INERTIAL EFFECTS IN THE DYNAMICS OF MARTENSITIC PHASE BOUNDARIES

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ABSTRACT

Localized phase transitions, as well as shock waves, can be modeled by material discontinuities satisfying appropriate jump conditions. One can show that the classical system of Rankine-Hugoniot jump conditions is incomplete in the case of subsonic phase boundaries. The supplementary condition which generalizes the condition of phase equilibrium, can be obtained from the traveling wave solution of the truly dynamic system of equations describing the interface structure.

1. INTRODUCTION

There is a long history of studies of highly localized "switching" waves in continuum mechanics; shock waves and combustion waves are among the most well known. Dynamic phase changes (condensation and liquefaction shocks, crystallization fronts, moving domain, martensitic, antiphase and twin boundaries, etc.) are similar to both shocks and flames; in all these cases, one homogeneous state gains at the expense of the other through the spatial advance of a transitional region. At a scale which is much larger than the width of the transition zone, these processes can be described by the motion of the surface of discontinuity. On this surface material parameters experience abrupt changes, so that modeling is possible in terms of corresponding *jump conditions*.

The use of Maxwell, Gibbs-Thompson, Hertz-Knudsen, and similar (supplementary to Rankine-Hugoniot) relations in the theory of dynamic phase changes suggest that the classical system of jump conditions being satisfactory for shocks is at least incomplete in the case of phase transitions [1]. We revisit the problem by considering a simple model of the internal structure of the fast moving *martensitic phase boundary* (see also [2, 3]). Our extended model of continuum, capable of describing a "thick" interface, incorporates a weak form of *nonlocality* together with a Maxwell type dissipative mechanism which simulates *interphase kinetics*. Analysis of a model-type solution of the structure problem clarifies the distinction between supersonic (*shock*) and subsonic (*kink*) discontinuities and provides explicit example of additional jump relation, different from the "normal growth" condition. An interesting prediction based on a smooth interface theory is the existence of a slow and a fast phase boundaries for a given state far ahead. This prediction is possibly related to the observations of "schiebung" and "umklapp" martensite [4].

2. JUMP CONDITIONS

Consider the classical Rankine-Hugoniot (RH) jump conditions on a moving surface of discontinuity in a heat-conducting thermoelastic body. Assume that eulerian cartesian coordinates are used and the moving interface is characterized by its normal vector $\mathbf{n}$ and its material velocity D (mass flux). Introduce: e-specific internal energy, $\mathbf{v}$-velocity vector, $\mathbf{P}$-Cauchy stress tensor and $\mathbf{q}$-heat flux vector. The balances of mass, momentum and energy on the jump take the form

$$D[\mathrm{v}] - [\mathbf{P}\mathbf{n}] = 0,\ D\left[e + \frac{\mathbf{v}^2}{2}\right] - [\mathbf{P}\mathbf{n}\cdot\mathbf{v} - \mathbf{q}\cdot\mathbf{n}] = 0, \tag{1}$$

where the square brackets denote a jump: [ ] : =($)_+$ - ($)_-$ and $\mathbf{n}$ faces the side +. Zeroes on the right hand sides of (1) indicate that we omit surface supplies of mass, momentum and energy; in particular, we ignore surface tension. We may not however, ordinarily ignore the surface entropy production $\Re = D[s] + \left[\frac{\mathbf{q}\cdot\mathbf{n}}{T}\right]$, where s and T are specific entropy and absolute temperature. According to the second law of thermodynamics, $\Re \geq 0$, which yields an inequality-type restriction on the possible jumps in the case of supersonic waves (shocks), and provides restrictions on the constitutive structure for the surface entropy production $\Re$ in the case of subsonic waves (kinks) [5, 6, 7]. Thus, a natural assumption

$$\Re = \Re(D), \tag{2}$$

offers an additional jump condition, which does not follow from (1) (kinetic relation).

One can show that (2) generalizes the classical Maxwell-Gibbs condition of phase equilibrium, which says $\Re = 0$. To represent it in more familiar terms, let us specify the model by taking a hyperelastic body with the energy $e = e(\mathbf{F}, s)$, where $\mathbf{F}$ is a deformation gradient. Then $T = \partial e/\partial s$, $\mathbf{P} = \rho(\partial e/\partial \mathbf{F})\mathbf{F}^T$. If both temperature and displacement are continuous on the jump, (1,2) yields [5, 6, 8, 9]

$$\Re T = D\left([f] - \left\{\frac{\partial f}{\partial \mathbf{F}}\right\}\cdot[\mathbf{F}]\right) \equiv DG.$$

Here, $f = e - Ts$ is a specific free energy and { } := $\frac{1}{2}$ (($)_+$+($)_-$). Assuming $\Re$ to be quadratic in D, theories of "normal growth" provide a linear relation between "thermodynamic force" G and the "flux" D. For a nondissipative process ($\Re = 0$), one obtains the dynamic generalization of the Maxwell ("equal area") condition G=0, which for stationary fluids further reduces to the classical Gibbs' equality of chemical potentials. The main problem for the truly dynamical theory of the interphase structure is the actual calculation of the function $G = G(D)$, when D is not small [7, 8].

3. INTERPHASE STRUCTURE

To be specific, consider an isothermal one dimensional simple shear motion of an elastic solid: $x = x_o$, $y = y_o + y(x,t)$, $z = z_o$. The governing equations in the absence of body forces are $u_t - v_x = 0$, $v_t - \tau_x = 0$ where $v = y(x,t)_t$ is a velocity, $u = y(x,t)_x$ is the only nontrivial component of the deformation gradient $\mathbf{F}$, and $\tau(u)$ denotes the corresponding component of the Piola stress tensor (sub-index denotes a partial derivative with respect to the corresponding variable, reference density is unity). The RH conditions take the form $D[u] + [v] = 0$, $D[v] + [\tau] = 0$, where $D = x^*(t)_t$ is the interphase velocity.

In order to smooth out sharp discontinuities, one is motivated to consider a regularized theory which includes the original model as a limiting case. There seem to be two known ways for the system to cope with the (nonlinearity driven) profile steepening, by dispersion and dissipation. Such a regularization can be accomplished by the introduction of nonlocal and memory effects. Usually that means a singular perturbation of an original system by terms with higher derivatives, which results in a formation of internal boundary layers simulating the discontinuity structure. In the classical theory of shock waves, the introduction of viscous dissipation is known to be sufficient to build a structure. This is not always the case in the theory of phase boundaries, because they may be nondissipative. Therefore, pure dispersive contributions to constitutive relations appear to be necessary [2, 3, 7, 10].

Consider a weakly nonlocal free energy in the Van der Waals form $f = f_0(u) + \varepsilon u_x^2$, where the local part f_0, taken as a function of u may be nonconvex for solids undergoing martensitic transformations . Although homogeneous spinodal states with $\frac{\partial^2 f_0}{\partial u^2} < 0$ are unstable, they would be expected to stabilize through evolution into narrow highly inhomogeneous zones (with the width $\sim \sqrt{\varepsilon}$) within which the nonlocal term in the energy dominates. The governing equation for the viscoelastic (Maxwell) solid with the nonlocal energy f read

$$u_t = v_x, \; v_t = (\tau(u) - 2\varepsilon u_{xx} + \eta v_x)_x\,, \tag{3}$$

where $\tau(u) = \frac{\partial f_0}{\partial u}$ and η is the viscosity coefficient. For kink-like traveling wave solutions, dependent on $z = x - Dt$ only, the system (3) integrates to give

$$-\tau(u) + D^2 u + 2\varepsilon u_{zz} + \eta D u_z = \pi, \tag{4}$$

where π is a constant of integration. Introduction of the extended coordinate $z' = z/\sqrt{\varepsilon}$ shows that η and ε will occur in (4) only in a non-dimensional combination

$$\mathbf{W} = \eta/\sqrt{\varepsilon}.$$

Suppose that the state ahead of the discontinuity with $u = u_2$ transforms to the state behind the discontinuity with $u = u_1$. Hence the boundary conditions for the second order O.D.E.(4) are

$$u(z) \to \begin{cases} u_2, & z \to +\infty \\ u_1, & z \to -\infty. \end{cases} \tag{5}$$

The equilibria of (4) clearly satisfy RH conditions $-\tau_1 + D^2 u_1 = -\tau_2 + D^2 u_2 = \pi$.

One can see that the problem (4, 5) is overdetermined, and the jump velocity D must be found as the eigenvalue from the condition of existence of the (traveling wave) solution. The spectrum of the nonlinear boundary value problem (4, 5) contains both continuous and discrete parts [11]. While points of the continuous spectrum (shocks) are distinguished by inequalities, those of the discrete spectrum (kinks) provide new jump relations, supplementary to the RH conditions. The analysis of nonlinear boundary value problem (4, 5) can be found in [10, 11, 12].

Since supersonic martensitic phase boundaries are similar to regular shock waves, we focus here on subsonic phase boundaries (kinks) and illustrates the idea of kinetic equation on an example. Suppose that the isotherm $T = T_0$ is given by the cubic polynomial (Fig.1):

$$\tau(u) = \tau_0 + K(u - u_\beta)(u - u_\alpha)\left(u - \frac{u_\beta + u_\alpha}{2}\right), \tag{6}$$

where the parameters have been chosen in such a way that $u_\alpha < u_\beta$ are Maxwell (equilibrium) deformations of coexisting phases, τ_0 is a Maxwell pressure and K characterizes the width of the pressure range $\Delta\tau$ between binodal and spinodal ($\Delta\tau = (\sqrt{3}/144)\, K(\Delta u)^3$, $\Delta u = u_\beta - u_\alpha$).

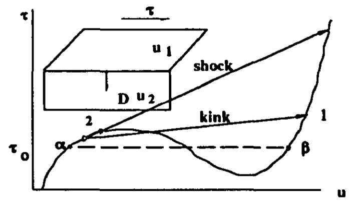

Figure 1. A typical isotherm $\tau=\tau(u,T=\text{const})$ for the solid which allows for martensitic phase transformation.

The desired solution of (4, 5) with $\tau(u)$ taken from (6) is [8, 11] :

$$u(z) = \frac{u_2 + u_1}{2} - \frac{u_2 - u_1}{2} th\left[\sqrt{\frac{K}{\varepsilon}}\frac{u_2 - u_1}{4}(z - z_0)\right], \tag{7}$$

where $D > 0$ so that the wave transforms the state with $u = u_2$ into the state with $u = u_1$. Substitution of (7) into (4,5) provides a relation between u_1 and u_2

$$y^2 + \zeta x^2 = 1,$$

$$x = (u_2 + u_1 - u_\beta - u_\alpha)/\Delta u, \quad y = (u_1 - u_2)/\Delta u.$$

where $\zeta = 3\left(1 - \frac{12}{\mathbf{W}^2}\right)$. This relation is represented in Fig.2 for different values of the nondimensional parameter $\mathbf{W}$.

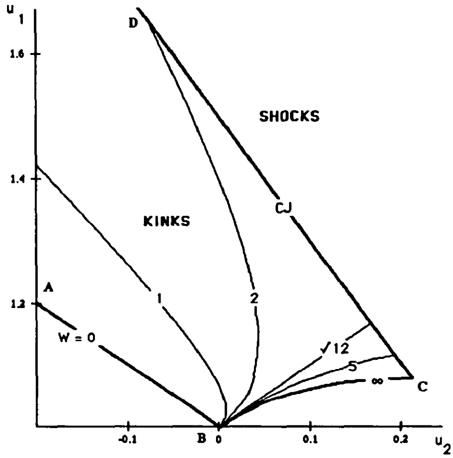

Figure 2. The deformation $(u_1/\Delta u)$ of the state behind the martensitic phase boundary, as a function of the deformation $(u_2/\Delta u)$ of the state in front of it. CJ regimes are sonic with respect to the state in front.

According to Fig.2 kinetic curves for kinks lie inside the domain ABCD, where AB corresponds to equilibrium (Maxwell) dynamic regimes, BC corresponds to the metastable phase equilibria, while CD describes marginal (sonic) Chapman-Jouget (CJ) regimes. We mention that for $\mathbf{W}^2 \ll 12$, two kinks-slow and fast- are possible for the given state far ahead [8, 11]. The straightforward calculation shows that $D = (3\sqrt{K}/\mathbf{W})\Delta u \cdot x$, which gives another type of kinetic curves (presented in Fig.3).

Now one can show that [8, 11]

$$\Re(D) = \frac{a}{T_0} D^2 (1 + bD^2)^{3/2} = \frac{aD^2}{T_0} + \frac{3ab}{2T_0} D^4 + O(D^6), \tag{8}$$

where

$$a = \frac{\mathbf{W}\sqrt{K}(\Delta u)^3}{12}, \quad b = \frac{12 - \mathbf{W}^2}{3(\Delta u)^2 K}.$$

Relation (8) gives in *explicit form* of an additional jump condition required for kinks. For slow kinks a quadratic (normal growth) approximation for the entropy production is adequate up to the terms of fourth order in D, moreover it is *exact* if $\mathbf{W}^2 = 12$. The first term in the expansion (8) provides a *mobility* of the phase boundary.

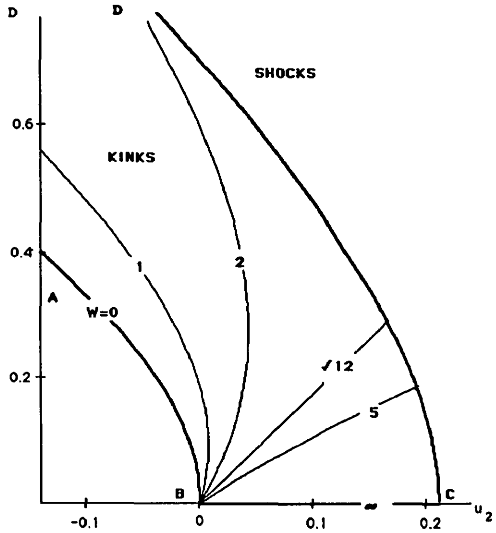

Figure 3. Phase boundary velocity ($D/\sqrt{K\Delta u}$) as a function of the state of deformation ahead of it ($u_2/\Delta u$) for different values of the non-dimensional parameter W.

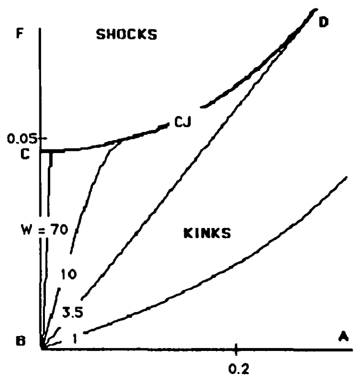

Figure 4. Kinetic laws, following from the exact solution for a different W; here F is the "driving force" measuring the degree of the metastability while $\tilde{D}$ is the conjugate mass flux.

It can be shown that the envelope of the family of kinetic curves $G = \Re T_0/D$ vs. D parameterized by $\mathbf{W}$, corresponds to the CJ regimes (D equals local characteristic speed and $u_1 + 2u_2 = 1.5(u_\beta + u_\alpha)$). Different kinetic relations between the normalized thermodynamic "force" $F = \frac{G}{K(\Delta u)^4}$ and the normalized "flux" $\tilde{D} = \frac{D}{\sqrt{K}\Delta u}$, stemming from (8), are presented in Fig.4.

An interesting property of this solution is that if the viscosity is sufficiently large ($\mathbf{W}^2 \gg 12$), then the phase transformation remains nearly "frozen" until the critical driving traction is achieved. At this point the phase boundary travels at a speed close to the local acoustic velocity. One can expect threshold phenomena to be associated with this case for $G^* \approx (3/64)K(\Delta u)^4 = (9\sqrt{3}/4)\Delta\tau\Delta u$. This also explains "stability" of the metastable states for $0 < G < G^*$ in the limit of $\varepsilon \to 0$, $\eta \to 0$, but $\mathbf{W} = \eta^2/\varepsilon \to \infty$.

4. SUMMARY

In this paper we deal with the problem of the internal structure of the interface for both shock waves and phase boundaries. In terms of the structure analysis, the first kind of discontinuity is associated with a continuous spectrum of the corresponding boundary value problem, while a discontinuity of the second kind relate to points of a discrete spectrum. Additional jump condition in the case of subsonic phase boundaries (kinks) can be regarded as constitutive relation for the discontinuity surface. The fact that kinks are subsonic and can adjust their velocity based on information from the state ahead, creates a basis for such a constitutive behavior. An unusual general property of the solutions of the truly dynamical problem is that two kinks-slow and fast-exist for the given state in front of the discontinuity. For slow kinks we obtained "normal growth" condition. An important prediction of this model is that the speed of the kink can be negligible until a critical level of metastability is achieved. After this "ignition", the speed suddenly increases considerably. This can explain burst-like transformation following the "normal growth" too slow to be observed.

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