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DYNAMICS OF NON-EQUILIBRIUM PHASE BOUNDARIES IN A HEAT CONDUCTING NON-LINEARLY ELASTIC MEDIUM*

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The phase transformation of the first kind in a non-linearly elastic heat conducting medium is simulated by the relationships on a strong discontinuity. A generalization of the Stefan formulation is given. An existence condition for stationary flow, analogous to the Gibbs phase equilibrium condition, is obtained for non-equilibrium phase boundaries. A pure dilatational phase transition in a compressible fluid and pure shear transformation of the twinning type in non-linearly elastic crystals are considered as model examples. The problem of the structure is solved for closure of the system of relationships on the shock.

A phase transformation ordinarily turns out to be localized in a narrow domain of space and it can be simulated in terms of the conditions on a strong discontinuity /1/. Formulation of the problem of the static equilibrium of liquid phases as well as of liquid and (non-linearly elastic) solid phases was given by Gibbs, who proposed a phase equilibrium criterion and formulated appropriate conditions on the shock; the extension of the Gibbs conditions to the case of the equilibrium of two solid phases is known in both the linear /2/ and non-linear /3/ theories of elasticity. The dynamic problem of the propagation of the equilibrium phase boundary is considered in the Stefan formulation as a rule, including the assumption about the continuity of the density (the strain tensor component) on the shock; the thermal problem is here separated from the mechanical one. Simulating the interphasal surface on the shock the temperature fields are merged by using the well-known Stefan conditions as well as the phase equilibrium condition that reduces to giving the temperature on the front.

The purpose of this paper is to extend the Stefan-Gibbs formulation to the case of the motion of a coherent isothermal phase boundary in a non-linearly elastic heat conducting medium and to derive the dynamic analogue of the phase equilibrium condition (and the Stefan conditions) with possible dissipation at the transformation front. Two dissipative mechanisms are examined, viscous and kinetic. The case of equilibrium phase boundaries was investigated in /4-6/.

1. The model of a coherent phase boundary is based on the assumption of the continuity of the displacements at the front. Let $x^i = x^i(\xi^a)$ be the deformation law for the elastic body, x^i the Euler Cartesian coordinates of the observer, and ξ^a the Lagrange coordinates that are in agreement with the Euler coordinates in the reference state. The phase boundary coherence condition is written in the form

$$[x^i] = 0 \tag{1.1}$$

where, as usual, $[A] = A^+ - A^-$ is the difference between the limit values of the function on the sides of the surface of discontinuity.

The system of relationships on the phase boundary at rest includes together with the isothermal condition

$$[T] = 0 \tag{1.2}$$

the standard requirement of equality of the forces

$$[\partial f/\partial x_a^i]\, n_a^\circ = 0 \tag{1.3}$$

as well as the additional scalar phase equilibrium condition

$$[f] - \{\partial f/\partial x_a^i\}[x_a^i] = 0 \tag{1.4}$$

Here $f(x_a, T)$ is the free energy per unit mass $x_a^i = \partial x^i/\partial\xi^a$ is the distortion tensor, T is the temperature, n_a° is the vector of the unit normal to the phase boundary in the reference

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*Prikl.Matem.Mekhan.,51,6,1009-1019,1987 configuration, and the latter is assumed to be common for both phases $\{A\} = {}^1/_2\,(A^+ + A^-)$.

Conditions (1.1)-(1.4) enable the equilibrium two-phase configuration with unknown boundary to be determined. In the special case of the equilibrium of two liquid phases relationship (1.4) reduces to the conditions, known in thermodynamics, of the equality of the chemical potentials $[f + pV] = 0$, where V is the specific volume and $p = -\partial f/\partial V$ is the continuous pressure on the phase boundary by virtue of (1.3). The static equilibrium problem is formulated as a problem to seek a broken-line extremal of the free energy functional; consequently, it is easy to identify the classical Weierstrass-Erdmann conditions in (1.3)-(1.4). Ordinarily, the normal vector n_a° is included explicitly in the condition analogous to (1.4) (see /3, 7, 8/), however, the mode of writing used here for the relationships on the broken-line extremal is also well-known (see /9-11/, say).

To obtain the dynamic conditions at the phase jump we write the system of equations of motion of the heat conducting non-linearly elastic medium in Lagrange coordinates (in the absence of mass forces and thermal sources)

$$\rho^\circ \frac{\partial v_i}{\partial t} = \frac{\partial}{\partial \xi^a}\left(\rho^\circ \frac{\partial e}{\partial x_a{}^i}\right), \quad \rho^\circ \frac{\partial}{\partial t}\left(e + \frac{v^2}{2}\right) = \frac{\partial}{\partial \xi^a}\left(\rho^\circ \frac{\partial e}{\partial x_a{}^i}\, v^i\right) - \frac{\partial}{\partial \xi^a}\, q^{\circ a} \tag{1.5}$$

Here $e\;(x_a{}^i, s) = f + Ts$ is the internal energy per unit mass, $x^i\,(\xi^a, t)$ is the law of motion, s is the entropy density, $v^i = \partial x^i/\partial t$ is the velocity vector, $\rho^\circ\,(\xi^a)$ is the density in the reference configuration, and $q^{\circ a}$ is the heat flux vector.

We assume that the phases are characterized by a different kind of dependence of the function e on its arguments; sometimes it is possible to speak about one (non-convex) function defined on a non-simply-connected or even non-connected domain. The discontinuities $([x^i] = 0,\ [x_a{}^i] \neq 0,\ [s] \neq 0)$ of the solution of system (1.5) correspond to coherent two-phases states. The Hugoniot conditions

$$\left[\rho^\circ D^\circ v^i + \rho^\circ \frac{\partial e}{\partial x_a{}^i}\, n_a{}^\circ\right] = 0, \quad \left[\rho^\circ D^\circ \left(e + \frac{v^2}{2}\right) + \rho^\circ \frac{\partial e}{\partial x_a{}^i}\, v^i n_a{}^\circ\right] = [q^{\circ a} n_a{}^\circ] \tag{1.6}$$

should be satisfied at the jump, where D° is the velocity of the jump in the reference configuration, and surface effects are neglected. Taking account of possible energy dissipation at the jump due to viscosity, heat conduction, transformation non-equilibrium etc., the entropy balance condition can be represented in the form /1/

$$[\rho^\circ D^\circ s] = [q^{\circ a} n_a{}^\circ/T] + \mathbf{R}^\circ \tag{1.7}$$

where $\mathbf{R}^\circ$ is the entropy production per unit surface area of the discontinuity in the reference configuration.

Following Stefan, and assuming that the time of heat transfer within the transformation front is much less than the time to heat a domain with the characteristic linear dimension of the external problem, we consider the temperature at the jump to be continuous (see (1.2)). It can be shown that relationships (1.2) and (1.6) turn out to be insufficient to determine the parameters behind the jump and the jump velocity by means of the state ahead of the jump. If the jump is evolutionary, a single discontinuous solution can sometimes be constructed by using the relationship (1.7), which is formulated as the inequality $\mathbf{R}^\circ \geqslant 0$. To determine the velocity of the front in the case of subsonic motion under consideration, it is necessary to have an additional relationship at the discontinuity, for instance (as is done in deflagration wave theory), the shock velocity D° or the dissipation $\mathbf{R}^\circ T$ can be given explicitly.

Assuming that $\mathbf{R}^\circ$ is a known function of the flow parameters, we obtain a relation, an analogue of (1.4), from (1.2), (1.6) and (1.7). Let us use the Hadamard compatibility conditions

$$[x_a{}^i] = \lambda^i n_a{}^\circ, \quad [v^i] = -\lambda^i D^\circ \tag{1.8}$$

which are corollaries of (1.1) and we eliminate the expression $[q^{\circ a} n_a{}^\circ]$ from (1.6) and (1.7). After reduction, we obtain

$$\rho^\circ D^\circ\,(([f] - (\partial f/\partial x_a{}^i)_\pm\,[x_a{}^i]) \mp {}^1/_2\,[v_i]\,[v^i]) = -\mathbf{R}^\circ T \tag{1.9}$$

This condition can obviously be rewritten in the form

$$\rho^\circ D^\circ\,([f] - \{\partial f/\partial x_a{}^i\}\,[x_a{}^i]) = -\mathbf{R}^\circ T \tag{1.10}$$

Relationship (1.10) is the desired extension of (1.4). We note that in the case of equilibrium (non-dissipative) phase jumps, the static condition (1.4) and the dynamic condition (1.10) are in identical agreement.

We assume that the points $x_a{}^{i+}$ and $x_a{}^{i-}$ can be connected smoothly in the space of the tensors $x_a{}^{i\cdot}$, lying entirely in the domain of definition of the function $f\,(x_a{}^i, T)$. Then transforming the left side of (1.10), we obtain

$$\tfrac{1}{2}\rho^\circ D^\circ \left(\int_{x_a^{i-}}^{x_a^{i+}} \left(\frac{\partial f}{\partial x_a{}^i} - \frac{\partial f}{\partial x_a{}^i}\bigg|_+ \right) dx_a{}^i + \int_{x_a^{i-}}^{x_a^{i+}} \left(\frac{\partial f}{\partial x_a{}^i} - \frac{\partial f}{\partial x_a{}^i}\bigg|_- \right) dx_a{}^i \right) = -\mathbf{R}^\circ T \tag{1.11}$$

For non-dissipative phase shocks in a liquid medium condition (1.11) yields the generalized "Maxwell area rule" /12/

$$\int_{V-}^{V+} (p - p_+)\, dV + \int_{V-}^{V+} (p - p_-)\, dV = 0 \tag{1.12}$$

The energy balance condition at the shock can be obtained in the form

$$\rho^\circ D^\circ (T\,[s] + ([f] - \{\partial f/\partial x_a{}^i\}\,[x_a{}^i])) = [q^{\circ a} n_a{}^\circ] \tag{1.13}$$

by using (1.6), (1.7) and (1.10).

It differs from the classical Stefan condition by the fact that the thermal effect of the transformation is computed taking the heat dissipated into account.

To close the system of relationships on the phase shock, it is necessary to determine the quantity $\mathbf{R}^\circ$ by relying on additional information about the non-equilibrium processes in the interphasal domain and by solving the problem of the structure of the discontinuity. In certain cases phenomenological models containing empirically determined parameters can be utilized.

By definition we introduce $[\mu] \equiv [f] - \{\partial f/\partial x_a{}^i\}\,[x_a{}^i]$ and we note that the expression $m_0 = -\rho^\circ D^\circ$ yields the mass flux across the phase boundary. Then condition (1.10) can be rewritten in the form $m_0\,[\mu] = \mathbf{R}^\circ T$. This relationship recalls the formula for the volume dissipation in a homogeneous chemically reacting mixture (monomolecular reaction); the vanishing of the "thermodynamic force" corresponds to the equilibrium state: $[\mu] = 0$. In the limit, the weak non-equilibrium of the "flux" and the "force" can be connected by the linear relationship

$$m_0 = \gamma_0^{-1}\,[\mu],\quad T\mathbf{R}^\circ = \gamma_0^{-1}\,[\mu]^2 = \gamma_0 m_0{}^2$$

The problem of investigating the structure reduces to determining the single parameter γ_0 in this approximation. A theory of the "normal" growth of crystals from a supercooled melt and a Hertz-Knudsen theory of non-equilibrium condensation are constructed according to the principle mentioned.

2. The passage from (1.10) to (1.4) for equilibrium phase boundaries is made under the assumption of a non-zero mass flux through the surface; consequently, the static equilibrium conditions found in this manner require additional foundation. To clarify this question we give an independent variational deduction of the conditions of the phase jump, while also keeping in mind a possible extension to the case of non-coherent transformations. This enables a natural tensor representation of the relationship (1.10) to be obtained.

To simplify the discussion and avoid unimportant details, we will confine ourselves to considering the isothermal problem by assuming $T \equiv T_0$ and neglecting dissipation. It is convenient to perform the subsequent analysis in four-dimensional form by supplementing the three Lagrange space coordinates ξ^a $(a = 1, 2, 3)$ by a fourth, the time $\xi^4 = t$. We denote the coordinates in R^4 by Greek letters $(\alpha, \beta = 1, 2, 3, 4)$ and in R^3 by Latin letters.

The equations of motion and boundary conditions on the transformation front can be obtained by using the Hamilton variational principle /1, 9/

$$\delta \int_{V^4} \Lambda^\circ (x_a{}^i, x^i, \xi^\alpha, T_0)\, d^4\xi = 0,\quad \Lambda^\circ = \rho^\circ (v^2/2 - f) \tag{2.1}$$

We will assume that $V_3(t)$ is a three-dimensional volume occupied by the medium in the reference configuration, ∂V_3 is its external surface, and V_4 is the four-dimensional volume formed by the locations of V_3 at different times $t \in (t_1, t_2)$. Let there be a two-dimensional strong surface of discontinuity $\Sigma_2(t)$ within the volume V_3 which moves over particles of substance forming a three-dimensional surface $\Sigma_3 \subset V_4$ in R^4. The position of the surface Σ_3 can be given by a set of functions $\bar{\xi}^a = \bar{\xi}^a(u^A, t), \bar{t} = t$ where u^A are coordinates in Σ_2 and $A = 1, 2$.

We consider variations of the law of motion of particles of the medium $\delta x^i = x^{i'}(\xi^a, t) - x^i(\xi^a, t)$ as well as variations of the position of the surface of strong discontinuity over the particles $\delta\bar{\xi}^\alpha = \bar{\xi}^{\alpha'}(u^A, t) - \bar{\xi}^\alpha(u^A, t)$. Setting all variations in ∂V_3 equal to zero and carrying out standard reduction /4, 9/, we obtain from (2.1)

$$\int_{V_4^+ \cup V_4^-} \frac{\delta\Lambda^\circ}{\delta x^i}\,\delta x^i\, d^4\xi + \int_{\Sigma_3} \left[\frac{\partial\Lambda^\circ}{\partial x_a{}^i}\,\Delta x^i + \left(\Lambda^\circ \delta_\beta{}^\alpha - \frac{\partial\Lambda^\circ}{\partial x_\alpha{}^i}\, x_\beta{}^i \right) \delta\bar{\xi}^\beta \right] \times n_\alpha{}^\circ\, d\sigma^\circ = 0 \tag{2.2}$$

$$\delta/\delta x^i = \partial/\partial x^i - (\partial/\partial\xi^\alpha)\,(\partial/\partial x_\alpha{}^i)$$
$$\Delta x^i = \delta x^i + x_\beta{}^i\delta\bar{\xi}^\beta$$

where $\delta/\delta x^i$ is the variational derivative, $n_\alpha{}^\circ$ is the unit 4-vector normal to Σ_3, $d\sigma^\circ$ is the invariant surface element in the reference configuration, and Δx^i are the total variations of coordinates of the surface. To take account of dissipation it is necessary to transfer from the variational principle (2.1) to the Sedov variational equation /1/ by adding the non-holonomic term

$$\delta W^* = \int\limits_{\Sigma_3} \mathbf{R}^\circ T_0 \delta\bar{\xi}^\alpha n_\alpha{}^\circ\, d\sigma^\circ$$

to (2.1).

Equating the coefficients of the volume variations δx^i in (2.2) to zero, we obtain the first of Eqs.(1.5). The energy equation is replaced by the isothermal condition. Because of the independence of the variations Δx^i and $\delta\bar{\xi}^\alpha$ on Σ_3 we have

$$\left[\frac{\partial\Lambda^\circ}{\partial x_a{}^i}\Delta x^i\right] n_\alpha{}^\circ = 0, \quad [(\Lambda^\circ\delta_\beta{}^\alpha - (\partial\Lambda^\circ/\partial x_\alpha{}^i)\, x_\beta{}^i)\,\delta\bar{\xi}^\beta]\, n_\alpha{}^\circ = 0 \tag{2.3}$$

For coherent boundaries $[\Delta x^i] = 0,\ [\delta\bar{\xi}^\beta] = 0$ consequently

$$[\partial\Lambda^\circ/\partial x_\alpha{}^i]\, n_\alpha{}^\circ = 0 \tag{2.4}$$
$$[\Lambda^\circ\delta_\beta{}^\alpha - (\partial\Lambda^\circ/\partial x_\alpha{}^i)\, x_\beta{}^i]\, n_\alpha{}^\circ = 0 \tag{2.5}$$

It is easy to recognize the first group of Hugoniot relations (1.6) that ensure continuity of the momentum flux ($n_4{}^\circ = -D^\circ$) in the three conditions (2.4). The expression in the square brackets in (2.5) taken with the opposite sign is called the energy-momentum tensor; its spatial part

$$T_b{}^a = \rho^\circ\,(f\delta_b{}^a - (\partial f/\partial x_a{}^i)\, x_b{}^i)$$

is known in the theory of elastic defects as the Eshelby tensor /13/. For coherent phase boundaries only one of the four relationships (2.5) is independent by virtue of the compatibility conditions $[x_\alpha{}^i] = \lambda^i n_\alpha{}^\circ$ and it can be written thus, for instance (compare /6/):

$$[\Lambda^\circ] - \{\partial\Lambda^\circ/\partial x_\alpha{}^i\}\, [x_\alpha{}^i] = 0 \tag{2.6}$$

Projecting (2.5) on the time axis ($\beta = 4$), we obtain condition (1.9). The difficulties noted above for deriving the static conditions from the dynamic conditions are associated with the fact that the projection on the ξ^4 axis is a degenerate operation in statics.

The spatial projection of (2.5) by using the Eshelby tensor can be written in the static case in the form

$$[T_b{}^a]\, n_a{}^\circ n^{\circ b} = 0 \tag{2.7}$$

In connection with the fact that relationship (2.7) is an extension of the condition of equality of the liquid phase chemical potentials, the tensor $T_b{}^a$ is sometimes called the chemical potential tensor /7/.

Using the known dualism between the Eshelby tensor and the Cauchy stress tensor /14/, the equations of motion can be rewritten in terms of $T_b{}^a$. Thus, for $\rho^\circ = \mathrm{const}$ we obtain the relationships $\rho^\circ\partial v_b/\partial t = \partial T_b{}^a/\partial\xi^a$ which are corollaries of the equations of motion (the Noether identity), here $v_b = v_i x_b{}^i$.

We note a case that is important for the sequel, when the utilization of these relationships simplify the investigation. Let $f = \bar{f}\,(\rho, \partial\rho/\partial x^i, T_0)$, $\rho = \rho^\circ/\det\|x_a{}^i\|$ then the Cauchy tensor, which is not spherical in the general case, has the form

$$P_i{}^k = \left(-\rho^2\frac{\partial\bar{f}}{\partial\rho} + \rho\frac{\partial\bar{f}}{\partial\rho_{,j}}\rho_{,j} + \rho^2\left(\frac{\partial\bar{f}}{\partial\rho_{,j}}\right)_{,j}\right)\delta_i{}^k - \rho\frac{\partial\bar{f}}{\partial\rho_{,k}}\rho_{,i} \tag{2.8}$$

(the comma before the subscript denotes differentiation). At the same time the Eshelby tensor

$$T_b{}^a = \rho^\circ\left(\bar{f} + \rho\frac{\partial\bar{f}}{\partial\rho} - \frac{\partial\bar{f}}{\partial\rho_{,i}}\rho_{,i} - \rho\left(\frac{\partial\bar{f}}{\partial\rho_{,i}}\right)_{,i}\right)\delta_b{}^a$$

turns out to be spherical, and consequently, the equilibrium equations can be integrated once /15/.

To construct models of non-coherent boundaries it is necessary to turn to (2.3) and to formulate the appropriate constraints on the variations $\Delta x^{i\pm}$, $\delta\bar{\xi}^{\beta\pm}$ /7, 8, 16/.

3. The simplest example of applications of the results obtained above is phase transition

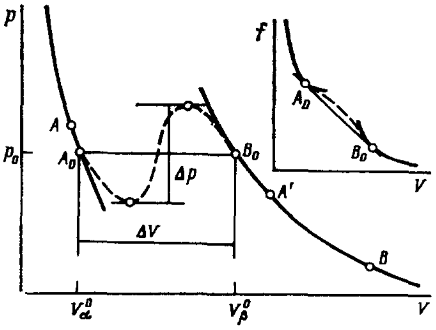

Fig.1

in a liquid. In this case the free energy depends on the single deformation characteristic that enables us to make the form of this function specific, to construct the structure of the isothermal phase shock, and to evaluate the dissipation due to viscous friction /5/.

We can write the equations of isothermal compressible fluid flows $(T \equiv T_0)$ in the form of plane waves

$$\frac{\partial \rho}{\partial t} + \rho\frac{\partial v}{\partial x} + v\frac{\partial \rho}{\partial x} = 0, \quad \rho\frac{\partial v}{\partial t} + \rho v\frac{\partial v}{\partial x} + \frac{\partial p}{\partial x} = 0 \tag{3.1}$$

The corresponding Hugoniot conditions have the form

$$[\rho(D - v)] = 0, \quad [\rho(D - v)^2 + p] = 0 \tag{3.2}$$

where D is the jump velocity in the observer's coordinate system. For a liquid undergoing a phase transition the function $f(V, T_0)$ has two branches corresponding to different phases.

The classical discontinuous solutions of (3.1) with a jump of the type $B - A'$ (shock waves, Fig.1) satisfy the conditions of the Zemplen theorem and are adetermined uniquely by relationships (3.2). Jumps of the type $B - A$ do not satisfy the evolutionarity condition

$$\left.\frac{\partial p}{\partial V}\right|_A \leqslant \frac{p(A) - p(B)}{V(A) - V(B)} \leqslant \left.\frac{\partial p}{\partial V}\right|_B$$

Consequently, relationship (3.2) turns out to be inadequate for constructing the discontinuous solution. In the case of equilibrium phase jumps $(\mathbf{R} = 0)$ the additional condition (1.10) can be written in the form

$$[f + p/\rho + {}^1/_2(D - v)^2] = 0$$

If the dissipation is different from zero, it is necessary to turn to the problem of the structure of a discontinuity to evaluate it.

A unique equation of state $f(V, T_0)$ in the range of values of V corresponding to the interphasal zone is required to obtain continuous solutions. The simplest model of an "equilibrium mixture" assumes the construction of the maximum convex continuation for f and reduces to determining the points A_0 and B_0 on the graph of $f(V, T_0)$ by using the relationships $[\partial f/\partial V] = 0$, $[f - V\partial f/\partial V] = 0$ (the Gibbs conditions), which are then connected by a line segment. Taking account of surface effects in the heterophasal domain results in a nonconvex (Fig.1) continuation of f /17/. Van der Waals proposed taking account of non-local terms in the equation of state by setting

$$\bar{f}(\rho, \nabla\rho, T) = f(\rho, T) + \varepsilon(\nabla\rho)^2 \tag{3.3}$$

in order to "suppress" the thermodynamic instability of the material in a domain with $\partial^2 f/\partial V^2 < 0$. Here $\varepsilon > 0$ is a function of the density and temperature that can be considered as a small parameter after reduction to dimensionless form. A medium with inhomogeneities can be a realistic physical model of a heterophase mixture; the disperion relationships corresponding to (3.3) for a medium with periodically located phase inclusions can be obtained by the methods from /18/.

We consider the solutions of (3.1) of the form $\rho(\xi)$, $v(\xi)$ where $\xi = x - Dt$ with the boundary conditions $\rho(\pm\infty) = \rho_{\beta,\alpha}$, $v(\pm\infty) = v_{\beta,\alpha}$ which models the jump structure. Taking into account the non-local components in the expression for the stress tensor (2.8) as well as the viscous stresses, we obtain after integration

$$\begin{gathered} \rho u = m_0, \quad u = v - D \\ p - \rho^2\frac{\partial\varepsilon}{\partial\rho}\left(\frac{\partial\rho}{d\xi}\right)^2 - 2\varepsilon\rho^2\frac{d^2\rho}{d\xi^2} - \eta\frac{du}{d\xi} + \rho u^2 = \pi_0 \end{gathered} \tag{3.4}$$

where η is the viscosity coefficient, m_0 and π_0 are constants of integration. Eliminating $u(\xi)$ from (3.4) and introducing the notation $y(\rho) = d\rho/d\xi$ we arrive at a boundary value problem for a first-order equation /5, 12, 19/

$$\begin{gathered} d(\varepsilon y^2 - \mu)/d\rho = m_0\eta y/\rho^4, \quad y(\rho_\alpha) = y(\rho_\beta) = 0 \\ \mu = f(\rho, T_0) - {}^1/_2 m_0^2/\rho^2 + \pi_0/\rho \end{gathered} \tag{3.5}$$

where $\rho_{\alpha,\beta}$ are two neighbours of the point $\min\mu(\rho)$.

The boundary value problem (3.5) has a solution only for special values of the parameters;

the corresponding relation $m_0(\pi_0, T_0)$ merely enables us to determine its velocity by means of the state in front of the shock. The necessary condition for the solution (3.5) to exist

$$m_0(\mu(\rho_\alpha) - \mu(\rho_\beta)) = \eta m_0^2 \int\limits_{\rho_\alpha}^{\rho_\beta} \frac{y(\rho)}{\rho^4} d\rho \tag{3.6}$$

agrees with (1.10), where the dissipation $\mathbf{R}T_0$, equal to the right-hand side of (3.6), can be calculated explicitly by means of the known function $y(\rho)$.

Questions of the existence and uniqueness of the solution of the boundary value problem (3.5) are examined in /12, 19/.

Let us approximate the function $p(V, T_0)$ by a cubic parabola. We assume that the Maxwell pressure $p_0(T_0)$ is known as are the specific volumes of the phases $V_\alpha^\circ < V_\beta^\circ$ in equilibrium with those which exist for $T = T_0$ and $p = p_0$. The isotherm $p = p_0 - k(V - V_\alpha^\circ)(V - V_\beta^\circ)\cdot(V - {}^1/_2(V_\alpha^\circ + V_\beta^\circ))$ is determined by this apart from a constant $k = 6\sqrt{3}\Delta p/\Delta V^3$, $\Delta V = V_\beta^\circ - V_\alpha^\circ$ that characterizes the attainable degree of metastability Δp (Fig.1). In the case of non-dissipative transformations $(\eta \equiv 0, \mu(\rho_\alpha^e) = \mu(\rho_\beta^e))$ we obtain $V_\alpha^e + V_\beta^e = V_\alpha^\circ + V_\beta^\circ$ which enables us to determine the state beind the jump $(V_\alpha^e;\ v_\alpha = D(2V_\delta^e - V_\alpha^\circ - V_\beta^\circ)$ and also the state velocity by means of the state ahead of the jump $(V_\beta^e;\ v_\beta = 0)$ $D^2 = k(V_\beta^e)^2(V_\beta^\circ - V_\beta^e)(V_\alpha^\circ - V_\beta^e)$. If $\eta \neq 0$, it is necessary to solve Eq.(3.5) numerically; however, the problem has an analytic solution

$$V(\xi) = \frac{V_\alpha + V_\beta}{2} + \frac{V_\alpha - V_\beta}{2} \operatorname{th}\left(\frac{\sqrt{k}(V_\alpha - V_\beta)}{4\sqrt{\varepsilon_0}}(\xi - \xi_0)\right)$$

in the case $\varepsilon = \varepsilon_0/\rho^4$, $\varepsilon_0 = \text{const}$

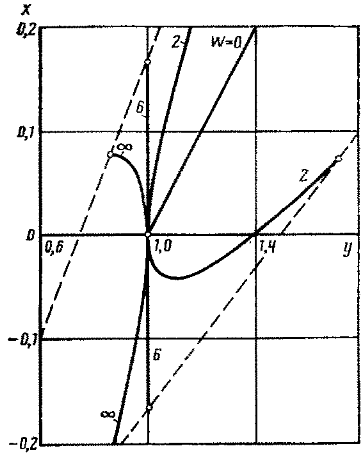

Fig.2

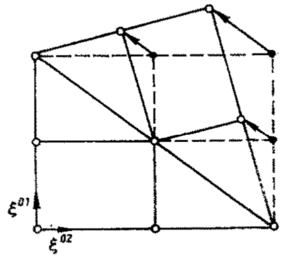

Fig.3

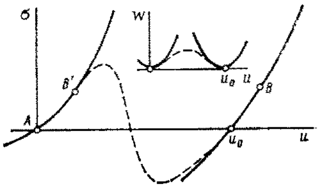

Fig.4

This solution can be regarded as approximate for other dependences $\varepsilon(\rho)$; its validity near the liquid-vapour critical point is noted in /20/.

The relation between the parameters before and after the shock is given by a second-order equation

$$3(1 - 6/\mathbf{W})(2x - y + 1)^2 + y^2 = 1,\ \mathbf{W} = {}^1/_2\eta^2/\varepsilon_0$$
$$x = (V_\beta^\circ - V_\beta)/\Delta V,\ y = (V_\beta - V_\alpha)/\Delta V$$

The dependence $x(y)$ is represented in Fig.2 for different values of the dimensionless parameter W; the Jouguet regimes correspond to the dashed lines /12/. For $2x - y + 1 \geqslant 0$ we have phase rarefactions jumps, and for $2x - y + 1 \leqslant 0$ compression jumps; for sufficiently small W two-flow modes with a compression jump are possible, a fast and a slow one (Fig.2).

The calculation of the dissipation at the jump according to (3.6) yields

$$\mathbf{R}T_0 = \gamma m_0^2(1 + a m_0)^3 \tag{3.7}$$
$$\gamma = \frac{\sqrt{2k\mathbf{W}}}{12}(\Delta V)^3(1 + 2x)^3,\quad a = -\frac{\sqrt{2\mathbf{W}/k}}{6(1 + 2x)\Delta V}$$

We turn our attention to the fact that although a linear model of dissipation (Newtonian viscosity) was used in the equations of the structure, a linear relationship between the thermodynamic force and the flux on the phase boundary is conserved only in the limit $m_0 \to 0$, in which case $\gamma \to \gamma_0$, where $\gamma_0^2 = (\sqrt{3}/12)\, W \Delta p\, (\Delta V)^3$.

4. Twinning in elastic crystalline substances, which generally occurs without a change in volume /21/, can serve as an alternative to the phase transition in the liquid phase; as an example we consider the very special case of twinning in tetragonal crystals.

We assume that the Lagrange coordinate axes $\xi^{\circ a}$ $(a = 1, 2, 3)$ are superposed on the crystal axes of symmetry. We use the notation: a, b, b are parameters of the elementary cell and we rotate the system of coordinates through the angle $\varphi = \mathrm{arctg}\,(b/a)$ in the $\xi^{\circ 1}$, $\xi^{\circ 2}$ plane by going over to a new material system ξ^1, ξ^2, ξ^3 (Fig.3). We consider shear deformations of the form

$$x^1 = \xi^1,\quad x^2 = u\xi^1 + \xi^2,\quad x^3 = \xi^3 \tag{4.1}$$

and we denote the free energy per unit volume of the crystal in this class of isochoric deformations with parameter u by $W(u) = \rho^\circ f\,(x_a^{\,i}, T_0)$.

It can be seen from Fig.3 that the function $W(u)$ has two minima corresponding to mirror-symmetric twins. This is the undeformed state with $u = 0$ and the simple shear state with $u_0 = 2\,(b^2 - a^2)/ab$. In the absence of external stresses piecewise-homogeneous (twinned) equilibrium configurations of the type displaced in Fig.3 are obviously possible.

We write the equations of isothermal motions in the form of plane waves $(u^i = u^i\,(\xi^1, t))$ of the non-linearly elastic medium under consideration

$$\rho^\circ \partial v^i/\partial t = \partial \sigma^{i1}/\partial \xi^1 \tag{4.2}$$

where $u^i = x^i - \xi^i$ is the displacement vector, $v^i = \partial x^i/\partial t$ is the velocity vector, and $\sigma^{i1} = \partial W/\partial\,(\partial x^i/\partial \xi^1)$ are the non-zero Piola-Kirchhoff stress tensor components.

The Hugoniot condition and compatibility relationships at the phase jump have the form

$$[\rho^\circ D^\circ v^i + \sigma^{i1}] = 0,\quad [v^i + D^\circ\,(\partial x^i/\partial \xi^1)] = 0 \tag{4.3}$$

The superscript i takes the single value $(i = 2)$ for the class of deformations (4.1) under consideration; consequently we will omit it henceforth. The evolutionarity conditions

$$\left.\frac{\partial \sigma}{\partial u}\right|_A \leqslant \frac{\sigma(B) - \sigma(A)}{u(B) - u(A)} \leqslant \left.\frac{\partial \sigma}{\partial u}\right|_B$$

are satisfied for ordinary shock waves of the type $A - B'$ but are not satisfied for phase jumps of the type $A - B$ (Fig.4). Condition (1.10) obtained above and which is written in the form

$$D^\circ([W] - \{\sigma\}\,[u]) = -\mathrm{R}^\circ T_0 \tag{4.4}$$

can be used as the additional condition on the shock.

In statics we have the equilibrium solution $u^+ = 0$, $u^- = u_0$, $\sigma^\pm = 0$.

According to (4.4), motion of the twinning boundary over the unperturbed background $(u^+ = 0,\ \sigma^+ = 0)$ is possible only when there is dissipation at the front, and is ensured by a homogeneous shear stress $(\sigma^- = \sigma_0)$ behind the jump. Therefore, (4.4) sets up a correspondence between the velocity of the twinning boundary motion and the applied stress for a known expression for R°, and can be used to determine the plastic flow law due to twinning, and to investigate the dynamics of the deformation of materials with a shape memory (pseudo-elasticity /22/).

To determine the dissipation, the problem of the structure of the discontinuity must be solved by using complicated equation of state and rheological relationships. The structure of the equilibrium twinning boundary can be constructed if, by following the analogy with the liquid case, energy of the form $\overline{W} = W(u) + \varepsilon\,(\nabla u)^2$ /23/ is considered. The question of the dissipation mechanism during twinning is substantially more complex, however, and a detailed micro-model of the displacement process for the twin boundary must be relied upon for its solution.

Let us present the simplest phenomenological scheme that enables the non-equilibrium of the transformation to be taken into account in the case of quasistatic processes when it can be assumed that $[\sigma] \cong 0$. We assume that the phase states are characterized by different values of a certain internal parameter η, while the Gibbs free energy per unit mass is written in the form $g\,(\eta, \nabla\eta, T, \sigma) = \overline{W} - \sigma u$. We consider the medium to be at rest and the density to be constant.

Relaxation of the internal parameter η can be described within the framework of the Ginzburg-Landau phenomenological model by using the kinetic equation /24/: $\partial\eta/\partial t = -\Gamma\delta g/\delta\eta$ where $\delta/\delta\eta$ is the variational derivative. In the isothermal case $(T \equiv T_0)$ soliton solutions exist for this equation, which depend on $\xi = x - Dt$ and describe the structure of the phase jump - the discontinuity of the variable η. Dissipation due to non-equilibrium of the transformation will obviously be proportional to the quantity /25/

$$\int_{-\infty}^{\infty} (d\eta/d\xi)^2\, d\xi$$

For instance, let $\eta = (u - u_2)/(u_1 - u_2)$, where $u_{1,2}(\sigma_0)$ are the roots of the equation $\sigma_0 = \partial W/\partial u$. We set

$$\bar{g}/g_0 = g(\eta, \sigma_0, T_0) + \varepsilon(\nabla\eta)^2, \quad \partial g/\partial\eta = \eta(\eta - 1)(\eta - \eta_0).$$

The parameter η_0 depends on the external shear stress σ_0. For $0 < \eta < 1/2$ the kinetic equation has an analytic solution of the desired form

$$\eta = (1 + \exp(\xi - \xi_0)/(2\sqrt{\varepsilon}))^{-1}$$

The wave velocity $D = -m_0/\rho_0$ is given by $D = (1 - 2\eta_0)g_0\Gamma\sqrt{\varepsilon}$. For dissipation at the jump we have

$$RT_0 = \gamma_0 m_0^2, \quad \gamma_0^{-1} = 3\rho_0^2\Gamma\sqrt{\varepsilon}$$

Therefore, for small m_0 we again arrive at a quadratic expression in the flux for the rate of entropy production. As in the case of viscous phase jumps in a compressible fluid, analysis of the structure of the discontinuity enables us to find the value of the phenomenological coefficient γ_0.

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