Phase transitions of the second kind in crystals containing dislocations

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The characteristics and the domain structure of ordered regions (OR), which occur in a disordered phase near dislocations, are considered. It is taken into account that such OR may form a random framework that penetrates the whole crystal but occupies a small fraction of its volume. In many systems, for typical values of the parameters, a phase transition proves possible, with establishment of definite order within the framework, at some temperature T_f considerably higher than the transition temperature T_c^0 in an ideal crystal. Because of the smallness of the volume of the framework, the mean order parameter $|\overline{\eta}|$ remains very small at $T \approx T_f$, and only in the range $T \approx T_c^0$ should there be observed experimentally a noticable increase of $|\overline{\eta}|$, manifesting itself as a smeared out phase transition. For other values of the parameters, a percolation transition, of the type considered by S. L. Ginzburg, [Sov. Phys. JETP 46, 1029 (1977)], proves possible in a crystal containing dislocations. The dependences of the singularities of thermodynamic quantities on the dislocation density and on the crystal parameters are investigated. Dislocation superparamagnetism at $T > T_f$ is considered.

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The crystals in which phase transitions are studied usually contain dislocations. The random strain field produced by them may substantially affect the singularities of thermodynamic quantities near the transition point. The nature of the effect of the random field on these singularities depends to a considerable degree on its correlation distance. The case of a δ -correlated field, representing, for example, crystals with point defects, has been treated by the ε -expansion method,¹⁻⁴ and it was found that in a nonideal crystal, power-law singularities are preserved. A different physical situation occurs for large-scale inhomogeneities, investigated by S. L. Ginzburg.⁵ In this case, it was found possible to introduce a local transition temperature $T_{c}(\mathbf{r})$ and to relate the phase transition to the occurrence of percolation over the region $T \leq T_c(\mathbf{r})$. Such a percolation phase transition is also clearly expressed (although to it correspond different critical indices).

The random fields produced by an ensemble of dislocations usually vary slowly with distance, and to describe the effects produced by them it is also possible to apply the local transition temperature approximation (LTTA); criteria for its applicability are discussed below. But the random field $T_c(\mathbf{r})$ in a crystal with dislocations is in general more complicated than the Gaussian field, with homogeneous and isotropic correlation function, considered in Ref. 5 (the regions with maximum $T_c(\mathbf{r})$ form cylinders near the dislocation lines), and the physical picture of the phase transition may differ significantly both from a percolation transition and from a transition in an ideal crystal. Ordered regions (OR) near dislocation lines may appear considerably above the transition temperature T_c^0 in an ideal crystal⁶ (and even in crystals in which, in the absence of dislocations, no phase transition at all is observed⁷).

Below, the important fact is taken into account that in a crystal with straight-line dislocations or with dislocation loops of large radius, the OR form a com-

plicated random framework, consisting of ordered domains with order parameter η of different signs, and penetrating the whole crystal, although still occupying a small fraction of its volume. At some temperature $T_f > T_c^0$, a structure consisting of an equal number of domains with opposite signs of η is transformed to a state with a predominant number of domains with a definite sign of η ; that is, a phase transition takes place in the dislocation framework. With lowering of the temperature, the thickness of the ordered elements of the framework increases; and when $T \approx T_c^0$, there should appear comparatively large ordered clusters, entrapping many dislocations. Therefore η in them takes the same sign as in the framework that links them in the infinite cluster. As a result, in the range $T \approx T_c^0$, where the order gradually spreads over the whole volume of the crystal, there occurs a continuous change of $\eta(T)$ and of its derivatives from very small values to values corresponding to an ideal crystal. Experimentally, this should manifest itself as a smeared out phase transition of the second kind. Thus the physical reason for the smeared out phase transition that is usually observed experimentally may be the formation of an ordered dislocation framework.

The picture described should hold for $T_f - T_c^0 \gg \delta T_{cr}$, where δT_c is the spread of $T_c(\mathbf{r})$. For other values of the crystal parameters, $T_f - T_c^0 \leq \delta T_{cr}$, no framework forms, and percolation occurs only if the infinite cluster directly includes an appreciable fraction of the volume. There then occurs a percolation transition of the type considered by Ginzburg.⁵

The purpose of the present paper is to discuss the general qualitative features of the effect of dislocations on various types of phase transition of the second kind, and to investigate the dependence of their characteristics on the parameters of the dislocation ensemble, such as the dislocation density and the radius of the dislocation loops. The numerical coefficients in the corresponding relations are in most cases determined only in order of magnitude. By the long-range order parameter $\eta(\mathbf{r})$ we shall understand a dimensionless parameter characterizing the corresponding transition; for example, the degree of long-range order in the case of ordered alloys, or the ratio \mathbf{M}/M_0 of the magnetization to the saturation magnetization at T=0 in the case of a ferromagnetic transition. The paper will consider only the equilibrium characteristics of the inhomogeneous ordered structure that arises; the kinetics of its formation will not be discussed. It is assumed that at a given temperature, the positions of the dislocations are fixed.

In Section 1, we present the strain field and the temperature field $T_c(\mathbf{r})$ produced by straight-line dislocations and by dislocation loops, and also by statistical ensembles of them. In Section 2, we discuss the formation of OR produced by individual dislocations. In Ref. 6, this problem was treated in the self-consistent field approximation, as a phase transition leading to establishment of an $\eta(\mathbf{r})$ of a single sign throughout the whole OR. But in the temperature range in which order is established, in a quasi-one-dimensional OR, fluctuations are very important that lead to the formation of domains with different η and to a considerably smeared out phase transition. In this connection, formation of OR near dislocations is treated in the LTTA for a system with arbitrary critical indices, with allowance for fluctuations. An estimate is given for the characteristic lengths of domains; it is necessary for investigation of the problem of the dislocation framework. In Section 3, we consider the formation of such frameworks, "true" phase transitions in them, and smeared out phase transitions in the volume of the crystal; we also analyze the temperature dependences of thermodynamic quantities in the presence of frameworks. We consider in Section 4 the order case, when $T_f - T_c^0 < \delta T_c$, no framework forms, and a percolation phase transition occurs. We discuss also the question of the applicability of the LTTA used earlier⁵ to describe such a transition, and we estimate the temperature interval near the transition point itself in which such an approximation ceases to be applicable.

1. THE STRAIN FIELD AND THE LOCAL TRANSITION TEMPERATURE FIELD IN A CRYSTAL CONTAINING DISLOCATIONS

For simplicity we shall suppose that there is no strain linear in η and that $T_c(\mathbf{r})$ is determined solely by the trace of the stress tensor, $\sigma = \sigma_{ii}$, or by the dilatation $u = u_{ii}$. Near the transition point in a strained crystal, the thermodynamic quantities depend on the difference $T - T_c[\sigma(\mathbf{r})]$. Outside an insignificant range of very small $T - T_c$, provided the criteria indicated below are satisfied, we may neglect the change δK of the bulk modulus K near T_c and the distortion of the dislocation-produced field $u(\mathbf{r})$ that results from the OR. Then

$$\tau_{\mathfrak{e}}(\mathbf{r}) = \frac{T_{\mathfrak{e}}(\mathbf{r}) - T_{\mathfrak{e}}^{\circ}}{T_{\mathfrak{e}}^{\circ}} = \kappa u(\mathbf{r}), \quad \kappa = -K \frac{1}{T_{\mathfrak{e}}^{\circ}} \frac{\partial T_{\mathfrak{e}}^{\circ}}{\partial P}, \quad \tau = \frac{T - T_{\mathfrak{e}}^{\circ}}{T_{\mathfrak{e}}^{\circ}}.$$
(1)

Here P is the pressure, and we have introduced convenient reduced temperatures: τ and the transition

temperature $T_c(\mathbf{r})$. For a straight-line dislocation,

$$\pi_{cn}(\mathbf{r}-\mathbf{r}_t) = \frac{\varkappa b}{|\mathbf{r}_{\perp}-\mathbf{r}_t|} f_n(\theta), \quad f_n(\theta) = -\frac{1}{2\pi} \frac{1-2\mu}{1-\mu} \sin \theta.$$
 (2)

Here the index *n* determines the type of dislocation, i.e., the directions of the Burgers vector **b** and of the dislocation line 1; the vector \mathbf{r}_t is the position of a site in the atomic plane perpendicular to 1 through which the dislocation line passes; \mathbf{r}_{\perp} is the projection of **r** on this plane; $\theta - \theta_n$ is the angle between $\mathbf{b} = \mathbf{b}_n$ and $\mathbf{r}_{\perp} - \mathbf{r}_t$. The explicit form of $f_n(\theta)$ is given for an edge dislocation in an isotropic medium (μ is Poisson's ratio). In elastically anisotropic crystals also, $|f_n(\theta)| \sim 0.1$.

In crystals containing several (\dot{p}) systems of randomly distributed dislocations, within linear elasticity theory one can determine the dilatation, and consequently $\tau_c(\mathbf{r})$, as the superposition of terms produced by the individual dislocations:

$$\mathbf{r}_{c}(\mathbf{r}) = \sum_{n=1}^{p} \sum_{t} c_{in} \tau_{cn} (\mathbf{r} - \mathbf{r}_{t}).$$
(3)

Here the numbers c_{in} are unity or zero, depending on whether a dislocation of type *n* passes through the site *t*. They are uncorrelated random quantities, taking the value unity with some probability $c_n \ll 1$ (we shall consider the c_n equal for dislocations with opposite signs). The probability distribution $w(\tau_c)$ of the random function (3) has the form

$$w(\tau_{c}) = \left\langle \delta \left[\tau_{c} - \sum_{ni} c_{in} \tau_{cn} (\mathbf{r} - \mathbf{r}_{i}) \right] \right\rangle$$
$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iz\tau_{c}} e^{-g(z)} dz, \qquad (4)$$
$$g(z) \approx \sum_{n} c_{n} \sum_{t} \left[1 - \cos z \tau_{cn} (\mathbf{r} - \mathbf{r}_{i}) \right], \quad c_{n} \ll 1.$$

An analysis of functions of the type g(z) and $w(\tau_c)$ for straight-line dislocations was carried out in an investigation of the scattering of x rays and of nuclear magnetic resonance and nuclear gamma resonance spectra.⁸⁻¹⁰ If the size R of the crystal is large in comparison with the mean distance r_d between dislocations, one may neglect terms of order unity in comparison with the large quantity $l \approx \ln(R/r_d)$. In this approximation, $w(\tau_c)$ in its central part is described by a Gaussian function, and in its tails decreases according to a power law:¹⁰

$$w(\tau_{c}) = \frac{(2\pi)^{-l_{h}}}{\delta\tau_{c}} \exp\left[-\frac{\tau_{c}^{2}}{2(\delta\tau_{c})^{2}}\right], \quad |\tau_{c}| \leq \delta\tau_{c},$$

$$w(\tau_{c}) = \frac{1}{2l\delta\tau_{c}} \left(\frac{\delta\tau_{c}}{|\tau_{c}|}\right)^{3}, \quad |\tau_{c}| \gg \delta\tau_{c},$$

$$\delta\tau_{c} = \varkappa f \left(ln_{d}b^{2}\right)^{1/2}, \quad l = \frac{1}{2} \ln\left[2\pi n_{d}R^{2}\ln\left(2\pi n_{d}R^{2}\right)\right] \approx \int_{r_{d}/l^{1/4}}^{R} \frac{dr_{\perp}}{r_{\perp}}, \quad (5)$$

$$n_{d} = \sum_{n=1}^{2} \frac{c_{n}}{\Delta} = r_{d}^{-2}, \quad f^{2} = \int_{0}^{2\pi} f_{n}^{2}(\theta) d\theta = \frac{1}{4\pi} \left(\frac{1-2\mu}{1-\mu}\right)^{2}.$$

Here Δ is the area per position t; $n_d = r_d^{-2}$ describes the dislocation density (the usual dislocation density per unit area is 2-3 times smaller than n_d); the second expression for f^2 pertains to an edge dislocation in an

isotropic medium.

From formulas (5) and (2) it is seen that the mean fluctuations $\delta \tau_c$ of the value τ_c are $l^{1/2}$ times larger than the inhomogeneity of τ_c produced by dislocations lying at the mean distance r_d . This is due to the slow decrease of $\tau_{cr}(\mathbf{r} - \mathbf{r}_t)$, which leads to the result that when $l \gg 1$, in a large part of the crystal the main contribution to the fluctuations of τ_c is produced not by a few near dislocations, but by a large number of distant dislocations. As a result, τ_c for $|\tau_c| \leq \delta \tau_c$ is distributed according to a Gaussian law. On the other hand, in a smaller part of the crystal volume (~1/l) near dislocation lines, when

$$|\mathbf{r}-\mathbf{r}_t| < r_1 \sim r_d/l^{\prime_1}$$

the main contribution to τ_c is obviously made by the nearest dislocation; here $|\tau_c| > \delta \tau_c$ may be quite large. It is these regions that lead to the power-law dependence of $w(\tau_c)$ at large $|\tau_c|$ in (5).

In the case of dislocation loops, at large distances from the center of a loop the dilatation and τ_{cm} decrease according to the law

$$\tau_{cn}(\mathbf{r}-\mathbf{r}_t) = \varkappa b R_0^2 f_t(\mathbf{m}) / |\mathbf{r}-\mathbf{r}_t|^2, \quad |\mathbf{r}-\mathbf{r}_t| \gg R_0.$$
(6)

Here πR_0^2 is the area of the loop; $f_i(\mathbf{m})$ depends on the directions of the vectors

 $\mathbf{m} = (\mathbf{r} - \mathbf{r}_t) / |\mathbf{r} - \mathbf{r}_t|,$

b, and the normal to the plane of the loop. But at small distances from the dislocation line of a loop, the dilatation is almost the same as near a straight-line dislocation, and τ_{cn} is determined by formula (2) (with an $f_n(\theta)$ that changes along the line of the loop).

If the density of loops N_i and their radius R_0 are large enough so that $N_i R_0^3 \gg 1$ (since $N_i R_0 \sim n_d$, this condition is equivalent to the requirement that $R_0 \gg r_d$ $= n_d^{-1/2}$), then the main contribution to the sum (4) for g(z) is made by regions distant from the dislocation lines by less than R_0 . In this case, the distribution $w(\tau_c)$ is determined by the same formula (5) as for straight-line dislocations.⁸⁻¹⁰ It is necessary only to make the substitutions

$$n_d \to N_i R_0 \sim n_d, \quad f^2 \to 2\pi \langle f_n^2(\theta) \rangle, \quad R \to R_0, \tag{7}$$

where $\langle \ldots \rangle$ denotes an average both over θ and over the perimeter of the loop. But if $N_i R_0^3 \ll 1$, then $w(\tau_c)$ changes significantly, and in its central part it has a Lorentzian form.

2. ORDERED REGIONS NEAR SINGLE DISLOCATIONS

At comparatively high temperatures, when $\tau \gg \delta \tau_{co}$ in the greater part of the crystal the strains are insufficient for the occurrence of ordering, and only near the dislocation lines can thin cylindrical OR originate. In order to investigate them, it is necessary first to consider ordering near single straight-line dislocations. If gradient terms in the thermodynamic potential Φ may be neglected, then in the LTTA the boundary $r_0(\theta)$ of the OR near such a dislocation, i.e., the region where $\tau \leq \tau_c(\mathbf{r})$, is determined according to (2) by the condition

$$0 < r_{\perp} < r_{\theta}(\theta) = \frac{\kappa b}{\tau} f_{\pi}(\theta),$$

$$r_{\theta}(\theta) = 0, \quad \kappa f_{\pi}(\theta) < 0.$$
(8)

Here \mathbf{r}_i is taken equal to zero. The order parameter $\eta(\mathbf{r})$ and its mean value $\tilde{\eta}$ in the OR are determined by the formulas

$$\eta(\mathbf{r}) = \eta_{\theta} \left[\tau_{en}(\mathbf{r}) - \tau \right]^{\theta} = \eta_{\theta} \tau^{\theta} \left[\frac{r_{\theta}(\theta)}{r_{\perp}} - 1 \right]^{\theta}, \quad \tilde{\eta} = \frac{\pi \beta (1 - \beta)}{\sin \pi \beta} \eta_{\theta} \tau^{\theta}, \quad (9)$$

where η_0 and β are the constants in the formula $\eta = \eta_0 (-\tau)^{\beta}$ for an ideal crystal.

The dependence of Φ on $\nabla \eta$, disregarded in the LTTA, may be neglected if

$$r_{e}^{3}[\tau-\tau_{e}(\mathbf{r})]|\Delta\eta| \ll \eta,$$

where $r_c[\tau - \tau_c(\mathbf{r})]$ is the correlation radius corresponding to $\tau_c(\mathbf{r})$ (see, for example, Ref. 11). In the greater part of the volume of the OR, $|\Delta\eta| \sim r_0^{-2}\eta$, where $r_0 = \max r_0(\theta), |\tau - \tau_c(\mathbf{r})| \sim \tau, r_c[\tau - \tau_c(\mathbf{r})] \sim r_c(\tau) \equiv r_c$. Therefore the indicated criterion is satisfied, and the LTTA is applicable, if

 $r_0 \gg r_c = a/\tau^{v}$

$$\tau^{i-\nu} \ll \tau_0^{i-\nu}, \quad \tau_0^{i-\nu} \sim \varkappa f b/a. \tag{10}$$

In a certain layer at the surface of the region, $|\Delta \eta| \sim (r_0 - r_\perp)^{-2} \eta$ is large,

 $r_{e}[\tau - \tau_{c}(\mathbf{r})] \ge r_{e}$

and the LTTA is inapplicable. But the thickness of this layer,

$$\Delta r \sim r_0 (\tau/\tau_0)^3$$
, $\xi = (1-v)/(1+v)$

is small in comparison with r_0 when the condition (10) is satisfied.

In formulas (2), (8), and (9), the strains due to the formation of the OR themselves were disregarded. In an actual region $r_{\perp} \sim r_0$ (or $\tau_c - \tau \sim \tau$) they have the order of magnitude

κτ^{ι-α}kT_e/vK

(v is the atomic volume, α the critical index for the specific heat) and are small in comparison with the strain bf/r_0 produced by the dislocation if

 $\kappa^2 \tau^{-\alpha} k T \sqrt{v} K \ll 1.$

The condition $\delta K \ll K$ for smallness of the renormalization of K near T_c has the same form. Since $kT_c \ll vK$ and $\alpha \ll 1$, this condition is usually satisfied outside a very narrow interval $\delta \tau$ near $\tau - \tau_c = 0$, corresponding to a very small region $\delta r \ll r_0, r_c$.

According to (10), if $\kappa fb \ge a$, then $\tau_0 \sim 1$; that is, the LTTA is valid, and OR of thickness $r_0 > r_c$ originate at all $\tau \ll 1$. But in other cases, especially in systems

with a large radius of interaction (where $a \gg b$ and $\nu = 1/2$), $\tau_0 \ll 1$, and the condition (10) is satisfied only at very small τ . In the region $\tau > \tau_0$, the LTTA is inapplicable, but $r_c > r_0$, and the disturbance produced by a dislocation is not yet sufficient for production of OR. Therefore τ_0 plays the role of the temperature of formation of such OR. It has been determined by Narbutovskii and Shapiro,⁶ with allowance for gradient terms in Φ , in the case of a transition to the superconducting state, by use of Landau's theory on the assumption that η is constant along the cylinder. Their expression⁶ for the ordering temperature agrees with the order-of-magnitude estimate τ_0 of (10) (if in it we set v = 1/2 and regard a as the coherence distance). But when $\tau \sim \tau_0$, the order should be appreciably nonuniform not only across but also along the cylinder. This is due to the fact that the interfaces between antiphase domains with different signs of η , or between ordered and disordered sections, have, when $\tau \sim \tau_0$, an interface energy $\sigma r_0^2 \sim \sigma r_c^2$ (σ is the specific surface energy) not greater, in order of magnitude, than kT_{c} . The formation of such a nonuniform quasi-one-dimensional OR (with domains of size $\sim r_0 \sim r_c$, whose energy of formation $\sim kT_c$) proceeds gradually, as a considerably smeared out phase transition (over a τ interval of width comparable with τ_0).

Even at $\tau \ll \tau_0$, when an OR has already formed, it may be split into antiphase domains. In the Ising model (for example, in the ordering of alloys), the interface energy is

 $\sim \sigma r_0^2 \sim kT_c r_0^2/r_c^2 \gg kT_c$

and there is a thermodynamic advantage in the formation of elongated cylindrical domains with a mean length L_0 of order

$$L_{0} \sim r_{e} \exp \left(\sigma r_{0}^{2} / \xi_{1} k T_{e} \right) \sim r_{e} \exp \left(r_{0}^{2} / \xi_{2} r_{e}^{2} \right) \gg r_{e}.$$
(11)

Here and hereafter, ξ_i (i = 1, 2, ...) are dimensionless constants of order of magnitude unity. In degenerate systems, for example in isotropic magnetic materials, there should occur, instead of distinct domains, a smooth distribution $\eta(\mathbf{r})$ along the cylinder axis, due to turning,

 $\eta(\mathbf{r}) = \mathbf{M}(\mathbf{r})/M_{o}$

with almost constant $|\eta(\mathbf{r})|$, leading to a relatively small increase of the density of Φ , of order $c(\nabla \eta_{\perp})^2$, where $c \sim kT_c \eta^{-2} r_c^{-1}$. The characteristic distance L_o , at which the change of $\eta(\mathbf{r})$ is comparable with η , is

$$L_{0} \sim r_{0}^{2} / r_{c}, \qquad M_{0}^{2} \eta^{2} r_{0}^{4} < k T_{c} r_{c}.$$
 (12)

In actual magnetic materials, turning of $\mathbf{M}(\mathbf{r})$ with respect to the cylinder axis z is impeded by the magnetostatic energy that arises, of density $\sim M_0^2 \eta^2$, when $\mathbf{M} \perp z$ (for simplicity, we limit ourselves to the case in which the energy density of anisotropy and of magnetostriction is less than $M_0^2 \eta^2$). Therefore the estimate (12) is correct only if

 $M_0^2 L_0 \ll c/L_0,$

and this energy may be neglected. The corresponding

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condition is indicated in (12).

But if

 $M_0^2 L_0 \gg c/L_o$,

then the magnetostatic energy leads to partition of the ordered cylinder in the magnet into distinct antiphase domains, with the magnetization parallel to its axis, and with wall thickness $L^0 \ll L_0$. The expressions for σ and for the domain length L_0 are then different, depending on the ratio between L^0 and r_0 :

$$L_0 \sim L^0 \exp (M_0 \eta r_0^2 / \xi_3 (kT_c r_c)^{1/4})$$

when

$$\begin{array}{l} L^{0} \sim (kT_{c}/r_{c}M_{0}^{2}\eta^{2})^{\frac{1}{2}} > r_{0}, \quad kT_{c}r_{c} < M_{0}^{2}\eta^{2}r_{0}^{4}; \\ L_{0} \sim r_{0} \exp \left(M_{0}^{2}\eta^{2}r_{0}^{3}/\xi_{k}kT_{c}\right), \quad L^{0} \sim r_{0} \end{array}$$

$$(13)$$

when

$$kT_c < r_0^2 r_c M_0^2 \eta^2 \sim M_0^2 a^3 (\kappa b f/a)^2 \tau^{-(2+\nu-2\beta)}.$$

For example, when $M_0 \sim 10^3$ G, $a^3 \sim 10^{-23}$ cm³, $\kappa b/f \sim 10^{-1}$, $T_c \sim 10^3$ K, and $\nu = 2\beta$, the last condition in (13) is satisfied if $\tau < 10^{-3}$.

Similarly, one can consider an OR near an isolated dislocation loop. If, for $\tau \sim \tau_0$, $r_0(\tau_c)$ is small in comparison with the loop radius R_0 , then the emerging OR at first has the shape of a torus, with a thickness and degree of order determined by formulas (8) and (9), as in the case of a straight-line dislocation. At lower temperatures, when $r_0 \sim R_0$, the OR becomes extended in all directions m, and its boundaries $r_0(m)$, with allowance for (6) and for the condition

 $\tau_{cn}(r_0(\mathbf{m})) \ge \tau$

are determined by the formula

$$r_0(\mathbf{m}) = [\times bR_0^2 f_l(\mathbf{m}) / \tau]^{th}, \quad \times f_l(\mathbf{m}) > 0, \tag{14}$$

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where $r_0 \sim \tau^{-1/2}$. At very small τ , as well as when $\tau > \tau_0$, according to (14)

*r*₀(τ)≤*r*_c(τ),

the LTTA ceases to be applicable in the greater part of the volume bounded by $r_0(m)$, and only in a small portion of it can one distinguish a region of local order exceeding the fluctuation background. If $r_0(\tau_0) > R_0$, then the LTTA is altogether inapplicable for description of the ordering near the loops.

3. PHASE TRANSITION DUE TO A DISLOCATION FRAMEWORK OF ORDERED REGIONS

The character of a phase transition in a crystal containing an ensemble of dislocations depends substantially on the ratio between the temperature τ_0 of formation of OR near individual dislocations and the mean spread $\delta \tau_c$ of the local ordering temperatures. According to (5) and (10), if the condition

$$B = \frac{r_a}{a} \left(\frac{xfb}{a}\right)^{\lambda} \sim \frac{l'^{h}\tau_0}{\delta\tau_c} \gg l'^{h}, \quad \lambda = \frac{v}{1-v}, \quad (15)$$

is satisfied, then $\tau_0 \gg \delta \tau_c$; that is, initially, at a com-

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paratively high temperature $\tau \sim \tau_0$, near individual dislocations there are formed cylindrical OR, whose size r_0 , for $\tau \gg \delta \tau_c$, increases as $1/\tau$.

If, however, there are several systems of straightline dislocations with nonparallel dislocation lines, then the OR are not isolated, but each of them must intersect OR forming near dislocations of other systems. As a result, the OR near randomly distributed dislocations form a complicated, nonperiodic framework, consisting of thin cylinders oriented in several characteristic directions and intersecting OR of other systems over intervals distributed according to some random law. From geometric considerations it is clear that (at least in the case of complete noncorrelation of the dislocations of different systems) the mean lengths L_1 of the sections between successive intersections are of order of magnitude

$$L_{i} \sim \frac{1}{n_{d}r_{0}} = \frac{r_{d}^{2}}{r_{0}} \sim \frac{r_{d}^{2}}{\kappa b f} \tau, \quad r_{d} = \frac{1}{n_{d}^{\gamma_{h}}} \gg r_{0}.$$
 (16)

The same type of continuous framework of OR, with a characteristic length (16) of sections, is formed in crystals containing randomly distributed dislocation loops of sufficiently large radius $R_0 \gg L_1$. If $R_0 \ll L_1$, then the OR near loops are isolated. In the other limiting case of dislocations distributed with incomplete randomness, when their lines are linked and form a Frank network, the characteristic lengths of the sections are obviously $L'_1 \sim r_d$.

The structure of the OR within the framework is determined to a considerable degree by the ratio between L_1 and the characteristic distance L_0 of change of sign of η , determined by formulas (11)–(13). At comparatively large τ , when $L_0 \ll L_1$, each section of the framework, and consequently the framework as a whole, is split into fluctuational domains with different signs of η . Therefore the mean value of η (the magnetization, in the case of ferromagnetism) is zero, and long-range order does not appear, although there is local order in each domain. In the case of lower temperatures, when according to $(11)-(13) L_0$ is large, in an isolated OR the change of sign of η at sufficiently large distances (but for $L_0 < R$) leads with ever increasing rapidity to the destruction of long-range order. But in the case of a two-dimensional (d=2) or three-dimensional (d = 3) framework with $L_0 \gg L_1$, a change of sign of η within individual sections is improbable; and for appearance in the ordered framework of a region with the opposite sign of η and with dimensions $\Lambda \gg L_1$, it is necessary to produce antiphase boundaries at $\sim (\Lambda/L_1)^{d-1}$ links of the framework, and the corresponding probability

 $q \sim \exp\left[-\left(\Lambda/L_{1}\right)^{d-1}\ln\left(L_{0}/r_{c}\right)\right]$

is exponentially small.

Therefore at some temperature $T = T_f$ (or $\tau = \tau_f$), for which

 $L_0(\tau_f) = \xi_{\mathfrak{s}} L_1(\tau_f),$

a phase transition should occur in the dislocation framework of OR. As a result of this transition, a

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framework consisting of equal numbers of antiphase domains with opposite signs of η transforms to a state with a predominant number of domains of a definite sign. From the condition $L_0(\tau_f) = \xi_5 L_1(\tau_f)$, with use of (11) and (16), it follows that in the Ising model with a completely random distribution of dislocations, we have

(17)

$$r_0^2(\tau_f)/r_c^2(\tau_f) = \xi_2 \ln (\xi_5 r_d^2/r_0 r_c),$$

or

 $\tau_{j} = \xi_{0} \tau_{0} \{ \ln \left[\xi_{0} B^{2} (\tau_{j} / \tau_{0})^{1+\nu} \right] \}^{-\lambda_{1}}, \quad \lambda_{1} = 1/2 (1-\nu).$

Here τ_0 is defined by formula (10), *B* by (15) $[B^2(\tau_f/\tau_0)^{1+\nu} \gg 1]$. According to (17) and (15), τ_f increases with increase of the dislocation density. If, for example, $\kappa fb \sim a/10$ and $r_d/a \sim 10^3 - 10^4$, then $B \sim 10 - 100$. Then τ_f may be several times smaller than τ_0 and several times (or several tens of times) larger than $\delta \tau_c$. We note that the qualitative estimate of τ_f from the condition $L_0 \sim L_i$ and the logarithmic dependence of τ_f on the length L_1 of the sections of the framework agree with the results of an exact solution of the two-dimensional Ising problem for a regular framework constructed from single-atom chains intersecting after a distance L_1 .¹²

In Heisenberg magnets with appreciable magnetostatic energy, according to (13) and (16) the condition $L_0 \sim L_1$ gives

$$\tau_{1} = \xi_{7} \tau_{0} E^{\phi_{1}} \{ \ln[\xi_{8} B^{2} E^{\prime / \nu} (\tau_{1} / \tau_{0})^{1 + \beta - \nu / 2}] \}^{-2\phi_{1}}, \quad \phi_{1} = 1 / (4 - 2\beta - \nu)$$

when

$$\begin{aligned} & (\tau_{i}/\tau_{0})^{2-2\nu} < E(\tau_{0}/\tau_{i})^{2-2\beta+\nu} < 1. \\ & \tau_{i} = \xi_{7}' \tau_{0} E^{\phi_{2}} \{ \ln [\xi_{0}' B^{2}(\tau_{i}/\tau_{0})^{2}] \}^{-\phi_{2}}, \quad \psi_{2} = 1/(3-2\beta) \end{aligned}$$
(17a)

when

 $E(\tau_0/\tau_f)^{2+\nu-2\beta} > 1, \quad E = M_0^2 \eta_0^2 a^3/kT_c \tau_0^{3\nu-2\beta}.$

At large E, formulas (17a) do not lead to values of τ_f less than τ_0 . In this case, with lowering of temperature there is no formation of OR with different numbers of oppositely oriented domains, but directly as a result of the phase transition at $\tau_f \sim \tau_0$ there appears in ordered framework with a predominant number of domains with definite directions of the magnetization.

With neglect of the magnetostatic energy, in an Ising magnet the energy at junctions of dislocations of different systems is minimal when the magnetization vectors \mathbf{M} in them are parallel. But if the magnetostatic energy is appreciable, and if the condition (13) is satsified, then in each dislocation \mathbf{M} is parallel to its line. Then there is an energetic advantage in the formation of an acute rather than an obtuse angle between the vectors \mathbf{M} of linking dislocations. As a result, a dominant direction of the resultant magnetization appears in the framework (a special situation arises if the lines of different systems are perpendicular, but ordinarily they do not form right angles; for example, in crystals with fcc lattice there is a system of lines of the type $\langle 211 \rangle$; OR near certain lines may make no contribution to the total nagnetization).

If the framework is formed on the basis of a Frank network and if $L_1 \sim r_d$, then in (17) and (17a) it is necessary to replace r_d^2/r_c by r_d , and correspondingly to divide the arguments of the logarithms by $B(\tau_f/\tau_0)$. This increases τ_f .

In degenerate systems (without appreciable longrange interaction), for a completely random distribution of dislocations, according to (12), (16), (10), and (15)

$$r_{f} = \xi_{s} \tau_{0} B^{-\psi}, \quad \psi = 2/(3 - \nu),$$
 (18)

while for a Frank network, $\psi = (2 - \nu)^{-1}$. Since $\nu \approx 2/3$, $\psi \approx 6/7$ or 3/4 differs little from unity, and τ_f cannot be appreciably larger than $\delta \tau_c$. Therefore in these systems, even when $B \gg 1$, the interval of a clearly expressed thin single-domain framework is absent, and τ_f may be below the temperature (23) of the percolation transition. On the other hand, in Heisenberg magnets a framework may form at τ_f determined by formulas (17a) if $M_0^2 L_0 \gtrsim c/L_0$ for all $\tau < \tau_0$, or at the temperature of transition from the degenerate to a quasi-Ising system

$$\tau_{i} = \xi_{7} \tau_{0} E^{*_{1}}, \quad \psi_{1} = (4 - 2\beta - \nu)^{-1},$$

if $E \ll 1$, and the condition $M_0^2 L_0 \gtrsim c/L_0$ begins to be satisfied only when $\tau < \tau_f < \tau_0$.

Thus in nondegenerate systems [in particular, in magnets when the condition (13) is satisfied], there can exist an appreciable interval of temperature $\tau_f > \tau \gg \delta \tau_c$ within which there is an ordered framework, occupying a small part of the crystal volume, while outside the framework $\eta = 0$. Within a small τ interval of order

$$\Delta \tau_j = \tau_j - \tau_j' \sim \tau_j / \ln(L_1/r_c) \sim \tau_j r_c^2(\tau_j) / r_0^2(\tau_j) \ll \tau_j$$

(for the Ising model), the mean (over domains) value of η in the framework increases from 0 to $\tilde{\eta}$. Below τ'_f , according to (9), the mean of $\eta(\mathbf{r})$ over the crystal is

$$\eta = \frac{\pi\beta(1-\beta)}{4\sin\pi\beta} \eta_0 b^2 n_d \varkappa^2 f^2 \tau^{\beta-2}, \quad \delta \tau_c \ll \tau < \tau_f'$$
(19)

and increases as $\tau^{\beta-2}$ (although the mean value over the OR, $\tilde{\eta} \sim \tau^{\beta}$, meanwhile decreases).

In the lower-temperature range, $\tau \sim \delta \tau_c$, where $r_0 \sim r_d/\ell^{1/2}$, the OR begin to be affected also by the fields of more distant dislocations, and as a result of superposition of these fields, there are gradually formed large OR that capture a considerable number of dislocations. Since these OR are connected with the framework, in ferromagnets the degree of order η has the same sign in all OR. The mean value of η can be found from the general formula

$$\overline{\eta} = \int_{-\infty}^{\infty} \eta(\tau - \tau_c) w(\tau_c) d\tau_c = \eta_0 \int_{-\infty}^{\infty} (\tau_c - \tau)^{\theta} w(\tau_c) d\tau_c, \quad \tau < \tau_f', \quad (20)$$

where $w(\tau_c)$ is determined by the expression (5). When

 $\tau \gg \delta \tau_c$, (20) and (5) lead to formula (19); when $\tau \leq \delta \tau_c$,

$$\overline{\eta} = \eta_o \frac{\Gamma(1+\beta)}{2\pi} (\delta\tau_c)^{\beta} \exp\left[-\frac{\tau^2}{4(\delta\tau_c)^2}\right] D_{-1-\beta}\left(\frac{\tau}{\delta\tau_c}\right), \ \tau \leqslant \delta\tau_c, \quad (21)$$

where $D_{-1-\beta}(x)$ is a parabolic-cylinder function. In the range of negative τ , when $-\tau \gg \delta \tau_c$, (21) goes over to the expression $\eta_0(-\tau)^\beta$ for η in an ideal crystal; and when $|\tau| \sim \delta \tau_c$, formulas (20) and (21) describe a continuous transition from the asymptotic law (19), corresponding to "framework ordering", to the law $\eta_0(-\tau)^\beta$, when order is established over the whole crystal.

In the range $\tau \gg \delta \tau_c$, $\overline{\eta}$ is very small, and the transition to an ordered state of the framework at $\tau = \tau_f$ may be experimentally undetectable. The transition will then be perceived as the establishment of a law $\eta \sim (-\tau)^{\beta}$ (and analogous laws for other materials) over a range $|\tau| \sim \delta \tau_c$, and experimentally such relations correspond to a smeared out (over the interval $\delta \tau_c$) phase transition of the second kind. Thus the presence of a dislocation framework leads to a smeared out transition in the vicinity of $\tau = 0$ along with a barely perceptible true transition at $\tau = \tau_f$. To estimate the interval of smearing out, we assume, for example, that $\times f l^{1/2} \sim 1$ and $n_d \sim 10^9$ cm⁻². Then according to (5), $\delta \tau_c \sim 10^{-3}$. As is well known, such smeared out phase transitions are actually often observed in solids. We note that in the absence of a framework, theory (including theory that starts from percolation concepts) predicts a transition with a singularity $\eta \sim (-\tau)^8$, where $\beta \approx 1/3.$

The variation of $y = (\overline{\eta}/\eta_0)(\sqrt{2} \delta \tau_c)^{-1/3}$ with $\tau/\delta \tau_c$ for $\beta = 1/3$ and l = 8.5 is shown in Fig. 1 (Curve 1). The same figure (Curve 2) shows the variation with $\tau/\delta \tau_c$ of $\overline{\beta} = d \ln \eta/d \ln |\tau|$, which describes the exponent when $\overline{\eta}(\tau)$ is approximated by the function $|\tau|^{\overline{B}}$. In a certain interval, $\overline{\beta} > \beta$; at the maximum, $\overline{\beta} \approx 0.5$. It is interesting that such an $\overline{\eta}(\tau)$ relation, with $\overline{\beta} \approx 0.5 > \beta$, has been observed at very small τ for the magnetic transition in Ni.¹⁴

It should be noted that a single sign of η in large OR is achieved only in ferromagnets. In the ordering of antiferromagnets or alloys, the Burgers vector **b** of dislocations produced in the disordered phase does not coincide with a lattice vector of the ordered phase; and when $\tau < \delta \tau_c$, isolated dislocations lead to the ap-



FIG. 1.

pearance of a complicated sign-variable field $\eta(\mathbf{r})$, consisting of domains of dimensions $\sim r_d$ produced by the dislocations and forming a peculiar glass (it disappears if the joining of dislocations in pairs is possible). Coupling of such large OR with the framework or with each other, in the presence of percolation, produces a one-sign field $\eta(\mathbf{r})$, determined by the condition for a minimum of the term in Φ containing $(\nabla \eta)^2$, and the discussions of the nature of the transition given here and in Section 4 remain valid. Then formulas (20) and (21) approximately determine not $\overline{\eta}$ but $|\overline{\eta}|$. But if the dislocations are produced in the ordered phase, then b is a lattice vector of the ordered phase, and in anti-ferromagnets or alloys, just as in ferromagnets, a single sign of η is established in large OR.

Also possible is a smearing out of a percolation phase transition (see Section 4) over an interval $\delta \tau_c/l$, due to the influence of the crystal boundaries on the dislocation field. It leads to the appearance in $\delta \tau_c$ of additional terms, *l* times smaller than those taken into account, but dependent on r and variable over distances comparable with the crystal size (additional smearing out may result from macroscopically inhomogeneous plastic strain).

We note that in the treatment given, it was assumed that the interval $\delta \tau$ in which $\delta K \ge K$ is small in comparison with $\delta \tau_c$. Under these conditions, the strictional phase transition of the first kind considered by Larkin and Pikin¹³ should not show up.

In analogy to (20), one can obtain an expression for the specific heat by averaging the expression

$$C_{p}^{o} = A_{\pm} \frac{kT_{c}}{v} |\tau - \tau_{c}|^{-\alpha},$$

corresponding to an ideal crystal (A_{+} and A_{-} refer to the regions $\tau > 0$ and $\tau < 0$). In the LTTA adopted, C_{p} does not become infinite and is determined by the formulas

$$C_{p}(\tau) = \frac{kT_{c}}{v} \int_{0}^{\infty} \frac{dt}{t^{\alpha}} [A_{+}w(t-\tau) + A_{-}w(t+\tau)], \quad \tau \ll \tau_{0},$$

$$C_{p}(\tau) = C_{p}^{\circ}(\tau) + \frac{kT_{c}}{2v} \frac{(\delta\tau_{c})^{2}}{\tau^{1+\alpha}} \left[\alpha A_{+} \left(1 + \frac{1}{l} \ln \frac{\tau}{\xi_{10}\delta\tau_{c}} \right) + (A_{-}-A_{+}) \frac{1}{2l} \frac{\pi\alpha}{\sin\pi\alpha} \right], \quad \tau \gg \delta\tau_{c}, \quad \alpha \ll 1,$$

$$C_{p}(0) = \frac{kT_{c}}{v} \frac{\Gamma[(3-\alpha)/2](A_{+}+A_{-})}{\pi^{t_{0}}(1-\alpha)2^{\alpha/2}(\delta\tau_{c})^{\alpha}}.$$
(22)

In the range $\tau < 0$ and $\delta \tau_c \ll |\tau| \ll 1$, there should exist disordered regions near the dislocations, when $\kappa f_n(\theta) < 0$, with thickness $\sim r_0$. The corresponding magnetostatic energy density $\sim M_0^2 \eta^2 r_0^2 n_d$, due to the mechanism pointed out by Lesnik,¹⁵ should lead at small τ to a large magnetic anisotropy, increasing with temperature in proportion to $\tau^{2\beta-2}$.

At temperatures $\tau_0 > \tau > \tau_f$ above the phase transition point, the OR framework in magnetic materials contains parts with different directions of the magnetization **M**, and in a certain sense the system behaves as a dislocation superparamagnet. Comparatively weak external fields should lead to a dominant orientation of **M**. An almost complete reorientation and establishment of a mean magnetization $\overline{M} = M_0 \overline{\eta}$ [$\overline{\eta}$ is determined by formula (19)] takes place when

$$HM_0\widetilde{\eta}r_0^2L_0\gg kT$$

or

$$H \gg H_1 = kTb\tau^{2-\beta}/M_0b^3(\varkappa f)^2L_0.$$

Here L_0 is determined by formulas (11) and (12) or should be replaced by the length R (or R_0) of the dislocation line if $R < L_0$; and it is assumed that $H_1 \gg 4\pi \bar{M}n$, where n is the demagnetizing factor of the specimen. For example, if

$$T_c \sim 10^3 \text{ K}, M_0 \sim 10^3 \text{ G}, L_0 \sim 10^4 b, \approx f \sim 10^{-1}, b^3 \sim 10^{-23} \text{ cm}^3,$$

 $n_a b^2 \sim 10^{-5}, \tau \sim 10^{-3},$

then $H_1 \sim 1$ Oe is small, and the mean magnetization according to (19) is of order $\overline{M} \sim 2 \cdot 10^{-3} M_0$. In the range $H \leq H_1$, a large susceptibility $\chi \sim \overline{M}/H_1$ should be observed.

4. PERCOLATION PHASE TRANSITION IN CRYSTALS WITH DISLOCATIONS

In crystals with small \varkappa or with $a \gg b$, at high dislocation density, instead of (15) the opposite condition $B \ll l^{1/2}$ may be satisfied. Then $\tau_0 \ll \delta \tau_c$, and OR are not formed near individual dislocations when $\tau \gg \delta \tau_{c}$. Only when $\tau \sim \delta \tau_c$ do OR originate, at once capturing a large number of dislocations. Initially these OR are disconnected, and the values of η in different clusters differ in sign (or, in magnetic materials, in the direction of M). With lowering of temperature, the sizes of the OR and their number increase, until at some temperature $\tau = \tau_{b}$ an infinite cluster originates and percolation occurs. In such a cluster, in the LTTA, η has a definite sign, and its appearance corresponds to a phase transition of the second kind in an inhomogeneous system.⁵ Cases are possible in which $B \gg l^{1/2}$ and a framework forms from OR near dislocations at $\tau \sim \tau_0 \gg \delta \tau$, but a phase transition in the framework appreciably above $\delta \tau_c$ does not occur ($\tau_f \leq \delta \tau_c$, for example, in degenerate systems). Then when $\tau \gg \delta \tau_c$, the sign of η in different OR is different, and only fusion of OR at $\tau = \tau_p \sim \delta \tau_c$ leads to the indicated percolation transition.

In both cases, at $\tau \approx \tau_p \sim \delta \tau_c$ the strains in the OR are chiefly caused not by the nearest dislocations, but by a large number of distant ones. Therefore the probability distribution of τ_c at $|\tau_c| \leq \delta \tau_c$ is Gaussian, and for approximate description of a percolation transition in a crystal with dislocations one can use directly the results of the calculation for a phenomenological model with a Gaussian distribution of inhomogeneities⁵ (using the parameter values that correspond to the case under consideration). In the three-dimensional case, a percolation transition, in the LTTA, takes place when the total volume x of the OR becomes equal to $x_c = 0.17$.¹⁶ For the Gaussian distribution (5), this value of x is reached when

$$\tau = \tau_{p} \approx 0.95 \delta \tau_{c} = 0.95 \varkappa f (ln_{d}b^{2})^{\frac{1}{2}} .$$
(23)

Thus dislocations shift the phase-transition point (when $\tau_f \leq \delta \tau_c$) by an amount proportional to $n_d^{1/2}$. For example, if $\kappa f l^{1/2} \sim 1$, then $\tau_p \approx \delta \tau_c \sim 10^{-4}$ at $n_d = 10^7$ cm⁻², and $\tau_p \sim 10^{-2}$ at $n_d = 10^{11}$ cm⁻². In the interval

 $|\tau-\tau_p| \ll \delta \tau_c$

an important role is played by processes of percolation fusion of clusters, and in the LTTA the dependence of $\overline{\eta}$, χ , and r_c on $\tau - \tau_p$ is characterized by the percolation critical indices β_p , γ_p , and ν_p , which differ from the usual indices β , γ , and ν of an ideal crystal. According to Ref. 16, $\beta_p \approx 0.35$, $\gamma_p \approx 1.7$, and $\nu_p \approx 0.9$. Only when $|\tau| \gg \delta \tau_c$ are the percolation dependences of χ and $\overline{\eta}$ (for $\tau < 0$) replaced by the critical dependences for ideal crystals. Formulas for $\overline{\eta}$ and χ in the transitional region $|\tau| \sim \delta \tau_c$ have been given by Ginzburg⁵ [the specific heat, in the LTTA, is determined by formula (22)].

The results of Sections 3 and 4 are correct not only for straight-line dislocations but also for loops of large radius $R_0 \gg r_d$ [with the substitution (7) in the expression for $\delta \tau_c$]. If, however, $R_0 < r_d$, then no connected framework forms, and the spread of τ_c is predominantly determined by the effect of the nearest loops. In the case $R_0 < r_d$ (but $r_0(\tau_0) < R_0$), there occurs percolation of isolated OR, whose boundaries are determined by formula (14) but are somewhat distorted by the influence of neighboring loops. On estimating τ_p from the condition $N_1 r_0^3(\tau_p) \sim 1$ with use of (14), we get

$$\tau_{p} \sim \varkappa f N_{l} R_{0}^{2} b, \qquad \varkappa f (N_{l} R_{0}^{3} R_{0} b^{2} / a^{3})^{1/2} > 1, \qquad N_{l} R_{0}^{3} < 1.$$
(24)

The necessary condition for applicability of the LTTA, $r_0(\tau_p) > r_c(\tau_p)$, is written out in (24) for $\nu = 2/3$. In this case τ_p is proportional to n_d .

These features of thermodynamic quantities at $\tau \approx \tau_p$ have been derived by Ginzburg⁵ by use of the LTTA, in which it is assumed that OR do not interact until contact, and that upon making contact they immediately unite into a cluster with a single sign of η . In some narrow interval

near the transition point itself, this approximation ceases to be applicable even when condition (10) is satisfied. This is due to the fact that with lowering of the temperature, the growing OR shortly before their fusion into an infinite cluster are already beginning to interact noticeably (with energy $\sim kT_c$), when the distance Δr between them is comparable with the local radius of correlation $r_c(\tau, \mathbf{r}) = a|\tau - \tau_c(\mathbf{r})|^{-\nu}$ in the region of proximity. The point of contact \mathbf{r}_s of the OR is a saddle point of the function $\tau_c(\mathbf{r})$;

$$\Delta \tau \sim \delta \tau_c (\Delta r/r_2)^2$$
, $\Delta r \sim r_c (\tau, \mathbf{r}_s)$,

where in the LTTA $\tau_p = \tau_c(\mathbf{r}_s)$, and r_2 is the characteristic correlation distance of variation of $\tau_c(\mathbf{r})$. By use of this estimate, from the conditions

$$\Delta \tau \sim \delta \tau_c (\Delta r/r_2)^2$$
, $\Delta r \sim r_c (\tau, \mathbf{r}_s)$

it is not difficult to find the interval of breakdown of the LTTA;

$$\Delta \tau \sim \delta \tau_c [a/r_2(\delta \tau_c)^{\nu}]^{\lambda_2} = \delta \tau_c [r_c(\delta \tau_c)/r_2]^{\lambda_2}, \ \lambda_2 = 2/(1+2\nu).$$
⁽²⁵⁾

The estimate (25) is applicable to the general case of large-scale inhomogeneities of $\tau_c(\mathbf{r})$, with characteristic distance r_2 , and indicates the interval $|\tau - \tau_p| < \Delta \tau$ in which the theory of Ref. 5 is inapplicable. In the case being considered, of inhomogeneities produced by randomly distributed dislocations, according to (4) and (5) the random field τ_c is a superposition of statistically independent fields with various scales of inhomogeneities: from $r_d/l^{1/2}$ to the crystal dimension R. For large $B \gg l^{1/2}$, even for the smallest-scale fluctuations with $r_2 = r_d/l^{1/2}$, in (25)

$$[r_c(\delta\tau_c)/r_2] \sim (l^{\frac{1}{2}}/B)^{1-\nu},$$

that is, $\Delta \tau \ll \delta \tau_c$. For small $B \ll l^{1/2}$, the small-scale inhomogeneities with $r_2 < r_c(\delta \tau_c)$ lead to small energy of interaction of OR that are approaching each other $(\ll kT_c)$, insufficient for the establishment of a single sign of η . But according to (5) they make only a small contribution to $\delta \tau_c$, of the order

$$\frac{1}{2}\ln\left(r_{c}(\delta\tau_{c})l^{\prime\prime}/r_{d}\right)/\ln\left(R/r_{c}(\delta\tau_{c})\right)\approx(2l)^{-1}(1-\nu)\ln\left(l^{\prime\prime}/B\right)\equiv\varepsilon.$$

A slight lowering of τ from τ_p by an amount

Δ'τ≈εδτ.≪δτ.

is sufficient for establishment of percolation of the large-scale inhomogeneities with $r_2 > r_c(\delta \tau_c)$, for which the LTTA and the results of Ref. 5 are valid.

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Deformation-potential operator for a screw dislocation

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Geometrical considerations are used to obtain the form of the operator of the deformation potential for a screw dislocation. It is shown that the spectrum of an electron moving along a dislocation in a parallel magnetic field differs from the usual parabolic spectrum.

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In the description of the interaction of an electron with lattice defects one frequently employs the deformation potential, which is a quantity proportional to the divergence of the displacement \mathbf{u} . In the case of screw dislocations of interest to us, div $\mathbf{u} = \mathbf{0}$, whereas the influence of the screw dislocation on the moving electron is subject to no doubt. We shall show how this difficulty can be overcome.

The interaction of an electron with a screw dislocation will be described with the aid of the metric theory. The undeformed medium is assumed to be isotropic. We consider first the situation in the classical approach. The electron spectrum prior to the deformation is then $E = (p_x^2 + p_y^2 + p_x^2)/2\mu$, μ is the particle mass, and p is the momentum. The principal assumption is that the trajectories are frozen into the medium and are deformed together with the medium. Then uniaxial tension by a factor k along the x axis corresponds to a spectrum

$$E = \frac{1}{2\mu} \left(\frac{1}{k^2} p_x^2 + p_y^2 + p_z^2 \right)$$

Any homogeneous deformation can be resolved into similar tensions and rotations. In the case of an inhomogeneous deformation it is possible to introduce a metric ds^2 such that the trajectories coincide with the geodesics. By, the same token, the behavior of a particle in a deformed medium is completely described. The transition to quantum mechanics is in standard fashion-a Laplace operator, followed by a Hamiltonian, is constructed from the metric ds^2 .

Let the screw dislocation in an isotropic medium be located along the z axis, and let a positive value of the Burgers vector $b = 2\pi a$ correspond to a right-hand screw. We express the metric in the form $ds^2 = \omega_1^2$ $+\omega_2^2 + \omega_3^2$. In the absence of the dislocation we have $\omega_1 = dr, \omega_2 = rd\varphi, \omega_3 = dz$. It is almost obvious that when the dislocation is introduced $\omega_3 = dz$ is replaced by ω_3 $-dz - ad\varphi$, while ω_1 and ω_2 remain unchanged. The corresponding Laplace operator can be easily calculated:

$$\Delta = \partial_{xx} + \partial_{yy} + \partial_{zz} + \frac{2a}{r^2} \partial_{z\varphi} + \frac{a^2}{r^2} \partial_{zz}.$$

It corresponds to a Hamiltonian

$$\mathscr{H} = \frac{1}{2\mu} (p_z^2 + p_y^2 + p_z^2) + V, \quad V = \frac{1}{2\mu} \left(\frac{2a}{r^2} (x p_y p_z - y p_z p_z) + \frac{a^2}{r^2} p_z^2 \right),$$

where $p_x = -i\hbar \partial_x$, and the operator V assumes here the role of the deformation potential. The eigenfunctions of this Hamiltonian are of the form $J_{\mu\nu}(kr)e^{im\varphi}e^{ixz}$ where $\nu = m + a\kappa$. They correspond to energies $\hbar^2(k^2 + \kappa^2)/2m$. If the wave-vector component along the z axis is $\kappa = 0$, then V = 0 and the dislocation does not influence the motion of the electron.

More meaningful results are obtained if a magnetic field H is directed along the z axis. Then the momentum operators in the Hamiltonian take the form

$$p_{x} = -i\hbar\partial_{x} + \frac{e}{2c}Hy, \quad p_{y} = -i\hbar\partial_{y} - \frac{e}{2c}Hx,$$
$$p_{z} = -i\hbar\partial_{z}$$

We seek the ψ function in the form $\psi = R(r)e^{i\pi\varphi}e^{i\pi z}$. The Schrödinger equation then becomes

$$-\frac{\hbar^2}{2m}\left(R_{rr}+\frac{1}{r}R_r-\frac{\nu^2}{r^2}R-\kappa^2R\right)+\frac{\hbar\omega\nu}{2}R+\frac{\mu\omega^2}{8}r^2R=ER$$

Here $\omega = |e| H/\mu c$, $\nu = m + a\kappa$. The eigenvalues and eigenfunctions are given by¹

$$\begin{split} E &= \frac{\hbar^2}{2\mu} \varkappa^2 + \hbar \omega \frac{|\nu| + \nu}{2} + \hbar \omega \left(l + \frac{1}{2} \right), \quad l \ge 0, \\ R &= e^{-\tau r^2/2} r^{|\nu|} F(-l, |\nu| + 1; \gamma r^2), \quad \gamma = \mu \omega/2\hbar. \end{split}$$

Since $a|\kappa| \ll 1$, it follows that at m < 0 the dependence of the electron energy on its velocity $v = \hbar \kappa / \mu$ along the dislocation is the usual parabolic one. At $m \ge 0$ this is