislocations affect adversely the observation conditions. One should therefore avoid annealing of the samples, which leads to an increased impurity density at the dislocations.

The supercriticality Δ_0 is determined by the value of the parameter λ, which characterizes the change of the elastic interactions in the region of the line defect.[1] Having only qualitative grounds for the possibility of realizing a value of λ that leads to instability, we cannot, of course, estimate reliably Δ_0 and hence T_c for the dislocations. We can nonetheless estimate the temperature interval in which the structural transition should be sought.

At weak supercriticality ($\Delta_0^2 \ll c^{1/2}$) or on going into an incommensurate (at $\Delta_0^2 \gg c^{1/2}$) phase, we can indicate only the upper bound of T_c. Namely, recognizing that the supercriticality should be less than the Debye temperature we obtain (at $c \sim 10^{-7}$) $T_c < 10^{-2}\Theta$. A transition into a commensurate phase is possible only at $\Delta_0^2 \gg c^{1/2}$, from which it follows that

$$\Theta c^{1/2}/\alpha \ln[(1/c)\ldots] < T_c < \Theta/\alpha \ln[(1/c)\ldots],$$

which yields $\Theta \cdot 10^{-3} < T_c < \Theta$ at $c \sim 10^{-7}$.

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