Equilibrium between elastically-interacting phases

I. M. Kaganova and A. L. Roitburd

L. V. Vereshchagin Institute of High-Pressure Physics, USSR Academy of Sciences

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We investigate the thermodynamics of the heterogeneous system which results when a solid undergoes a first-order phase transition, and derive equations for equilibrium between the phases in the presence of elastic interactions. These equations are solved by finding the shape of the region containing the new phase, embedded in the infinite matrix of the old phase, which minimizes the elastic energy. For the case of elastically-isotropic phases, this equilibrium inclusion has the shape of an ellipsoid, possibly degenerate, i.e., a cylinder or a plane-parallel plate. We determine the regions of stability for the various equilibrium shapes as a function of the intrinsic strain tensor which characterizes the phase transition, and the relations between the elastic properties of the phases. We investigate the influence of an external homogeneous stress field on an equilibrium inclusion, and show that an external shear field does not penetrate the inclusion and does not interact with it. We construct the equilibrium surface of the inclusion and the matrix in the space of the shear and hydrostatic components of the external stress field. This surface bounds the region in which the matrix phase is stable against transformation into the inclusion phase. As the equilibrium shape of the inclusion is varied in an external stress field, there is a line of special points on this surface which can be interpreted as phase transitions to the resulting phase inclusion ("morphological" phase transitions for the phase inclusion). We determine the thermodynamic hysteresis of the phase transition.

INTRODUCTION

As a rule, there is an elastic interaction between phases coexisting in a solid, caused by the differing crystal lattices and elastic properties of the phases in contact. The elastic fields are long-range, i.e., they extend from the interphase boundaries out to a distance on the order of the size of the surface of contact. The long range means that even for phases having macroscopic dimensions (when the surface energy can be neglected compared to the elastic energy), the equilibrium depends on the volume, shape and mutual positions of the phase regions. This constitutes the principal peculiarity of equilibrium between phases in a solid compared to equilibrium in liquid or gaseous phases.

In these investigations we will treat heterogeneous-phase ("heterophase") solids as continuous media, represented by originally homogeneous crystals in which a certain part has undergone conversion to the other phase (Fig. 1). If the connectivity of such a crystal is not disrupted, i.e., if there are no breaks in its continuity and plastic deformation has not taken place, then an internal stress field appears in the crystal as a result of compensation for the changes in volume and shape of the transformed local region relative to its original state. In the transformed phase there is no elastic strain other than the so-called intrinsic strain, which is characteristic of the phase transformation and determines the changes in structure and symmetry during the transition. It can be determined from the change in the dimensions and shape of the whole crystal after the latter has been completely converted to the homogeneous new phase. This concept of an intrinsic strain is fundamental to the following exposition.

Using the intrinsic strain, the conditions for equilibrium between the phases in a homogeneous stress field $\hat{\sigma}$, which are expressed by equating the thermodynamic potentials of the original (φ_1) and final (φ_2) homogeneous states of the crystal, within the linear theory of elasticity can be written in the form[1]:

$$\Delta\varphi=\varphi_2-\varphi_1=\Delta f_0-{}^1/_2\hat{\sigma}\Delta\hat{S}\hat{\sigma}-\hat{\varepsilon}\hat{\sigma}=0,$$
$$\varphi_i=f_i-\hat{\varepsilon}_i\hat{\sigma},\quad \Delta f_0=f_{02}-f_{01},\quad \Delta\hat{S}=\hat{S}_2-\hat{S}_1. \tag{0.1}$$

Here, $\hat{\varepsilon}$ is the intrinsic strain of phase 2 relative to phase 1; $f_1=f_{01}+1/2\hat{\sigma}\hat{S}\hat{\sigma}$ is the free energy density of the deformed phase, where f_{01} is the density for the undeformed phase; $\hat{\varepsilon}_1$ and $\hat{\varepsilon}_2$ are strains, where $\hat{\varepsilon}_1=\hat{S}_1\hat{\sigma}$ and $\hat{\varepsilon}_2=\hat{S}_2\hat{\sigma}+\hat{\varepsilon}$; $-\hat{\varepsilon}_1\hat{\sigma}$ and $-\hat{\varepsilon}_2\hat{\sigma}$ are the amounts of work done against the stress field $\hat{\sigma}$. The elastic compliances $\hat{S}_1$ are taken to be independent of the stress $\hat{\sigma}$. The potentials φ_i are normalized to unit volume. (Here and below we will use a notation without subscripts for the tensors and their contractions: $\hat{\varepsilon}$ is a second-rank tensor, $\hat{S}$ is a fourth-rank tensor).

The differential form of Eqs. (0.1) for equilibrium between the phases

$$d\Delta f_0=\hat{\varepsilon}(\hat{\sigma})d\hat{\sigma},\ \hat{\varepsilon}(\hat{\sigma})=\hat{\varepsilon}+\Delta\hat{S}\hat{\sigma} \tag{0.2}$$

is a generalized Clausius-Clapeyron equation,[1] in which

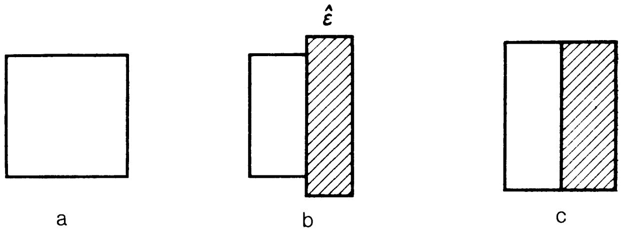

FIG. 1. (a) Crystal before a phase transformation. (b) The phase transformation, characterized by an intrinsic strain $\hat{\varepsilon}$, has occurred in the cross-hatched region. (c) Internal stresses compensate for the mismatch in the crystal lattices of the phases.

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$\hat{\varepsilon}(\hat{\sigma})$ is a renormalized intrinsic strain which includes a term connected with the differing deformabilities of the phases in addition to the intrinsic strain $\hat{\varepsilon}$ connected with the phase transformation, which depends only on temperature. Taking into account the temperature dependence of the left side of (0.2), i.e., $d\Delta f_0 = q dT/T$, where q is the latent heat of the transition, we can use Eq. (0.2) to construct the phase equilibrium surface $T = T_{\text{eq}}(\hat{\sigma})$, which serves as a phase diagram in the space of tensor components of the stress $\hat{\sigma}$ and temperature T. This surface separates regions in which one of the homogeneous phases is more stable than the other.

From the continuum-mechanics point of view, a heterophase crystal is a medium in which there is a certain spatial distribution of the intrinsic strain. In what follows we will limit ourselves to heterophase systems in which the intrinsic strains and moduli of elasticity are constant throughout each of the phases. In this case, the interphase boundaries are sources of internal stress. Treating the energy of the heterophase system as a functional of the interphase boundary configuration, we can find the equilibrium conditions of the system; along with the conditions of mechanical equilibrium $\nabla\hat{\sigma} = 0$, they include equilibrium conditions related to displacement of the interphase boundaries. Formally, this condition, which should be fulfilled at each point of the interphase boundary, coincides with the condition of phase equilibrium (0.1), where by $\hat{\sigma}$ we must now understand not the external stress but rather the local stress caused by all the internal and external sources, with the exception of the intrinsic stress of the portion of the boundary under study.[2,3]

The solutions to the equilibrium equations describe the various heterophases of the structure, which are characterized by definite spatial distributions of the phases under study. In order to investigate the initial stages of the transformation, it is sufficient to discuss a two-phase system consisting of a finite region of one phase (an inclusion) within an unbounded region of the other phase (the matrix). The boundary for stability of the matrix phase against a transition to the inclusion phase (i.e., a transition which takes place with a gradual increase in the fraction of the transformed phase) is determined by the existence or nonexistence of an equilibrium macroscopic inclusion whose shape has the property of minimizing the elastic energy (we will call such an inclusion an " equilibrium" inclusion). In $(T,\hat{\sigma})$ space, this stability boundary corresponds to a certain surface $T = T_{\text{tr}}(\hat{\sigma})$ which we will refer to as the phase transformation surface: reacing this surface is a necessary condition for the evolution of the phase transition. In a solid, this surface does not coincide with the phase equilibrium surface $T = T_{\text{eq}}(\hat{\sigma})$ as a rule. The equation for the transformation surface is

$$\Delta\varphi + e(\hat{\varepsilon}(\hat{\sigma}),\ \hat{S}_1,\ \hat{S}_2) = 0, \tag{0.3}$$

where e is the elastic energy of an equilibrium inclusion of phase 1 in phase 2, referred to unit volume of the latter phase. The surface for the inverse transformation, i.e., from phase 2 to phase 1, is described by an analogous equation:

$$-\Delta\varphi + e'(-\hat{\varepsilon}(\hat{\sigma}),\ \hat{S}_2,\ \hat{S}_1) = 0, \tag{0.4}$$

where $-\hat{\varepsilon}(\hat{\sigma})$ is the intrinsic strain of phase 1 relative to phase 2, e' is the energy of an equilibrium inclusion of phase 1 in phase 2; this inclusion can have a shape which differs considerably from an inclusion of phase 2 into phase 1 (Fig. 2). Therefore, the phase equilibrium surface is split into two phase transformation surfaces, between which there lies a region where the homogeneous phase is stable against the formation of inclusions of the other phase, and hence where nucleation of the latter is impossible. This region where the transformation is forbidden determines the thermodynamic hysteresis between the direct and inverse phase transformations.

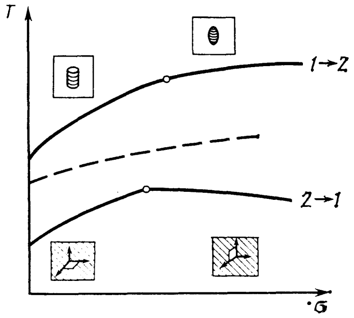

FIG. 2. Cross-section of the phase transformation diagram in $T - \hat{\sigma}$ space (σ is one of the principal values of the tensor $\hat{\sigma}$). Dashed line—equilibrium curve; solid line—phase transformation line. The shapes of the inclusions of the new phase are shown (the phase 2 region is crosshatched). The points where the morphological phase transitions occur are marked.

Hence, the thermodynamic behavior of the initial stages of a first-order phase transition in a solid is determined to a significant degree by the energies of the equilibrium inclusions.

Up until now, the problem of an equilibrium inclusion has been solved only for the case of phases with identical elastic moduli, for which the equilibrium inclusion has the shape of a thin plate.[4,5] The natural parameter which characterizes the equilibrium inclusion is its orientation relative to the crystallographic axes of the phases; this parameter is determined primarily by the anisotropy of the intrinsic strain, that is the orientation of its principal axes, and the ratio of the spherical component to the shear components of the intrinsic strain ε. Including the elastic anisotropy of the phases does not fundamentally change the results obtained for an isotropic medium, and as a rule leads only to a lifting of the degeneracy in the case of an intrinsic strain of symmetrical form.[6]

This allows us to assert that even in the general case in which the phases have different moduli a qualitatively correct solution of the problem can be obtained, if we likewise do not include the elastic anisotropy of the phases. In this approximation, the problem of the shape and energy of an equilibrium inclusion is solved in Sec. 2 of this article. The result depends significantly on the ratios of the elastic moduli of the phases.

If the inclusion phase is more rigid than that the matrix phase, and there is a dilatational component present in the intrinsic strain, the equilibrium inclusion has the form of an ellipsoid. As the fraction of shear in the intrinsic strain increases, the ellipsoid degenerates into a plate or cylinder. If the rigidity of the inclusion phase is smaller than that of the matrix phase, the equilibrium inclusion is a plate. The characteristic feature of these elastic equilibrium shapes is homogeneity of the elastic strain field inside the inclusion and the absence of dilatational components in the elastic field outside the inclusion. As a consequence of this, the Gibbs thermodynamic potential is constant along the entire interphase surface.

Once we have found the dependence of the energy of an equilibrium inclusion on the intrinsic strain, we can construct a phase transformation surface on the temperature-external stress diagram. Since the components of the intrinsic strain depend on the external stress [see Eq. (0.2)], the shape and energy of the equilibrium inclusion are changed along the transformation surface. At certain values of the external parameters, this change can have a qualitative character. Correspondingly, there appear anomalous features on the phase transformation surface, as if the phase which forms could be precipitated out in various states between which there are "morphological" phase transitions.[1]

Formally, the presence of anomalies on the phase transformation surface is explained by the fact that in the differential equation for this surface,

$$d\Delta f_0=[\hat{\varepsilon}(\hat{\sigma})+de/d\hat{\sigma}]\,d\hat{\sigma}, \tag{0.5}$$

the term $de/d\hat{\sigma}$ enters in; this term undergoes a discontinuity, or a discontinuity in its derivative, at the boundary of the transition from one equilibrium phase to another. In analogous fashion, we can investigate the phase transformation surface in a multicomponent system, where along with the external stress there is an additional parameter: the concentration, which also changes the ratio between the hydrostatic and shear components of the intrinsic strain.

For the model under discussion here, we have succeeded in giving a full thermodynamic description of the initial stages of the phase transformation in a solid, and have solved the problem of thermodynamic hysteresis. As an example, we carry out this program in Sec. 3 for the case of a purely external stress.

In addition to the assumption noted above, viz., that it is possible to neglect anisotropy in the elastic properties of the phases, the model we are investigating is based also on a series of other simplifications. Certain qualitative consequences which more complicated models lead to, in particular the inclusion of relaxation of the internal stresses, are discussed in the Conclusion of the article.

1. EQUILIBRIUM EQUATIONS FOR ELASTICALLY INTERACTING PHASES

Let us discuss an isothermal system consisting of two phases with volumes V_1 and V_2, separated by an interphase boundary S. Certain prescribed forces F_i act on the external surface S' which bounds the system. The thermodynamic potential of the system is

$$\Phi=\int\limits_{V_1} f_1(\eta,c,\nabla_i u_k)\,dV+\int\limits_{V_2} f_2(\eta,c,\nabla_i u_k)\,dV -\int\limits_{S'} F_i u_i\,dS-\mu\int\limits_{V_1+V_2} c\,dV. \tag{1.1}$$

The local free energy density f_i depends on the local values of the order parameters: a nonconserved one η and a conserved one c (for example, the concentration of the second component in a two-component system), and also on the gradient of the displacement u_i ($\nabla_k\equiv\partial/\partial x_k$); μ is a Lagrange multiplier which takes into account the condition that the parameter c be conserved. Equilibrium corresponds to vanishing of the variation of the functional (1.1) with respect to variation in the functions η, c, and u_i, and also with respect to arbitrarily small displacements of the interphase boundary δx_i:

$$\delta\Phi=\int\limits_{V_1+V_2}\left\{\frac{\delta f_{1,2}}{\delta\eta}\delta\eta+\left(\frac{\delta f_{1,2}}{\delta c}-\mu\right)\delta c+\frac{\delta f}{\delta u_i}\delta u_i\right\}dV +\int\limits_{S'}(\sigma_{ik}n_k-F_i)\,\delta u_i\,dS+\int\limits_{S}[\sigma_{ik}\delta u_i+\varphi_{ik}\delta x_i]\,n_k\,dS=0, \tag{1.2}$$

where

$$\varphi_{ik}\equiv(f-\mu c)\,\delta_{ik}-\sigma_{ik}\nabla_k u_i,$$

$\delta/\delta a$ is the variational derivative; $\sigma_{ik}=\partial f/\partial\nabla_k u_i$ is the stress tensor; $[a]=a_2-a_1$; a_2, a_1 are the values of the quantity a on the two sides of the phase boundary for phase 1 and phase 2, respectively; and n_i is a vector normal either to the surface S or to S'.

Equation (1.2) implies an equilibrium equation in the volume of each phase:

$$\delta f/\delta\eta=\partial f/\partial\eta=0, \tag{1.3}$$

$$\delta f/\delta c=\partial f/\partial c=0, \tag{1.4}$$

$$-\delta f/\delta u_i=\nabla_k\partial f/\partial\nabla_k u_i=\nabla_k\sigma_{ik}=0, \tag{1.5}$$

and a boundary condition on the external surface

$$\sigma_{ik}n_k|_{S'}=F_i. \tag{1.6}$$

The different phases correspond to different regions of definition of the order parameters η and c.

If the phase transformation proceeds without disrupting the continuity of the media (i.e., $[\delta u_i]=0$) and without plastic deformation (i.e., there is no slip at the interphase boundary, so $[\delta x_i]=0$), then, because the variations δu_i and δx_i are independent, setting the last integral in (1.2) to zero implies that on the boundary S

$$[\sigma_{ik}]\,n_k=0, \tag{1.7}$$

$$[\varphi_{ik}]\,n_k=0. \tag{1.8}$$

As a consequence of the condition of compatibility of the strains at the boundary S, i.e., curl $\nabla_i u_k=0$, the jump in the gradient of the displacement can be represented in the form of a dyadic product

$$[\nabla_k u_i]=S_i n_k,$$

where S_i is an arbitrary vector. If we take Eq. (1.7) into account, this latter assertion implies that a vector enters into the left-hand side of Eq. (1.8) which is parallel to the normal n_i. Consequently, the vector equation (1.8) is equivalent to a single scalar equation, which can be written in an invariant form which has no explicit dependence on the normal vector:

$$[f-\mu c]-{}^1/_2(\sigma_{ik}^{(1)}+\sigma_{ik}^{(2)})\,[\nabla_i u_k]=0. \tag{1.9}$$

In our model (in which the interphase boundary is a geometric surface), $\nabla_i u_k$ undergoes a discontinuity on S, and Eq. (1.9) becomes the Weierstrass-Erdman condition for a broken extremal.

Equations (1.3)–(1.5) for equilibrium in the volume of the phases and the interphase boundary equilibrium equation (1.9), together with the boundary conditions (1.6), (1.7), fully determine the equilibrium of the two-phase system under discussion here. We note that Eq. (1.9) has a simple physical meaning: it asserts that the local thermodynamic potentials are equal on the interphase boundary. Actually, $\sigma_{ik} = 1/2\ (\sigma_{ik}^{(1)} + \sigma_{ik}^{(2)})$ is the "external" stress with respect to the region of the boundary under study, because we have excluded the self-action of this region from the summation. Therefore, $f - \mu c - \{\sigma_{ik}\}\ \nabla_i u_k$ is the Gibbs potential of the near-boundary regions of the phases. Equation (1.9) is easily generalized to the case of other long-range fields which arise in heterophase bodies, e.g., electric and magnetic fields.[3]

From here on, we will limit ourselves to the case in which only elastic fields are present in the system, and the phases are spatially homogeneous with regard to order parameter and concentration. In particular, such heterophase systems arise during deformational phase transitions (e.g., ferroelastic or martensitic), where the strain components are the parameters of the transition. The simplest case is a polymorphic transition in a single-component system. For such a transition, to second order we have

$$f_i = f_{0i}(\eta, c, \hat{\varepsilon}_i) + {}^1/_2[\hat{\varepsilon} - \hat{\varepsilon}_i(\eta, c)]\hat{C}_i[\hat{\varepsilon} - \hat{\varepsilon}_i(\eta, c)]. \quad (1.10)$$

Here, $\varepsilon_{ik} = 1/2\ (\nabla_k u_i + \nabla_i u_k)$, and $\hat{C}_i$ is the elastic modulus tensor for the ith phase. In keeping with the definition given in the Introduction, the intrinsic strain $\hat{\varepsilon}_i$ of the ith phase is specified by the condition

$$(\partial f/\partial \hat{\varepsilon})_{\hat{\varepsilon} = \hat{\varepsilon}_i} = \hat{C}_i(\hat{\varepsilon} - \hat{\varepsilon}_i) = 0, \quad (1.11)$$

i.e., this is the strain acquired by the homogeneous phase as a result of variation of the order parameter within it when there are no stresses. If we assume that $\hat{\varepsilon}_1 = 0$, while $\hat{\varepsilon}_2 = \hat{\varepsilon}$ is the intrinsic strain of phase 2 measured from the unstressed state of phase 1, then taking (1.10) into account we can transform Eq. (1.9) to the form

$$\Delta f_0 - {}^1/_2\hat{\sigma}_1 \Delta \hat{S} \hat{\sigma}_2 - {}^1/_2(\hat{\sigma}_1 + \hat{\sigma}_2)\hat{\varepsilon} = \Delta f_0 - {}^1/_2\hat{\sigma}_2\hat{\varepsilon} - {}^1/_2\hat{\sigma}_1\hat{\varepsilon}^* = 0. \quad (1.12)$$

The second form of Eq. (1.12) is obtained from the first by using an identity transformation and by introducing an equivalent intrinsic strain

$$\hat{\varepsilon}^* = \hat{\varepsilon} + \Delta \hat{S} \hat{\sigma}_2, \quad (1.13)$$

which allows us to replace the system of phases under study, in which the phases have different elastic moduli, by an equivalent system of phases (in the mechanical and geometric sense) with identical moduli, specifically those of phase 1. The strain $\hat{\varepsilon}^*$ is defined by the system of equations

$$\hat{\sigma}_2 = \hat{C}_2(\hat{\varepsilon}^{(2)} - \hat{\varepsilon}) = \hat{C}_1(\hat{\varepsilon}^{(2)} - \hat{\varepsilon}^*). \quad (1.14)$$

This replacement preserves the stress and strain invariants of the system ($\hat{\varepsilon}^{(2)}$ is the total strain in phase 2).

As we will show below, the boundary equilibrium equation in the form (1.12) is extremely convenient for determining the equilibrium shape of the inclusion: it allows us to easily "guess" the solution of the problem we are looking for.[1)]

2. EQUILIBRIUM SHAPE OF AN INCLUSION IN AN ELASTICALLY ISOTROPIC MEDIUM

Let us discuss two elastically-isotropic phases whose elastic moduli are different. The intrinsic strain of the transformation $\hat{\varepsilon}$ is given, and we will assume that the external stress $\hat{\sigma} = 0$. We will prove that for an isotropic elastic medium there exists a region of values of the components of the intrinsic strain $\hat{\varepsilon}$ within which an ellipsoid is the equilibrium shape of an inclusion.

We begin with the equilibrium equation for the interphase boundary in the form (1.12). An ellipsoidal inclusion differs from an inclusion of arbitrary shape in that the elastic field within such an inclusion is homogeneous ($\hat{\sigma}_2 = \text{const}$). The stress has a discontinuity at the interphase boundary S; in addition, the value of $\hat{\sigma}_1$ at a given point of this boundary depends on the direction of the normal to the surface S at that point.[17] It is obvious that in this case Eq. (1.12) can be satisfied at all points on the surface S only if the slip reduces to zero:

$$\hat{\sigma}_1 \hat{\varepsilon}^* = 0. \quad (2.1)$$

Then Eq. (1.12) is transformed to the relation

$$\Delta f_0 - {}^1/_2\hat{\sigma}_2\hat{\varepsilon} = \Delta f_0 + e = 0, \quad (2.2)$$

which expresses the fact that the variation of the free energy as the volume of the inclusion is varied equals zero[17] (compare with Eq. (0.3) for $\hat{\sigma} = 0$).

In the elastically homogeneous isotropic medium which we are dealing with here, after the transformation to the equivalent strain, condition (2.1) is satisfied if $\hat{\varepsilon}^*$ is a pure dilatation, i.e., the stress outside the center of dilatation is a pure shear,[17] and the slip $\hat{\sigma}_1 \hat{\varepsilon}^*$ reduces to zero at any point of the inclusion surface.

The components of the tensor $\hat{\varepsilon}^*$ depend on $\hat{\varepsilon}$ and on the shape of the ellipsoid. Consequently, the problem consists of choosing the shape of the ellipsoid for a given tensor $\hat{\varepsilon}$ so that the equivalent strain, which is the solution to Eq. (1.14), is a pure dilatation.

In order to calculate the strain $\hat{\varepsilon}^{(2)}$ inside the ellipsoidal inclusion which enters into Eq. (1.14), we use the solution given by J. D. Eshelby[17]: $\hat{\varepsilon}^{(2)} = \hat{\mathscr{S}}\hat{\varepsilon}^*$, where $\hat{\mathscr{S}}$ is a linear operator given in the system of coordinates connected with the axes of the ellipsoid. The components of the matrix $\hat{\mathscr{S}}$ are expressed in terms of the integral

$$I_i = \frac{1}{2} a_1 a_2 a_3 \int_0^\infty \frac{du}{\Delta(a_i^2 + u)}, \qquad i = 1, 2, 3,$$
$$\Delta = \prod_{i=1}^{3} (a_i^2 + u)^{1/2}, \qquad \sum_{i=1}^{3} I_i = 1, \qquad 0 \leqslant I_i \leqslant 1, \quad (2.3)$$

which characterizes the shape of the ellipsoid: the values I_i depend on the ratios of the semi-axes of the ellipsoid a_i. For $I_1 = I_2 = I_3 = 1/3$, the shape of the inclusion is a sphere; for $I_i = 0$, $I_{j \neq i} \neq 0$, the ellipsoid degenerates into an infinite elliptic cylinder with axis along the ith axis; for $I_1 = 0$, $I_{j \neq i} = 0$, it becomes an infinite thin plate with its normal along the ith axis.

In calculating the matrix elements of $\hat{\mathscr{S}}$, we can show that for $\hat{\varepsilon}^* = \varepsilon^* \hat{E}$ ($\hat{E}$ is the unit matrix), then

$$\hat{\varepsilon}^{(2)} = \varepsilon^* \left(\frac{1 + \nu_1}{1 - \nu_1}\right) \begin{pmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{pmatrix}, \quad (2.4)$$

where ν_i is the coefficient of the Poisson matrix. Substituting

$\hat{\varepsilon}^{(2)}$ into Eq. (1.14) and taking into account the fact that the medium under investigation is isotropic ($\hat{C}_i$ are the isotropic moduli of elasticity), we obtain a system of equations for determining ε^* and I_i. This system has a solution only when the principal axes of the ellipsoid coincide with the principal axes of the intrinsic strain $\hat{\varepsilon}$:

$$I_i={}^1/_3[1+x_i\varphi(\gamma,\nu_2)/(1-\gamma)], \tag{2.5}$$

$$x_i=\frac{\tilde{\varepsilon}_i}{\varepsilon},\quad \varphi(\gamma,\nu_2)=1+\frac{2\gamma(1-2\nu_2)}{1+\nu_2},\quad \varepsilon^*=3\varepsilon\varphi^{-1}\left(\frac{1-\nu_1}{1+\nu_1}\right),$$

where $\gamma=\mu_1/\mu_2$, μ_i are the shear moduli, ν_i is the Poisson coefficient for the ith phase, ε is the dilatation, $\tilde{\varepsilon}_i$ is the principal value of the deviator for the intrinsic strain $\hat{\varepsilon}$, and consequently $\Sigma^j_{i=1}x_i=0$. Eq. (2.5) proves the assertion we made earlier. (The problem of equilibrium of a nucleus in a melt, which was formulated in a way analogous to this, was solved in Ref. 18. However, the solution obtained there for an ellipsoidal inclusion corresponded not to a minimum but to a maximum in the elastic energy).

The stress within an equilibrium ellipsoidal inclusion is

$$\hat{\sigma}_2=-p_2\hat{E}+\hat{\tau}_2, \tag{2.6}$$

where

$$p_2=4\mu_1\varepsilon/\varphi,\quad \hat{\tau}_2=2\mu_1\hat{\tilde{\varepsilon}}/(1-\gamma).$$

We note that only the purely dilatational part of the intrinsic strain is "responsible" for the pressure p_2, while only the purely deviator part is "responsible" for the shear τ_2.

The energy of the equilibrium ellipsoidal inclusion, measured relative to a unit of its volume, is

$$e_{\text{el}}=-\frac{1}{2}\hat{\sigma}_2\hat{\varepsilon}=\frac{6\mu_1\varepsilon^2}{\varphi}\left\{1-\frac{\varphi}{6(1-\gamma)}\frac{\tilde{\varepsilon}^2}{\varepsilon^2}\right\},\qquad \tilde{\varepsilon}^2=\hat{\tilde{\varepsilon}}\hat{\tilde{\varepsilon}},\quad \tilde{\varepsilon}^2/\varepsilon^2=2(x_1^2+x_2^2+x_1x_2). \tag{2.7}$$

In addition to the ellipsoidal inclusions under study here, Eq. (2.1), which is a necessary condition for equilibrium, admits as solutions inclusions in the form of ellipsoids of degenerate form, i.e., thin plates or long elliptic cylinders (the end surfaces are not taken into account). We can show that for $\gamma>1$ (i.e., the inclusion is less rigid than the matrix) the optimal oriented film-shaped inclusion always corresponds to a smaller elastic energy (for a given inclusion volume) than e_{el}. The equilibrium ellipsoidal inclusion is energetically favored only for values of $\gamma<1$.

Let us investigate the solution (2.5) for $\gamma<1$. The inequality

$$0\leqslant I_i\leqslant 1 \tag{2.8}$$

determines the region in which an equilibrium ellipsoidal inclusion exists. In the coordinates x_1, x_2 ($x_3=-(x_1+x_2)$, where the x_i are the values of the intrinsic shear divided by the intrinsic dilatation) the solution to the system of inequalities (2.8) is the interior of a triangle ABC (Fig. 3), whose vertices have coordinates $A(-a,-a)$, $B(2a,-a)$, $C(-a,2a)$, where $a=(1-\gamma)/\varphi$. As $\gamma\to 1$, this triangle collapses to a point which coincides with the coordinate origin.

Along the sides of ΔABC, one of the values I_i vanishes and the ellipsoid degenerates into an infinite elliptic cylinder whose axis coincides with the direction of the ith principal axis of the intrinsic strain $\hat{\varepsilon}$: $I_1=0$ on the side AC, $I_2=0$ on side AB, and $I_3=0$ on side CB. At the vertices of ΔABC, the ellipsoid degenerates into a film ($I_i=1$) whose normal coincides with the direction i: $I_1=1$ at point B, $I_2=1$ at point C, $I_3=1$ at point A.

Suppose now that the inclusion has the form of a long elliptic cylinder. We can show that condition (2.1) for equilibrium of the interphase boundary will be fulfilled if the axis of the cylinder coincides with one of the principal axes of the

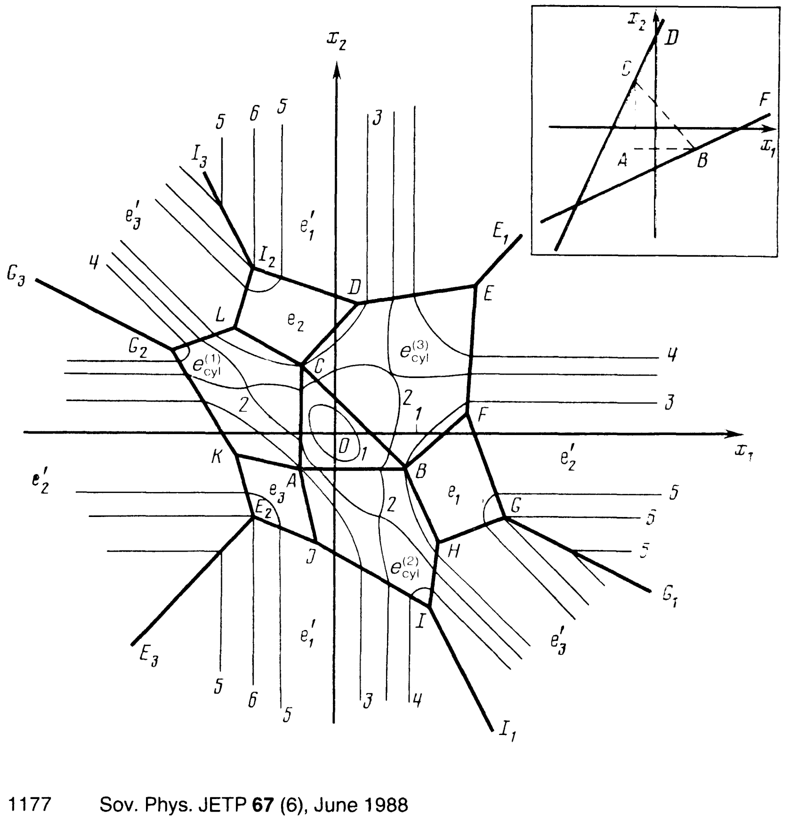

FIG. 3. Diagram of the morphological states for $\gamma<1$ ($\gamma=0.5$, $\nu_2=0.25$). The values of the elastic energy in the regions of stability of the various equilibrium states are shown: within the polygon $BCDEF$, marked with $e^{(3)}_{\text{cyl}}$, the stable shape of the equilibrium inclusion is an elliptic cylinder with its axis along the 3 axis; in the polygon $BFGH$, this shape is a plate with normal $\mathbf{n}=(1,0,0,)$, etc. The energy e/e_0 takes the following values on the numbered isoenergetic lines: 1—0.9, 2—0.8, 3—0.5, 4—1.5, 5—0.2, 6—0.

intrinsic strain $\hat{\varepsilon}$, while the equivalent strain $\hat{\varepsilon}^*$ is tetragonal. Thus, if the axis of the cylinder is directed along axis 3 ($I_3 = 0$), the equivalent strain must have the form

$$\hat{\varepsilon}^* = \begin{pmatrix} \varepsilon_1{}^* & 0 & 0 \\ 0 & \varepsilon_1{}^* & 0 \\ 0 & 0 & \varepsilon_3{}^* \end{pmatrix}. \tag{2.9}$$

Now Eq. (1.14) is a system for finding the three unknowns $\varepsilon_1{}^*$, $\varepsilon_3{}^*$ and, e.g., I_1,

$$I_1 = [\varepsilon_1(1-\nu_2\gamma) - \varepsilon_2\gamma(1-\nu_2) + \varepsilon_3\nu_2(1-\gamma)]/$$
$$(1-\gamma)[\varepsilon_1+\varepsilon_2+2\nu_2\varepsilon_3], \tag{2.10}$$

where ε_i are the principal values of the tensor $\hat{\varepsilon}$.

The elastic energy of this cylindrical inclusion, which is asymptotically in equilibrium, is

$$e_{\text{cyl}}^{(3)} = \mu_2\left\{(1+\nu_2)\varepsilon_3{}^2 + 2\gamma\left[\frac{[\nu_2\varepsilon_3+(\varepsilon_1+\varepsilon_2)/2]^2}{1+\gamma(1-2\nu_2)} - \frac{1}{(1-\gamma)}\left(\frac{\varepsilon_1-\varepsilon_2}{2}\right)^2\right]\right\}. \tag{2.11}$$

(In Ref. 19, the extrema of the function $e_{\text{cyl}} = e_{\text{cyl}}(\hat{\varepsilon})$ were studied for the special case $\varepsilon_3 = 0$). If the axis of the cylinder coincides with some other principal axis of $\hat{\varepsilon}$, the corresponding expressions for I_i and $e_{\text{cyl}}^{(i)}$ are obtained from (2.10), (2.11) by a cyclic permutation of the subscripts.

Just as for the case of triaxial ellipsoids, the equilibrium elliptic cylinders are energetically favored compared to the plate-shaped inclusions only for values $\gamma < 1$.

For each direction of the axis of the cylinder, inequality (2.8) specifies an angle in the plane (x_1, x_2) within which there exists a given solution. Thus, if the axis of the cylinder coincides with the 3 axis of the tensor $\hat{\varepsilon}$, the angle is given by the straight line (see inset to Fig. 3)

$$x_2 = [k_1 + (1-\nu_2)x_1]/k_2,$$
$$x_2 = [-k_1 + k_2x_1]/(1-\nu_2),$$
$$k_1 = (1-\gamma)(1+\nu_2), \quad k_2 = \nu_2 + \gamma(1-2\nu_2).$$

On these straight lines the cylinder degenerates into a plate whose normal coincides either with the direction of the first (the line *BF*) or the second (the line *CD*) principal axis of the tensor $\hat{\varepsilon}$. As $\gamma \to 1$, the angle "collapses" and the lines reduce to the line $x_2 = x_1$.

Let us discuss inclusions in the form of flat plates. The equilibrium conditions (2.1) in this case are fulfilled identically, because $\hat{\sigma}_1 \equiv 0$.[5] The elastic energy e of the inclusion depends on the orientation of the normal n to the plate relative to the principal axes of the intrinsic strain $\hat{\varepsilon}$. As a function of the form of $\hat{\varepsilon}$, the minimum is attained[6] either for a plate oriented along one of the principal axes, when $e = e_i$:

$$e_1 = \frac{\mu_2\varepsilon^2}{1-\nu_2}[(1+x_2)^2 + (1+x_3)^2 + 2\nu_2(1+x_2)(1+x_3)],$$
$$n_1{}^2 = 1, \quad n_2 = n_3 = 0, \tag{2.12}$$

or, when the plane of the plate is inclined and $e = e_i'$:

$$e_1{}' = \mu_2\varepsilon^2(1+\nu_e)(1+x_1)^2,$$
$$n_1 = 0, \quad n_2{}^2 = (1+\nu_2+\nu_2x_1+x_2)/(x_2-x_3), \quad n_3{}^2 = 1-n_2{}^2 \tag{2.13}$$

(the values e_2, e_3 and e_2', e_3' are obtained by cyclic permutation of the subscripts).

Ellipsoids, elliptic cylinders and plates exhaust all the possible shapes of inclusions within which the elastic field is homogeneous. By comparing the elastic energies for these various equilibrium inclusion shapes, we can construct a diagram of the morphological states in the (x_1, x_2) plane, i.e., we can bound the regions of stability of the various equilibrium shapes as the geometric characteristics of the transformation change.

The results of this analysis are shown in Fig. 3 for the case $\gamma < 1$: the heavy lines separate the stability regions of the various equilibrium shapes. The figure was drawn using $\gamma = 0.5$, $\nu_2 = 0.25$, but the qualitative form of the diagram is preserved for other parameter values.

Equilibrium ellipsoidal inclusions are possible only for the relatively small intrinsic shears in the regions bounded by ΔABC. Outside this region, as the intrinsic shears increase, the energetically-favored inclusions are either cylinders (the region in which these can occur adjoins the sides of ΔABC), or (near the vertices of ΔABC) plates whose normals are directed along one of the principal axes of the intrinsic strain. With further increase of the intrinsic shears, the equilibrium inclusion becomes a plate whose orientation depends on the value of x_i.

On the boundaries of the stability regions for the various equilibrium shapes there are singularities of the derivatives of the function $e = e(\hat{\varepsilon})$. Thus, as we pass through the line EE_1 the orientation of the equilibrium plate changes discontinuously; for a transition through the line *DEF* the equilibrium elliptic cylinder is replaced by an inclusion in the shape of an inclined plate. On these lines, the derivatives $de/d\hat{\varepsilon}$ undergo a discontinuity; on the remaining lines the second derivatives $d^2e/d\hat{\varepsilon}^2$ are discontinuous.

In Fig. 3, we use thin lines to denote contours of constant elastic energy of the equilibrium inclusions, i.e., $e = e(x_1, x_2) = \text{const}$, normalized to the value of energy $e_0 = 6\mu_1\varepsilon^2/\varphi$ for $x_1 = x_2 = 0$. If the intrinsic strain is close to a pure dilatation, the intrinsic shear causes the system energy to decrease. This dependence on shear takes place in the region where the ellipsoidal inclusion exists and for plates oriented perpendicular to one of the principal axes of the intrinsic strain. The elastic energy decreases most rapidly as the shear x_1 approach the points E_2, G and I_2. From these points, lines extend (e.g., line 6 in Fig. 3) and pass into the region of stability for the inclined plates; along these lines the elastic energy of the system reduces to zero, i.e., the function $e(x_1, x_2)$ attains an absolute minimum. In the region of existence of equilibrium cylindrical inclusions the function $e = e(x_1, x_2)$ has a saddle point (line 2 of Fig. 3).

For $\gamma > 1$ the plate is a natural candidate for the equilibrium shape of an inclusion, where the orientation of the plate depends on the value of the relative intrinsic shears x_i (Fig. 4): for small shear the plates are oriented perpendicular to one of the principal axes of the intrinsic strain, while as the shears increase it becomes energetically favorable to have inclined plates. The boundaries of the regions of stability for plates of various orientations do not depend on γ, and are determined solely by the value of ν_2. On the sides of the polygon $EGIE_2G_2I_2$ the orientations of the plates change smoothly, while there is a jump on the radial lines, e.g., EE_1 and GG_1.

In Fig. 4 we have normalized the elastic energy

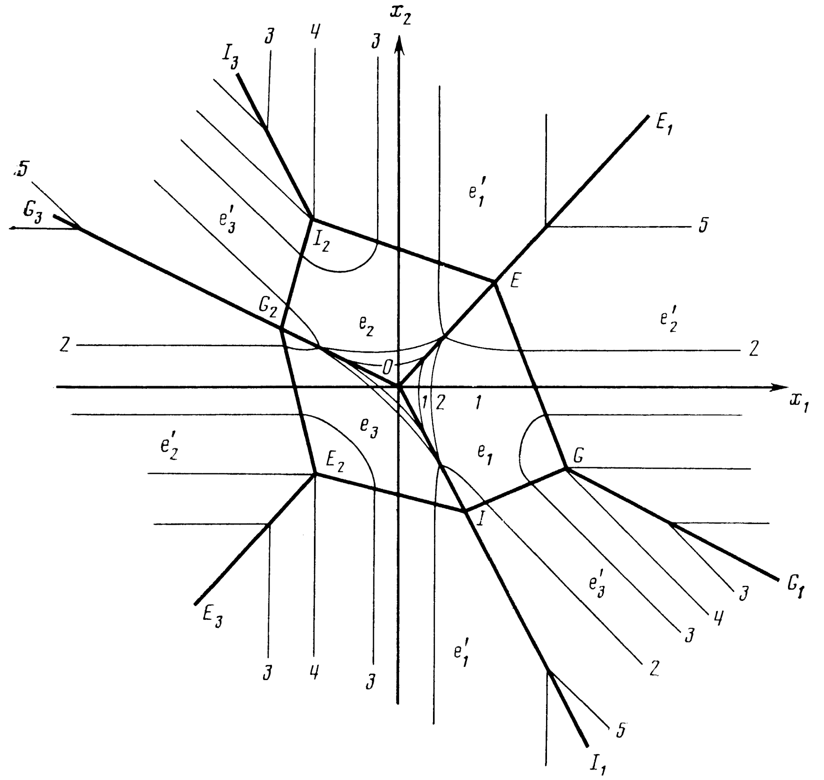

FIG. 4. Diagram of the morphological states for $\gamma > 1$. The notation is the same as for Fig. 3. The energy e/e_0 takes the following values on the numbered isoenergetic lines: 1—0.9, 2—0.8, 3—0.1, 4—0, 5—2.

$e = e(x_1, x_2)$ by the value $e_0 = 2\mu_2(1 + \nu_2)\varepsilon^2/(1 - \nu_2)$ for $x_1 = x_2 = 0$. As in the case $\gamma < 1$, the function $e = e(x_1, x_2)$ has a maximum at the coordinate origin, and the position of the absolute minimum does not change ($e = 0$, line 4 of Fig. 4). The saddle points represented by the isoenergetic line 2 are located on the boundaries of the stability region for plates oriented perpendicular to one of the principal axes of the intrinsic strain.

Let us now discuss the intersection of Figs. 3 and 4 with the line $x_1 = x_2 = x$ (the tetragonal intrinsic strain). If $\gamma < 1$, then for

$$-(1-\gamma)/\varphi < x < (1-\gamma)/2\varphi$$

the equilibrium shape of the inclusion is a biaxial ellipsoid. Outside this interval the following shapes are energetically favorable:

(1) If $(1 - \gamma)/2\varphi x < x_*$, where

$$x_* = (1+\nu_2)\{3+\gamma(1-2\nu_2) +3[1-2\gamma\nu_2-\gamma^2(1-2\nu_2)]^{1/2}\}/[3(1+\nu_2)+\gamma(1-2\nu_2)(5-\nu_2)],$$

the favored shape is a circular cylinder with its axis along the third principal axis of the intrinsic strain;

(2) For $-1 < x < -(1 - \gamma)/\varphi$, the favored shape is a plate orthogonal to the 3 axis;

(3) If $x < -1$ or $x > x_*$, the film is oriented at an angle:

$$n_3^2 = [x(2-\nu_2)-(1+\nu_2)]/3x,$$

while one of the projections n_1 and n_2 equals zero (the two equally acceptable orientations of the film).

In Fig. 5a we show the energy e of an equilibrium inclusion as a function of the tetragonality parameter x. For $x = x_*$ the derivative de/dx undergoes a jump, while for the rest of the boundary points the function $e = e(x)$ varies smoothly, although there is a discontinuity in d^2e/dx^2.

For $\gamma > 1$ the shape of the inclusion is a plate, which is asymptotically in equilibrium:

(1) For $x > (1 + \nu_2)/(2 - \nu_2)$ or $x < 1$, the inclined

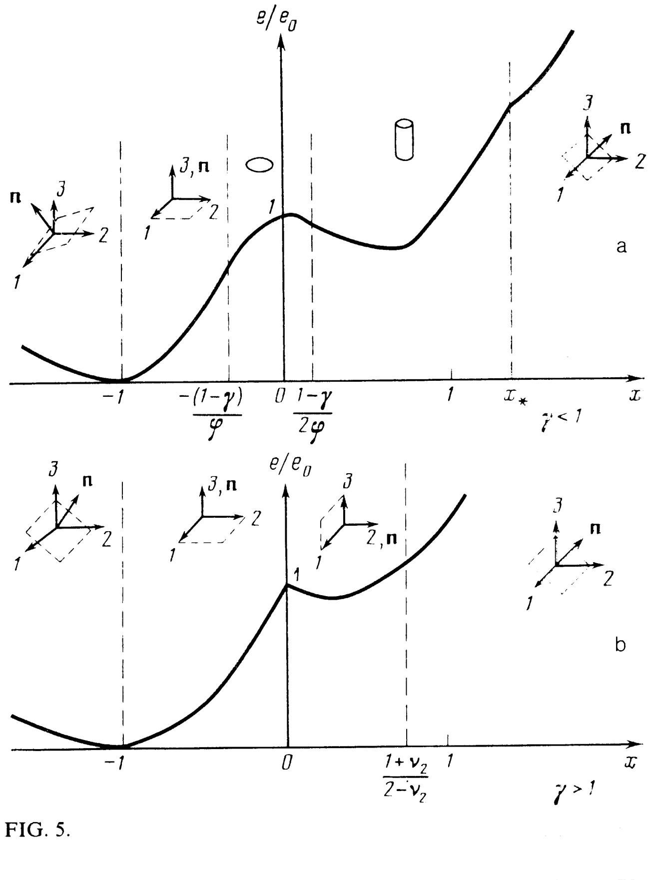

FIG. 5.

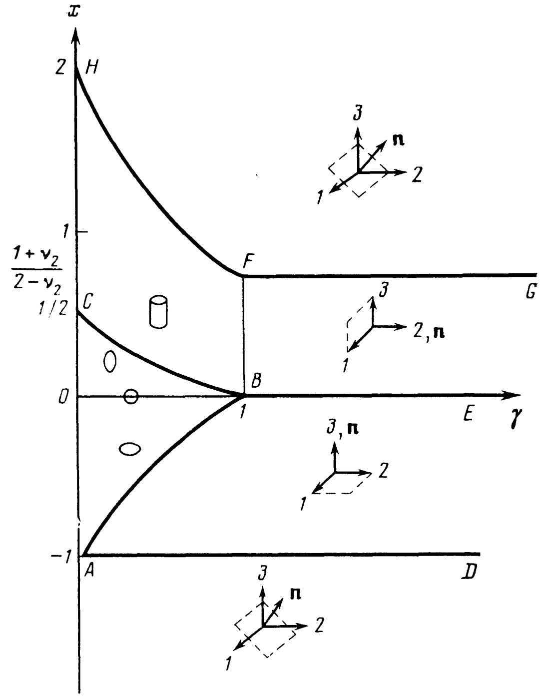

FIG. 6.

plate is energetically favored (with two equally acceptable orientations);

(2) For $0 < x < (1+\nu_2)/(2-\nu_2)$, the plate is oriented normal to either the first or the second principal axis (two equally acceptable orientations);

(3) For $-1 < x < 0$, the equilibrium plate normal is directed along the third principal axis. In Fig. 5b we show the function $e = e(x)$ for $\gamma > 1$. The derivative de/dx undergoes a jump at $x = 0$.

In Fig. 6 we show the region of existence of an equilibrium ellipsoidal inclusion in the (γ, x) plane for the case of a tetragonal intrinsic strain, and the relative stability of the near-equilibrium shapes (the plate and the cylinder). On the line AB $(x = -(1-\gamma)/\varphi)$ the ellipsoidal inclusion transforms into a plate with its normal **n** along axis 3. On the line BC $(x = (1-\gamma)/2\varphi)$ it transforms into a circular cylinder. On the lines AD $(x = -1)$, BE $(x = 0)$, and FG $(x = (1+\nu_2)/(2-\nu_2))$, there are changes in the relative stabilities of plates of various orientations. On the line HF $(x = x_*(\gamma))$, the energies of the inclined plate and the cylindrical inclusion are equal. On line $BF(\gamma = 1)$ the cylinder transforms into a plate oriented normal either to axis 1 or axis 2.

3. EQUILIBRIUM INCLUSIONS IN A HOMOGENEOUS EXTERNAL FIELD

Let the phase transformation proceed under the action of an external stress $\hat{\sigma} = -p\hat{E} + \hat{\tau}$. The total stresses in the two-phase system are conveniently expressed as sums: $\hat{\sigma}_1 = \hat{\sigma} + \hat{\tilde{\sigma}}_1$, $\hat{\sigma}_1 = \hat{\sigma} + \hat{\tilde{\sigma}}_2$. The tildes denote the internal stresses which are responsible for the phase transformation. Let us rewrite the original equation for local equilibrium (1.12) in the form

$$\begin{gathered}\Delta\varphi(\hat{\sigma}) - {}^1/_2\hat{\tilde{\sigma}}_2\hat{\varepsilon}(\hat{\sigma}) - {}^1/_2\hat{\tilde{\sigma}}_1\hat{\varepsilon}^*(\hat{\sigma}) = 0,\\ \Delta\varphi(\hat{\sigma}) = \Delta f_0 - \hat{\sigma}\hat{\varepsilon} - {}^1/_2\hat{\sigma}\Delta\hat{S}\hat{\sigma},\\ \hat{\varepsilon}(\hat{\sigma}) = \hat{\varepsilon} + \Delta\hat{S}\hat{\sigma}, \quad \hat{\varepsilon}^*(\hat{\sigma}) = \hat{\varepsilon}(\hat{\sigma}) + \Delta\hat{S}\hat{\tilde{\sigma}}_2.\end{gathered} \tag{3.1}$$

Here, $\hat{\varepsilon}(\hat{\sigma})$ is the intrinsic strain as a function of the external stresses, and $\hat{\varepsilon}^*(\hat{\sigma})$ is the equivalent strain corresponding to it. The stresses $\tilde{\sigma}_1, \tilde{\sigma}_2$ are calculated with respect to $\hat{\varepsilon}(\hat{\sigma})$ as if the external stresses were absent. Comparing (3.1) and (1.12), we see that the introduction of the external stresses reduces[1] to a renormalization of $\hat{\varepsilon}$ and to the replacement of Δf_0 by $\Delta\varphi(\hat{\sigma})$, which implies that all the conclusions of section 2 are still valid.

From this it is immediately clear that the external shear does not change the value of the shear stresses in an equilibrium ellipsoidal inclusion, and that such an inclusion does not interact with external shear. Actually, according to (2.6) and (2.7) we have

$$\hat{\tau}_2 = \hat{\tau} + \hat{\tilde{\tau}}_2, \quad \hat{\tilde{\tau}}_2 = 2\mu_1\hat{\tilde{\varepsilon}}(\hat{\sigma})/(1-\gamma).$$

Since $\hat{\tilde{\varepsilon}}(\tilde{\sigma}) = \hat{\tilde{\varepsilon}} - (1-\gamma)\hat{\tau}/2\mu_1$, the shear $\hat{\tau}_2 = 2\mu_1\hat{\varepsilon}/(1-\gamma)$ does not depend on $\hat{\tau}$. The pressure in the inclusion is renormalized only because of the external pressure p:

$$p_2 = (1 + 4\mu_1/3K_2)^{-1}[4\mu_1\varepsilon + (1 + 4\mu_1/3K_1)p],$$

where K_i is the modulus of hydrostatic compression. The change in the thermodynamic potential $\delta\Phi$ for such a two-phase system relative to the single-phase state also is independent of $\hat{\tau}$:

$$\begin{gathered}\frac{\delta\Phi}{V} = \Delta f_0 + \frac{9}{2}\Delta K\varepsilon^2 + \Delta\mu\hat{\varepsilon}^2\\ -\frac{9}{2}\Delta K\frac{1 + 4\mu_1/3K_1}{1 + 4\mu_1/3K_2}\left(\varepsilon - \frac{p}{3\Delta K}\right)^2,\\ 1/\Delta\mu = 1/\mu_2 - 1/\mu_1, \quad 1/\Delta K = 1/K_2 - 1/K_1,\end{gathered} \tag{3.2}$$

in which V is the volume of the inclusion. Consequently, the "fine adjustment" of the shape of the inclusion which ensures a minimum in the thermodynamic potential gives rise to an "expulsion" of the external shear field from the region occupied by the ellipsoidal inclusion.

Let us construct the surface of the equilibrium phases (0.1) and the surfaces (0.3) and (0.4) for the direct $(1 \to 2)$ and inverse $(2 \to 1)$ transformations. In the approximation of linear elasticity theory this surface is one of second order whose specific form depends on the ratio of the elastic moduli of the phases.

The equation of the equilibrium surface $\Delta\varphi = 0$ can be rewritten as a quadratic form in the components of the total intrinsic strain

$$\hat{\varepsilon}(\hat{\sigma}) = \varepsilon(p)\hat{E} + \hat{\tilde{\varepsilon}}(\hat{\tau}) = (\varepsilon - p/3\Delta K)\hat{E} + (\hat{\tilde{\varepsilon}} + \hat{\tau}/2\Delta\mu).$$

Then we obtain

$$\begin{gathered}\varkappa - {}^9/_2\Delta K\varepsilon^2(p) - \Delta\mu\hat{\tilde{\varepsilon}}^2(\hat{\tilde{\tau}}) = 0,\\ \varkappa \equiv \Delta f_0 + {}^9/_2\Delta K\varepsilon^2 + \Delta\mu\hat{\tilde{\varepsilon}}^2, \quad \Delta f_0 \approx q(T - T_0)/T_0,\end{gathered} \tag{3.3}$$

where T_0 is the transition temperature for the non-interacting unstressed phases. Eq. (3.3) approximates the actual phase equilibrium surface. The limits of the approximation are determined by the requirement that the stresses and strains in the system be small.

For ΔK and $\Delta\mu$ the same sign, Eq. (3.3) has a solution only if the sign of the parameter $\varkappa$ coincides with the sign of ΔK and $\Delta\mu$. In this case, the transformation can only take place starting with a certain critical temperature T_* ($\varkappa(T_*) = 0$); the sign of the difference $T_{\rm eq} - T_0$ ($T_{\rm eq} = T_{\rm eq}(\hat{\sigma})$ is the phase equilibrium temperature) is determined unambiguously. If the signs of ΔK and $\Delta\mu$ are different, a solution to Eq. (3.3) exists for arbitrary signs of $\varkappa$. The equilibrium temperature $T_{\rm eq}$ can be either larger or smaller than T_0, depending on the form of the external stresses $\hat{\sigma}$.

Let us analyze the following example: let the intrinsic strain be tetragonal:

$$\tilde{\varepsilon}_1(\tau)=\tilde{\varepsilon}_2(\tau)=\tilde{\varepsilon}(\tau), \quad \tilde{\varepsilon}_3(\tau)=-2\tilde{\varepsilon}(\tau), \quad \Delta K, \Delta\mu<0.$$

In the coordinate system $(T, \varepsilon(p), \tilde{\varepsilon}(\tau))$ the phase equilibrium surface is an elliptic paraboloid, within which the homogeneously stressed phase 2 is stable. In order to construct the transformation surface, we note that for a given form of $\hat{\varepsilon}(\hat{\sigma})$ the tetragonality parameter $x = \tilde{\varepsilon}(\tau)/\varepsilon(p)$. Various intervals of x correspond to regions of stability for different equilibrium shapes of the inclusions. Sectors in the plane $(\varepsilon(p), \tilde{\varepsilon}(\tau))$ are associated with these intervals; these sectors are formed by straight lines which pass through the coordinate origin. To each of these sectors there corresponds a specific dependence of the elastic energy on the components of the intrinsic strain. Therefore, although qualitatively the phase transformation surfaces $1\to2$ and $2\to1$ replicate the phase equilibrium surface, they are only piecewise-smooth surfaces. We note that for $x = -1$ the thermodynamic hysteresis reduces to zero [$e(x = -1) = 0$ both for the direct and for the inverse transition]. This implies that the transformation surfaces, direct and inverse, are tangent to the equilibrium surface along their lines of intersection with the plane $\varepsilon(p) + \tilde{\varepsilon}(\tau) = 0$.

The phase equilibrium surfaces and the phase transformation surfaces we have constructed allow us to explain the observed effect of shear stresses on the hysteresis of the phase transformation under pressure. In the case of large shear components in the intrinsic strain, the action of external shear can turn out to be very significant (because of the linear term[2] $\hat{\tau}\hat{\varepsilon}$ which enters into the expression for $\Delta\varphi(\hat{\sigma})$). Here, the high pressure plays an auxiliary role, hindering fracture under the action of the shear stresses.

To illustrate this, let us discuss the intersection of these surfaces with the plane $T = $ const. The solid line in the plane $(\varepsilon(p), \tilde{\varepsilon}(\tau))$ shown in Fig. 7 is a phase equilibrium line; the phase transformation lines $1\to2$ and $2\to1$ are shown by the dashed and dotted-dashed lines, respectively. Let the intrinsic strain ε be represented by the point A. In the framework of this model, we can choose to use only the portions of the curves close to the point A in describing the transformation. The straight line $\tilde{\varepsilon}(\tau) = \tilde{\varepsilon}$ which passes through the point A, by intersecting the equilibrium and transformation lines, determines the value of $\varepsilon(p)$, and consequently the equilibrium pressure $p_{\rm eq}$ along with the direct and inverse transformation pressures $p_{1\to2}$ and $p_{2\to1}$ at $\tau = 0$. The thermodynamic hysteresis of the transformation is proportional to the distance between the points $\varepsilon(p_{1\to2})$ and $\varepsilon(p_{2\to1})$. In our example, for $\tau = 0$ the shape of the equilibrium inclusion for the transition $1\to2$ is an ellipsoid, while for the inverse transformation $2\to1$ it is a plate with a normal $\mathbf{n} = (0,0,1)$. If $\tau\neq0$, the corresponding pressures are obtained from the intersections of the planes in the figure with the lines $\tilde{\varepsilon}(\tau) = $ const. As long as the external shear does not shift the point of intersection of the straight line $\tilde{\varepsilon}(\tau) = $ const. with the $1\to2$ transformation line from the sector corresponding to an equilibrium ellipsoid, the pressure $p_{1\to2}$ is independent of the external stress. However, the pressures $p_{\rm eq}$ and $p_{2\to1}$ change as τ varies; for $\tilde{\varepsilon}\neq0$, depending on the sign of τ, this change can lead both to smaller [the straight line $\tilde{\varepsilon}(\tau) = \tilde{\varepsilon}_1$ in Fig. 7] and larger (the straight line $\tilde{\varepsilon}(\tau) = \tilde{\varepsilon}_2$) hysteresis.

CONCLUSION

The thermodynamic analysis presented here is based on investigation of an isolated inclusion and, strictly speaking, pertains only to the initial stages of the phase transformation, when the fraction of the phase in the inclusion is vanishingly small. However, if the formation of an equilibrium inclusion is thermodynamically favored, then because such an inclusion causes a pure shear field in the matrix while the shear stresses do not interact with the inclusion, the conclusions arrived at here are valid up to those stages of the transformation when the spacing between inclusions becomes comparable to their sizes. These structural states are often observed in experiment and are used in practice.

In comparing the conclusions obtained here about the thermodynamics of the transformation and equilibrium shape of the inclusion with the actual data, it is necessary to keep in mind the assumptions which are contained in the computational model, and which limit the sphere of its applicability. The first assumption, which prevents us from ob-

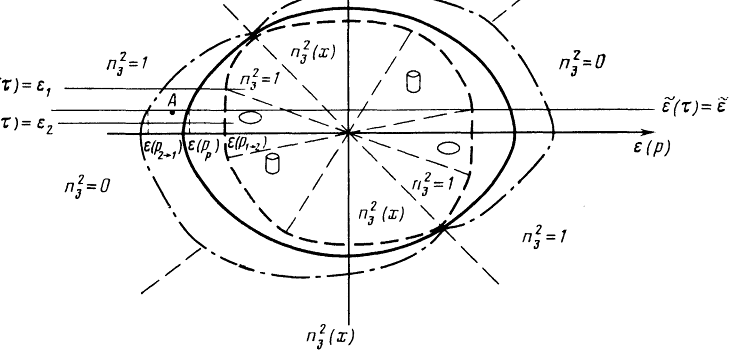

FIG. 7. Intersection of the phase equilibrium and phase transformation surfaces with the plane $T = $ const. Sectors corresponding to regions of stability of the various equilibrium shapes are marked.

taining an exact description of the transformation process, is that the phases are elastically isotropic. It is possible to show that the fundamental conclusions concerning the equilibrium inclusion remain valid when the anisotropy of the inclusion phase is included; however, we have not succeeded in estimating the role of anisotropy of the matrix. Apparently, in the case where the elastic anisotropy is not very large, the isotropic approximation gives a satisfactory description of real systems. Test of the continuum theory of defects persuasively confirm these intuitive considerations.

In addition to the assumptions about elastic isotropy, which, as with application of the linear theory of elasticity, basically affect the quantitative results of the theory, the computational model is based on a number of physical assumptions whose failure can qualitatively change the picture. It is assumed that in the heterophase system no processes occur which decrease the energy of the internal stresses except for shifts in the interphase boundary. Along with these processes there can be division of the phases into elastic domains, plastic deformation and redistribution of the order parameters or concentration. Let us discuss the possible roles of these processes in the thermodynamics of the transformation.

Elastic domains: in those cases when the phase transition is accompanied by lowering of the symmetry, the new phase appears at various oriented positions relative to the original phase, forming structural domains. These domains can also act as elastic domains, lowering the elastic interaction energy of the phase because of the variation of the mean intrinsic strain.[21] As a result, a polydomain phase forms in which the relative fraction of domains of various kinds is determined by the minimum of the free energy of the heterophase system. For an inclusion in a polydomain phase, the results we have obtained must be modified to take into account the fact that the mean intrinsic strain depends on the volume fractions of the various domains. However, in a number of cases the single-domain phase, of the sort we have assumed in our calculations, is selected out: first of all, if the phase transition is not accompanied by a lowering of symmetry; secondly, when the formation of domains leads to a decrease in the shear components in the intrinsic strain. Thus, if the dilatational components predominate in the intrinsic strain (in particular if the equilibrium shape of the single-domain inclusion is an ellipsoid) the division into domains must lead to an increase in the relative fraction of these components, and to an increase in the elastic energy. In this case, the formation of domains is not thermodynamically favored, and the structural domains cannot be elastic domains. Thirdly, separation into domains is connected with the appearance of additional stresses at the interphase boundary and with a cost in energy for the formation of domain boundaries. This leads to an increase in the effective surface energy of the interphase boundary. Correspondingly, the energy barrier grows for nucleating the polydomain phase; therefore, the beginning of the phase transformation is determined by the equilibrium of the matrix with a single-domain inclusion: the new phase nucleates in the single-domain state, and only enters into the polydomain state as a result of the growth process.

Plastic deformation: plastic deformation is a universal mechanism for lowering internal stresses. However, as with domain formation, it leads to an increase in the effective interphase surface energy. This makes removal of the elastic stresses by plastic deformation thermodynamically unfavorable for inclusions of small size. In addition, plastic deformation will be kinematically forbidden if the plastic yields of the phases are sufficiently high.

Redistribution of concentration and order parameter: in our calculations we assumed that the intrinsic strain is an invariant characteristic of the phase transition. However, by virtue of the homogeneity of the elastic field in the inclusion, it is not difficult to include a possible change in the order parameter or concentration within the inclusion, and to find the corresponding equilibrium values of these quantities along with the intrinsic strains corresponding to them.

It is more difficult to include a redistribution of the order parameters or concentrations in the matrix, where the elastic field is inhomogeneous. However, in many cases which are important for applications it is not necessary to do this. In particular, the shear field in the matrix does not result in redistribution of the centers of dilatation, which are usually assumed to be impurity atoms in a solid solution. If the symmetric phase serves as the matrix and the intrinsic strain depends quadratically on the order parameter, then in this case the matrix remains homogeneous since the elastic stresses do not affect the equilibrium zero value of the order parameter. Thus, the model investigated in this article allows us to give a thermodynamic description of a wide range of first-order phase transformations in solids.

[1)] The equilibrium equations obtained here agree with those of Refs. 2, 3; however, it should be noted that in various forms these equations have been obtained by several different authors (Refs. 5, 7–16). These authors paid no attention to the equivalence of the results they obtained in linear approximation.

[2)] In Ref. 20 the authors discussed only the dilatational components of $\hat{\varepsilon}$. Then the influence of shear reduces to quadratic corrections and is determined by the difference in elastic moduli of the phases.

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[1] A. L. Roitburd, Fiz. Tverd. Tela (Leningrad) **25**, 33 (1983) [Sov. Phys. Solid State **25**, 17 (1983)].

[2] A. L. Roitburd, Fiz. Tverd. Tela (Leningrad) **26**, 2025 (1984) [Sov. Phys. Solid State **26**, 1229 (1984)].

[3] A. L. Roitburd, Fiz. Tverd. Tela (Leningrad) **28**, 3051 (1986) [Sov. Phys. Solid State **28**, 1716 (1986)].

[4] A. G. Khachaturyan, Fiz. Tverd. Tela (Leningrad) **8**, 2709 (1966) [Sov. Phys. Solid State **8**, 2163 (1966)].

[5] A. L. Roitburd, Dokl. Akad. Nauk SSSR **197**, 1051 (1971) [Sov. Phys. Dokl. **16**, 305 (1971)].

[6] A. L. Roitburd and N. S. Kosenko, Phys. Status Solidi **A35**, 735 (1976).

[7] P. A. Privorotskii, Zh. Eksp. Teor. Fiz. **60**, 1525 (1971) [Sov. Phys. JETP]; Usp. Fiz. Nauk **108**, 43 (1972) [Sov. Phys. Usp. **15**, 555 (1973)].

[8] P. S. Zhitomirskii and I. N. Nechporenko, Fiz. Tverd. Tela (Leningrad) **19**, 859 (1977) [Sov. Phys. Solid State **19**, 498 (1977)].

[9] P. I. Robin, Am. Miner. **59**, 1286 (1974).

[10] F. C. Larche and J. W. Cahn, Acta Metall. **26**, 1579 (1978).

[11] F. C. Larche and J. W. Cahn, J. Res. Nat. Bur. Stand. **89**, 467 (1984).

[12] R. D. James, Archive for Rational Mechanics and Analysis **77**, 143 (1981); J. Mech. Phys. Solids **34**, 359 (1986).

[13] M. E. Gurtin, Archive for Rational Mechanics and Analysis **84**, 1 (1983).

[14] A. Grinfeld, Dokl. Akad. Nauk SSSR **251**, 824 (1980) [Sov. Phys. Dokl. Earth Sci. **251**, 11 (1982)]; Dokl. Akad. Nauk SSSR **258**, 567 (1981) [Sov. Phys. Dokl. Earth Sci. **258**, 13 (1983)]; Dokl. Akad. Nauk SSSR **265**, 836 (1982) [Sov. Phys. Dokl. Earth Sci. **265**, 21 (1984)].

[15] L. M. Truskinovskii, Geokhimiya (Geochemistry) **12**, 1730 (1983).

[16] W. C. Johnson and J. I. D. Alexander, J. Appl. Phys. **59**, 2735 (1986).

[17] J. D. Eshelby, Continuum Theory of Lattice Defects, Solid State Phys. **3**, 79 (1956).

[18] V. L. Berdichevskii, Dokl. Akad. Nauk SSSR **273**, 80 (1983) [Sov. Phys. Dokl. Earth Sci. **273**, 1 (1985)].

[19] V. M. Kardonskii and A. L. Roitburd, Fiz. Met. Metalloved. **33**, 662 (1972) [Phys. Met. Metallogr. (USSR) **33**, 210 (1972)].

[20] Yu. Ya. Boguslavskii, Fiz. Tverd. Tela (Leningrad) **27**, 140 (1985) [Sov. Phys. Solid State **27**, 81 (1985)].

[21] A. L. Roitburd, Usp. Fiz. Nauk **113**, 69 (1974) [Sov. Phys. Usp. **17**, 326 (1974)].

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