Rigidity of a condensed substance at high temperatures

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Using the screened interaction approximation we study the high-temperature phase of the dislocation model of melting. We show that the system can be in two states characterized by an exponential (liquid) and a power-law (intermediate phase) decrease in the rigidity at large distances.

1. INTRODUCTION

The description of a condensed substance at high temperatures is a vital problem in theoretical physics. Different stages in our understanding of the phenomena which occur in a substance near the melting temperature are reflected in the books by Frenkel',[1] Fisher,[2] and Ubbelohde.[3] The concept of local order first used by Frenkel' without giving a clear specific definition makes it easier qualitatively to understand the properties of a condensed substance. To make this approach more productive one must give a definition of local order and introduce parameters which characterize it. The volume in which one assumes this order to be present contains many atoms so that one must expect the description of the system in terms of the order parameter fields to be universal and independent of the details of the interatomic interactions. Experimental data support the local-order concept but do not give reliable information about its nature and the size of the ordered volume.

The local order exists on the background of the thermal fluctuations of the atomic positions. These fluctuations are characterized by a parameter $\Delta = \Delta'/d$ where Δ' is the square root of the mean square displacement of the atoms from their assumed ideal positions and d is the interatomic distance. At the melting point $\Delta = \Delta_m = 0.07$–0.17 (Lindemann criterion). Since Δ_m is small, each configuration of N atoms can be considered as a small deviation from an idealized one. For the latter, different investigators have chosen different geometric figures. For instance, in Refs. 4–7 the local structure of a melt was assumed to be equivalent to the local structure of the initial crystal, and the authors of Refs. 8 and 9 assumed it to be icosahedric. Especially popular was the random close packing of Bernal[10] and the random bond grid of Zachariasen.[11]

As a rule the melting temperature is so high that a classical description of the system is possible (hydrogen and helium are exceptions), i.e., one can use the classical Gibbs probability distribution

$$d\omega = Z^{-1}\exp\left[-\frac{H[n]}{T}\right]dn, \tag{1}$$

$$Z = \int \exp\left[-\frac{H[n]}{T}\right]dn. \tag{2}$$

The set of parameters giving the state of the system are denoted by $[n]$. For a classical system the momenta are distributed according to the universal Maxwell law so that one needs study only the configurational part of the energy H.

The physical configuration of N atoms is a set of points with coordinates $\mathbf{r}^\alpha$, $\alpha = 1,2,\dots,N$. Its description in terms of spatial order means that the configuration $\tilde{\Gamma}(\mathbf{r}^\alpha)$ is a deformed state of some ideal shape $\Gamma(\mathbf{r}_0^\alpha)$ and

$$\mathbf{r}^\alpha = \mathbf{r}_0^\alpha + \delta\mathbf{r}^\alpha, \tag{3}$$

where the $\delta\mathbf{r}^\alpha$ are small quantities. This statement must be considered to be the definition of local order. For a given configuration the problem of constructing an ideal shape may not have a unique solution. For a system of interacting particles one can use the principle of minimum interaction energy to construct a set of ideal shapes Γ_n which may vie for the role of components of the structure. For instance, for close-packed systems with binary Lennard-Jones interactions the set consists of fcc and hcp lattices and icosahedra. After the base of ideal shapes has been formed the problem is reduced to choosing the "best" one. To do this one must use numerical characteristics of a real physical structure dividing the phase space of these characteristics into regions corresponding to deformed states of the ideal shapes Γ_n. It is clear that such a division is probabilistic in nature. In the general case the above mentioned regions may overlap.

Numerical characteristics of a structure were introduced in the papers by Mitus' and Patashinskiĭ.[5,12,19] The crystal structure of most elements near the melting point is close-packed so that in Ref. 12 clusters of fcc and hcp lattices and isosahedra were studied as the Γ_n. A numerical simulation carried out in Ref. 12 showed that the overlap of the probability distributions corresponding to different Γ_n is small up to temperatures $T < 2T_m$ (T_m is the melting temperature). This means that for those temperatures the thermal fluctuations do not destroy the local order. The inequality $T < 2T_m$ indicates the region where there exist substances with a local structure but it does not answer the question what this structure is. We assume that the local order is crystal-like. Such an assumption makes it possible to introduce a single parametrization of the states of the system for the melt and the crystal.

2. PARAMETRIZATION OF THE STATES

The above mentioned parametrization was carried out in Refs. 4, 19, and 20 and in the present section we shall follow these papers. The assumption of a crystal-like local order means that we must choose fragments of crystal lattices as the ideal components of the structure. For the physical configuration of N points we define a one-to-one mapping on the lattice points of an ideal crystal lattice: $\Gamma \to \Gamma_0$: $(\mathbf{r}^\alpha \to \mathbf{r}_0^\alpha)$. This mapping retains neighbor relations: images of nearest neighbors are again nearest neighbors. We define a

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touching position with respect to a configuration of N atoms. It is reached, if:

1) The image of the central atom is superposed upon its original.

2) The whole lattice is rotated with respect to the central atom in such a way that the non-coincidence of the image and the pre-image is a minimum.

Let us clarify the second requirement. Minimum coincidence means that the quantity

$$\tilde{\Delta} = \Sigma_\alpha (\mathrm{r}^\alpha - \mathrm{r}_0^\alpha)^2 \tag{4}$$

is a minimum. A touching position of the lattice is described by a rotation matrix U which changes the lattice from its initial position into a touching one. We note that for separate atoms chosen as the center a touching position may not be realizable because the local order has been destroyed. The whole volume of the substance turns out to be split into two kinds: "good" and "bad" material. In an ideal crystal all atoms belong to the "good" material and one can at once map all atoms onto the lattice sites. In that case $U(\mathbf{r}) = \text{const}$. A liquid is isotropic and must therefore contain "bad" material—structural defects producing the isotropy. The problem of the ratio of the volumes of "good" and "bad" material and of their geometrical shapes is an important one. The concept of local order implies that "good" material occupies a large part of the volume. We assume that the region occupied by it is connected. One can substantiate this assumption by the following considerations. The definition of local order, given above, applies also to a two-dimensional system. Minimum disorder which one must introduce into a two-dimensional system to make it isotropic is described by a distribution of point defects. Considering arbitrary two-dimensional cross-sections of a three-dimensional system one can show that in that case the minimum defect of the order is described by a distribution of line defects. Hence follows the validity of our assumption.

The next step is to map the whole of the "good" material onto the lattice. We choose a cluster with its center at the point $\mathbf{r}_1$ and find $U(\mathbf{r}_1)$ for it. After that we find for a cluster with its center at $\mathbf{r}_2$ ($\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of nearest neighbors) the minimum change in $U(\mathbf{r})$ necessary to reach a new touching position. Repeating this procedure we construct $U(\mathbf{r})$ along some path. Repeating it for all paths in the connected region of "good" material, we determine the field $U(\mathbf{r})$. The mapping which is single-valued for each two consecutive steps along the path may turn out not to be single-values for a closed contour. The procedure of mapping along a path is known as the Burgers-Frank procedure.[15,14] A contour in the substance is here mapped upon a contour formed by bonds of an ideal lattice. The discrepancy of a closed contour is not changed when it is deformed provided the contour does not intersect a line of "bad" material. The problem of describing "bad" material is thus reduced to considering discrepancies of contours around separate defect lines. Local defects are equivalent to dislocations and disclinations. The difference consists in that in our case the Burgers vector $\mathbf{b}$ and the Frank vector $\mathbf{\Omega}$ may change along the defect line:

$$\mathbf{\Omega}(\mathrm{r}') = U(\mathrm{r}')U^{-1}(\mathrm{r})\mathbf{\Omega}(\mathrm{r}), \tag{5}$$

$$\mathrm{b}(\mathrm{r}') = U(\mathrm{r}')U^{-1}(\mathrm{r})\mathrm{b}(\mathrm{r}). \tag{6}$$

For a more precise description of the atomic coordinates of the chosen cluster of "good" material we must give not only the rotation, but also the deformation which is uniform on the scale of the cluster and which is described by a symmetric tensor $u(\mathbf{r})$.

It turned out that the atomic configurations of a condensed substance can be parametrized as follows:

1. "Good" material: the field of the deformation tensor $u_{ij}(\mathbf{r})$ and the rotation matrix $U_{ij}(\mathbf{r})$.

2. Defects: the fields of the dislocation density $\alpha_{ij}(\mathbf{r})$ and of the disclination density $\tau_{ij}(\mathbf{r})$. For isolated defects the α and τ fields are defined in the standard way:

$$\begin{aligned} \alpha_{ij} &= \sum_D \delta_i(\mathrm{r} - \mathrm{r}_D) b_j, \\ \tau_{ij} &= \sum_D \delta_i(\mathrm{r} - \mathrm{r}_D) \Omega_j, \end{aligned} \tag{7}$$

where the $\delta_i(\mathbf{r})$ are the components of the delta-function on the defect line.

3. STATEMENT OF THE PROBLEM

To describe the system in the framework of the proposed parametrization we must write down the Hamiltonian in terms of the α, τ, U, and u fields and calculate the Gibbs partition function. The first steps to realize this program were taken in a paper by Obukhov.[16] In it the fields τ and U were assumed to be unimportant and were dropped. It was shown that in such an approximation at a temperature $T_D = \epsilon/\ln(n)$ (ϵ is the average energy per unit length of the core of the dislocation and n the number of nearest neighbors in the crystal lattice) a system of dislocation lines with infinite length is formed in the crystal and this phase transition was identified with melting.

It was noted in Ref. 4 that the main feature of melting is the loss of long-range orientational order, and in it the $U_{ij}(\mathbf{r})$ fields were taken into account. It was then assumed that disclinations which require for their generation large elastic deformations cannot exist as equilibrium defects without a mechanism for plastic relaxation, i.e., without dislocations. The disclinations can thus be represented as a system of dislocations and thus do not require to be introduced explicitly. Considering the Gibbs statistics of the α, u, and U fields showed that the phase transition obtained in Ref. 16 is not, in general, melting. The orientational disordering is described by an effective Hamiltonian of the U fields which turned out to be identical with the Hamiltonian of the phenomenological theory of Ref. 5. According to Ref. 4 there can thus exist between the crystal and the liquid an intermediate phase which is characterized by the presence of a dislocation network of infinite length while at the same time retaining the orientational order.

It was indicated in Ref. 17 that a liquid must be characterized by the loss of rigidity over scales larger than some characteristic one and there an attempt was undertaken to calculate one of the characteristics of the rigidity—the large-scale effective shear modulus. It was only possible to do this below T_D where it turned out to be nonvanishing, as was expected. The aim of the present paper is a determination of the rigidity of the system above the dislocation transition. As in Ref. 4 we shall here assume that one needs not introduce the disclinations explicitly. In that case one can, provided the deformations are small, introduce instead of the rotation and the deformation of a single distortion field $\beta(\mathbf{r})$:

$$\beta_{ij} = u_{ij} + \frac{1}{2}(U_{ij} - U_{ji}). \qquad (8)$$

Calculating the rigidity enables us to answer the question whether there is a high-temperature phase[16] of the liquid and it also makes it possible to characterize the intermediate phase, predicted in Ref. 4, in more detail.

First of all we give a more precise definition of the quantity to be calculated. The rigidity of the system is defined by the Gibbs average

$$B_{ijkl}(\mathrm{r}, \mathrm{r}') = \langle \beta_{ij}(\mathrm{r})\beta_{kl}(\mathrm{r}')\rangle. \qquad (9)$$

It will become clear from what follows that it is convenient to use the quantity

$$\Omega_{\alpha\beta} = \frac{1}{4}\varepsilon_{\alpha ij}\varepsilon_{\beta kl}B_{ijkl}, \qquad (10)$$

where the ε_{ijk} are the Levi–Civita symbols. It is natural to name Ω the rotational rigidity since

$$\Omega_{\alpha\beta}(\mathrm{r}, \mathrm{r}') = \langle \omega_\alpha(\mathrm{r})\omega_\beta(\mathrm{r}')\rangle, \qquad (11)$$

$$\omega_\alpha = \frac{1}{2}\varepsilon_{\alpha ij}U_{ij}, \qquad (12)$$

where ω is the rotation vector: Its direction is the same as the rotational axis, and its absolute value is equal to the sine of the rotational angle of the axes of the local anisotropy with respect to the global coordinate system. It is clear from Eqs. (11) and (12) that the quantity Ω characterizes also the orientational order in the system.

4. HAMILTONIAN AND CONSISTENCY CONDITION

The Hamiltonian consists of two parts—the energy of the core of the dislocations and the energy of their interactions:

$$H = H_c + H_{int}. \qquad (13)$$

The energy of the core can be written in the form:

$$H_c = \sum_D \int_D \varepsilon\, dl, \qquad (14)$$

where ε is the energy of the core of a dislocation per unit length, the integration is along the dislocation line, and the summation is over all dislocations. We can write the interaction energy down starting from the well known expressions:[13,18]

$$H_{int} = \frac{1}{2}\int \beta_{ij}(\mathrm{r})\beta_{kl}(\mathrm{r})\Lambda_{ijkl}dv, \qquad (15)$$

$$\beta_{mn} = \int \varepsilon_{pmk}\Lambda_{ijkl}G_{jn,i}(\mathrm{r} - \mathrm{r}')\alpha_{pl}(\mathrm{r}')dv', \qquad (16)$$

where Λ is the elastic-constants matrix,

$$G_{jn,i}(\mathbf{r}) = dG_{jn}(\mathbf{r})/dx_i,$$

G_{jn} is the Green tensor of the crystal, and α is the dislocation-density tensor. For simplicity we shall assume the system to be simple cubic and elastically isotropic so that

$$\Lambda_{ijkl} = \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl},$$
$$G_{jn}(\mathrm{r}) = \frac{1}{4\pi\mu}\left(\frac{\delta_{jn}}{r} - \frac{1}{4(1-\nu)}\frac{d^2r}{dx_j dx_n}\right), \qquad (17)$$

where ν is the Poisson coefficient and μ and λ are the Lamé coefficients. Calculations using Eqs. (15)–(17) give:

$$H_{int} = \frac{1}{2}\int \alpha_{li}(\mathrm{r})D_{ij}^{\mathrm{ln}}(\mathrm{r} - \mathrm{r}')\alpha_{nj}(\mathrm{r}')dvdv', \qquad (18)$$

where the matrix D in the momentum representation is:

$$D_{ij}^{ln} = \frac{2\mu}{q^2}\left[\frac{1+p}{1+2p}S_{ij}S_{ln} + \frac{p^2}{2(1+2p)^2}S_{ij}n_l n_n - \frac{1}{2}S_{il}S_{jn} + \frac{p}{1+2p}S_{in}S_{jl}\right]. \qquad (19)$$

Here

$$n_i = q_i/q; \quad S_{ij} = \delta_{ij} - n_i n_i, \quad p = -\nu/(1+\nu).$$

Equation (19) is the same as the one used in Ref. 16 apart from the second term. In Ref. 16 this term was dropped since it gives zero for dislocation configurations of closed loops with a constant Burgers vector along the loop. We, however, assume that the rotation is not small and that the Burgers vector may change along the defect line:

$$\alpha_{li} = \alpha_{ls}^0 U_{is} = \sum_D \delta_l(\mathrm{r} - \mathrm{r}_D)b_s^0 U_{is}(\mathrm{r}), \qquad (20)$$

where the b_s^0 are the components of the Burgers vector in the system of coordinates the axes of which coincide with the axes of the local anisotropy. Using Eq. (20) the interaction energy takes the form:

$$H_{int} = \frac{1}{2}\int \alpha^0(\mathrm{r})U(\mathrm{r})D(\mathrm{r} - \mathrm{r}')\alpha^0(\mathrm{r}')U(\mathrm{r}')dvdv' \qquad (21)$$

(to simplify the notation we have dropped the indices). When evaluating the partition function using the Hamiltonian of (13), (14), and (21) and the fields α^0, U we must bear in mind that the above-mentioned fields are not independent but connected by a consistency condition.[4] In our case this condition can easily be obtained from Eq. (16):

$$\omega_\alpha = \frac{1}{2}\int \varepsilon_{\alpha mn}\varepsilon_{pmk}\Lambda_{ijkl}G_{jn,i}(\mathrm{r} - \mathrm{r}')\alpha_{ps}^0(\mathrm{r}')U_{ls}(\mathrm{r}')dv'. \qquad (22)$$

The matrix U is recovered from the vector $\boldsymbol{\omega}$ as follows:

$$U_{ij} = \delta_{ij}\cos\phi + (1 - \sin\phi)\frac{\omega_i\omega_j}{\omega^2} + \varepsilon_{ijk}\omega_k, \qquad (23)$$

where $\sin\phi = \omega$.

5. SCREENED INTERACTION APPROXIMATION

Using condition (22) and (23) when evaluating the partition function requires the introduction of a nontrivial weight factor in the functional integral since this condition is not linear. To avoid this difficulty we shall use an approximation similar to the Debye–Hückel approximation in the theory of a rarefied plasma. We proceed as follows. We assume that we have succeeded in solving the problem and in calculating the average:

$$A_{ijkl} = \langle U_{ij}(\mathrm{r})U_{kl}(\mathrm{r}')\rangle. \qquad (24)$$

If we replace in Eq. (21) the produce of the rotation matrices by A, the expression obtained will serve as an approximation for the effective Hamiltonian of the dislocations:

$$H^D_{eff} = H_c + \frac{1}{2}\int \alpha^0(\mathrm{r})\tilde{D}(\mathrm{r}-\mathrm{r}')\alpha^0(\mathrm{r}')dvdv',$$
$$\tilde{D}^{ln}_{ij}(\mathrm{r}-\mathrm{r}') = D^{ln}_{sk}(\mathrm{r}-\mathrm{r}')A_{sikj}(\mathrm{r}-\mathrm{r}'). \tag{25}$$

We can interpret Eq. (25) as the change in the Green tensor in comparison with an ideal crystal: if in an ideal crystal with a small dislocation density we have $\alpha^0 = \alpha$ and

$$\beta = \int \varepsilon\Lambda G(\mathrm{r}-\mathrm{r}')\alpha^0(\mathrm{r}')dv', \tag{26}$$

after integration over the rotation fields Eq. (26) changes to

$$\beta = \int \varepsilon\Lambda\tilde{G}(\mathrm{r}-\mathrm{r}')\alpha^0(\mathrm{r}')dv'. \tag{27}$$

Here $\tilde{D}$ is calculated in terms of $\tilde{G}$ in the same way as D is calculated in terms of G:

$$\tilde{D}^{pp_1}_{ll_1} = \Lambda_{mnm_1n_1}\varepsilon_{pmk}\varepsilon_{p_1m_1k_1}\Lambda_{ijkl}\Lambda_{i_1j_1k_1l_1}\tilde{G}_{jn,i}(\mathrm{q})\tilde{G}_{j_1n_1,i_1}(\mathrm{q}). \tag{28}$$

The consistency condition is in the approximation (25)

$$\omega_\alpha = \frac{1}{2}\int \varepsilon_{\alpha mn}\varepsilon_{pmk}\Lambda_{ijkl}\tilde{G}_{jn,i}(\mathrm{r}-\mathrm{r}')\alpha^0_{pl}(\mathrm{r}')dv'. \tag{29}$$

It can be written in another, more convenient form if we take the average of the product $\omega_\alpha(\mathbf{r})\omega_\beta(\mathbf{r}')$ and change to the momentum representation:

$$\Omega_{\alpha\beta} = \frac{1}{4}\varepsilon_{\alpha mn}\varepsilon_{\beta m_1n_1}\varepsilon_{pmk}\varepsilon_{p_1m_1k_1}\Lambda_{ijkl}\Lambda_{i_1j_1k_1l_1}\tilde{G}_{jn,i}(q)$$
$$\times\tilde{G}_{j_1n_1,i_1}(-\mathrm{q})L^{pp_1}_{ll_1}(\mathrm{q}), \tag{30}$$

where

$$L^{ln}_{ij}(\mathrm{r}-\mathrm{r}') = \sum_{\alpha^0}\alpha^0\exp\left(-\frac{H_d}{T}\right)\alpha^0_{li}(\mathrm{r})\alpha^0_{nj}(\mathrm{r}'). \tag{31}$$

The summation is over the dislocation configurations.

The obvious relation

$$\Omega_{\alpha\beta}(\mathrm{r}) = \frac{1}{4}\varepsilon_{\alpha ij}\varepsilon_{\beta kl}A_{ijkl}(\mathrm{r}) \tag{32}$$

together with Eqs. (28), (30), and (31) is the system of equations for Ω. This system is rather complicated and we use simplifying assumptions. We shall assume that

$$\tilde{D}(\mathrm{q}) = 2\mu f(q)[\ldots], \tag{33}$$

where the expression in the square brackets is identical to Eq. (19). This means that we assume the index form of the interaction to be the same as in an ideal crystal but the power-law dependence, $D \propto 1/r$, is replaced by a screening. Moreover, we shall assume that the quantity $A(\mathbf{r}-\mathbf{r}')$ is independent of the choice of the global system of coordinates. Hence it follows that the average relative rotation matrix of the axes of the local anisotropy, $g_{jl}(\mathbf{r}) = A_{ijil}(\mathbf{r}) = A_{jili}(\mathbf{r})$, is an isotropic tensor:

$$g_{jl}(\mathrm{r}) = g(\mathrm{r})\delta_{jl}. \tag{34}$$

One can also show easily that in that case the trace A_{iijl} vanishes: it is independent of the orientation of the global coordinates so that it can be averaged over these orientations without any changes. Interchanging that averaging with the statistical one we verify that $A_{iijl} = 0$. Starting from this we write down an expression for $\Omega_{\alpha\alpha}$:

$$\Omega_{\alpha\alpha}(\mathrm{r}) = \frac{1}{4}\varepsilon_{\alpha ij}\varepsilon_{\alpha kl}A_{ijkl} = \frac{1}{4}(A_{ijij} - A_{ijji}) = \frac{3}{4}g(r). \tag{35}$$

The function $g(r)$ characterizes the rotational rigidity of the system.

We consider the relation:

$$\tilde{D}^{ln}_{ii} = D^{ln}_{ij}A_{isjs} = D^{ln}_{ii}(\mathrm{r})g(r). \tag{36}$$

Integrating this equation over the angles, which can be done in the momentum representation, and using Eq. (33), we get:

$$f(r) = -\frac{g(r)}{4\pi r}, \tag{37}$$

where $f(r)$ is the Fourier transform of $f(q)$ from Eq. (33). Contracting condition (30) over the indices α and β we get the equation

$$F[-3\pi rf(r)] = \frac{1}{4}\varepsilon_{\alpha mn}\varepsilon_{\alpha m_1n_1}\varepsilon_{pmk}\varepsilon_{p_1m_1k_1}\Lambda_{ijkl}$$
$$\times\Lambda_{i_1j_1k_1l_1}G_{jn,i}(q)G_{j_1n_1,i_1}(-q)L^{pp_1}_{ll_1}(q), \tag{38}$$

where we have denoted by $F[\ldots]$ the operation of taking the spatial Fourier transform. It is now necessary to evaluate the correlator L, using Eqs. (25) and (31).

6. EVALUATION OF THE DISLOCATION CORRELATOR

We must evaluate the partition function

$$Z_D = \sum_{\alpha^0}\exp -\frac{H^D_{eff}}{T}, \tag{39}$$

where

$$H^D_{eff} = \sum_D \int_D \varepsilon dl + \frac{1}{2}\int \alpha^0_{li}\tilde{D}^{ln}_{ij}\alpha^0_{nj}dvdv', \tag{40}$$

and $\tilde{D}$ is given by Eq. (33). For simplicity we assume that ε is independent of the orientation of the Burgers vector and that with an appreciable probability dislocations are realized only with the minimum b^0. We introduce the conjugate field:

$$Z_D = \sum_{\alpha^0}\int D\phi_{ij}\exp[-\sum_D\int_D\frac{\varepsilon}{T}dl$$
$$-\frac{T}{2}\int\phi_{li}(\mathrm{r})(\tilde{D}^{-1})^{ln}_{ij}\phi_{nj}(\mathrm{r}')dvdv' - i\int\phi_{ij}(\mathrm{r})\alpha^0_{ij}(\mathrm{r})dv]. \tag{41}$$

Changing from Eq. (39) to (41) raises a problem, since the matrix $\tilde{D}$ is transverse, i.e., it does not have an inverse. To avoid this difficulty we note that in the continuum approximation we can write the core energy in the form:

$$H_c = \varepsilon\int(\alpha^0_{ij})^2dv. \tag{42}$$

Using this relation we can redefine the quantities $\tilde{D}$ and ε in Eq. (39):

$$\varepsilon \to \varepsilon - \beta,$$
$$\tilde{D}^{ln}_{ij} \to \tilde{D}^{ln}_{ij} + 2\beta\delta_{ij}\delta_{ln}\delta(\mathrm{r}). \tag{43}$$

In the final expressions we put $\beta \to 0$. In Ref. 4 we proposed a transformation reducing the summation over the configurations of dislocation loops to a path integral over three complex local fields ψ^ν ($\nu = 1,2,3$):

$$\sum_{\alpha^0} \exp\left[-\frac{H_c}{T} + i\int \alpha^0_{ij}(\mathrm{r})\phi_{ij}(\mathrm{r})dv\right]$$

$$= \int \Pi_\nu D\psi^\nu D\psi^{\nu *}\exp[-H_d], \qquad (44)$$

$$H_d = \int\sum_\nu [(1 - nJ)|\psi^\nu|^2 + g|\psi^\nu|^4$$

$$+ J|(d_k - i\phi_{kj}b^{0\nu}_j)\psi^\nu|^2]dv, \qquad (45)$$

where n is the number of nearest neighbors in the crystal lattice,

$$J = \lambda(g)\exp\left(-\frac{\varepsilon}{T}\right), \quad \lambda(g) = \frac{\int_0^\infty \exp(-x - gx^2)dx}{\int_0^\infty x\exp(-x - x^2)dx},$$

g is a model constant taking into account the distortion of the dislocation interaction at small distances. Since the dislocations with minimum Burgers vectors are equally probable, the average $\langle R\rangle$ for an arbitrary functional $R[\psi^\nu]$ is independent of the index ν. We integrate over the ψ fields in the mean-field approximation:

$$Z_D = \int D\phi_{ij}\exp[-\int \phi_{li}M^{ln}_{ij}\phi_{nj}dvdv'],$$

$$M^{ln}_{ij} = J\langle|\psi|^2\rangle\delta_{ij}\delta_{ln}\delta(\mathrm{r}) + \frac{T}{2}(\tilde{D}^{-1})^{ij}_{ln}. \qquad (46)$$

Adding in Eq. (41) a term with a source we see easily that

$$L^{ln}_{ij} = -J^2\langle|\psi|^2\rangle^2(M^{-1})^{ln}_{ij}. \qquad (47)$$

Evaluating it and substituting it into Eq. (38) gives the following expression for $f(r)$:

$$F[3\pi rf(r)] = \frac{2\mu p^2\tilde{J}^2}{T(1+2p)^2}\frac{f^2(q)}{[2(1+2p)^2/p^2 + (4\mu/T)\tilde{J}f(q)]}, \qquad (48)$$

where $\tilde{J} = J = \langle|\psi^2|\rangle$. Equation (48) allows yet one more simplification. The concept of crystallike local order in a condensed substance assumes that the "bad" material, i.e., the dislocation cores, take up a small part of the whole volume. Since $\langle|\psi^2|\rangle$ is proportional to the density of the dislocation segments we may assume $\tilde{J}$ to be a small quantity. We expand the right-hand side of Eq. (42) in $\tilde{J}$ and retain the first nonvanishing term:

$$F[rf(r)] = Cf^2(q), \qquad (49)$$

$$C = \frac{\mu\tilde{J}^2}{3\pi T}\left(\frac{p}{1+2p}\right)^4.$$

7. SOLUTION OF (49) AND DISCUSSION OF THE RESULTS

Before solving Eq. (49) we determine the limits of its applicability. The basis of its derivation was the approximation (25) which is based upon the assumption that $l_U \gg l_\alpha$, where l_U and l_α are characteristic scales over which the fields U and α change. The dislocation interaction is thus distorted in Eq. (25) over scales of the order l_α. This distortion does not affect the evaluation of L^{ln}_{ij} since it can be compensated by a suitable choice of the constant g but it imposes a restriction on the applicability of Eq. (49): its solutions characterize the rigidity of the system only for scales $r \gg l_\alpha$.

Equation (49) has two solutions:

$$f_1(r) = -\frac{1}{4\pi^3Cr^2},$$

$$f_2(r) = -\frac{a}{2\pi Cr}e^{-ar}, \qquad (50)$$

where α is a constant which is determined below. The function $g(r)$ corresponding to these solutions is:

$$g_1(r) = \frac{1}{C\pi^2 r},$$

$$g_2(r) = \frac{2a}{C}e^{-ar}. \qquad (51)$$

One of these functions must give the solution $g(r) = \text{const}$ for a rigid crystal as $\tilde{J}\to 0$. It is clear that this function is g_2 where we must have

$$a = \text{const}\frac{C}{2}. \qquad (52)$$

The state in which g_2 is realized is clearly the liquid. Equation (52) enables us to estimate the scale over which the liquid does not lose its rigidity with respect to torsional deformations: $r_l = \text{const}\times 10^2$ interatomic distances, where the constant is of order unity.

The state with g_1 is the intermediate phase the existence of which was predicted in Ref. 4. It is clear from Eq. (51) that this phase is characterized by a power-law decrease of the rotational rigidity at large distances: $\Omega_{mn}(r) \propto 1/r$ as $r\to\infty$.

An analysis of the thermodynamic advantages and stabilities of the solutions obtained is problematic in the framework of the approximations of the present paper: assumptions (33) and (34) enable us only to talk about the qualitative form of Ω.

Relations (51) are possible scenarios for the behavior of the rigidity of the system above T_D. Although the solution of the problem of their realization and stability is impossible in the framework of the present paper, Eqs. (51) give us a chance to study this problem experimentally.

We note that the liquid solution is most likely to be unstable: this is indicated by the nonphysical increase of r_l with temperature [see Eqs. (51), (52), and (49)]. In that case melting does not take place in the framework of the model considered here—it is necessary to introduce disclinations explicitly. A detailed consideration of this problem is the contents of a separate paper.

APPENDIX

The matrices met with in the text—the kernels of the quadratic forms in the momentum representation—have the form

$$V^{ln}_{ij} = Q(q)[\nu_1 S_{ij}S_{ln} + \nu_2 S_{ij}n_l n_n + \nu_3 S_{ln}n_i n_j$$

$$+ \nu_4 S_{il}S_{jn} + \nu_5 S_{il}n_j n_n + \nu_6 S_{jn}n_i n_l + \nu_7 S_{in}S_{jl}$$

$$+ \nu_8 S_{in}n_j n_l + \nu_9 S_{il}n_j n_n + \nu_{10}n_i n_j n_n n_l]. \qquad (53)$$

The coefficients μ_i and the factor Q' for the inverse matrix can be calculated using the following relations:

$$Q' = \frac{1}{Q}, \quad \mu_1 = \frac{\nu_1}{d_1}, \quad \mu_2 = \frac{\nu_3}{d_2}, \quad \mu_3 = \frac{\nu_2}{d_2},$$

$$\mu_4 = \frac{\nu_4\nu_{10} - \nu_5\nu_6}{(\nu_1 + \nu_7)d_3}, \quad \mu_5 = \frac{\nu_5}{d_3}, \quad \mu_6 = \frac{\nu_6}{d_3},$$

$$\mu_7 = -\frac{\nu_7}{d_1}, \quad \mu_8 = -\frac{\nu_8}{d_2}, \quad \mu_9 = -\frac{\nu_9}{d_2},$$

$$\mu_{10} = -\frac{\nu_1 + 2\nu_4 + \nu_7}{d_3}, \tag{54}$$

$$d_1 = \nu_1^2 - \nu_7^2, \quad d_2 = \nu_2\nu_3 - \nu_8\nu_9,$$

$$d_3 = 2\nu_5\nu_6 - \nu_{10}(\nu_1 + 2\nu_4 + \nu_7).$$

Below we give the coefficients and the factors for the matrices encountered in the text.

$D^{ln.}_{ij}$:

$$Q = \frac{2\mu}{q^2}, \quad \nu = \frac{1 + p}{1 + 2p}, \quad \nu_2 = \frac{p^2}{2(1 + 2p)^2},$$

$$\nu_4 = -\frac{1}{2}, \quad \nu_7 = \frac{p}{1 + 2p}; \tag{55}$$

$(\tilde{D}^{-1})^{ln.}_{ij}$:

$$Q = \frac{1}{2\mu f(q)}, \quad \nu_1 = \frac{\tilde{\beta} + (1 + p)/(1 + 2p)}{(\tilde{\beta} + 1)(\tilde{\beta} + 1/(1 + 2p))},$$

$$\nu_2 = \frac{1}{\tilde{\beta} + p^2/2(1 + 2p)^2}, \quad \nu_3 = \frac{1}{\tilde{\beta}}, \quad \nu_4 = \frac{1}{2\tilde{\beta}(\tilde{\beta} + 1)},$$

$$\nu_7 = \frac{-p}{(1 + 2p)(\tilde{\beta} + 1)(\tilde{\beta} + 1/(1 + 2p))},$$

$$\nu_{10} = \frac{1}{\tilde{\beta}}, \quad \tilde{\beta} = \frac{\beta}{\mu f(q)}; \tag{56}$$

$L^{ln.}_{ij}$:

$$Q = -\frac{4\mu}{T}\tilde{J}^2 f(q), \quad \nu_1 = \frac{b + 1 + p}{(b + 1)(b + 1 + 2p)},$$

$$\nu_2 = \frac{1}{b + 2(1 + 2p)^2/p^2},$$

$$\nu_4 = -\frac{1}{2(b + 1)}, \quad \nu_7 = \frac{p}{(b + 1)(b + 1 + 2p)}, \tag{57}$$

$$b = \frac{4\mu}{T}\tilde{J}f(q).$$

We show in Eqs. (55)–(57) only the nonvanishing ν_k. The matrix L^{ln}_{ij} is written down in the limit as $\tilde{\beta} \to 0$.

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