

NUCLEATION AND GROWTH IN ELASTODYNAMICS

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INTRODUCTION

Structures made of transforming materials exhibit a striking capacity to hysteretically recover significant deformation with a controllable amount of energy absorbed in the process. The unusual properties of these materials are due to the fact that large deformations and inelastic behavior are accomplished by coordinated migration of mobile phase or domain boundaries. Intensive research in recent years has led to well-defined static continuum theories for some of the transforming materials (see Pitteri and Zanzotto (1997) for a recent review). Within the context of these theories, the main unresolved issues include history and rate sensitivity in the constitutive structure.

In this overview we focus on the elastodynamical aspects of the transformation and intentionally exclude phase changes controlled by diffusion of heat or constituent. To emphasize ideas we use a one dimensional model which reduces to a nonlinear wave equation. Following Ericksen (1975) and James (1980), we interpret the behavior of transforming material as associated with the nonconvexity of elastic energy and demonstrate that a simplest initial value problem for the wave equation with a non-monotone stress-strain relation exhibits massive failure of uniqueness associated with the phenomena of nucleation and growth.

The multiplicity of solutions at the continuum level can be viewed as arising from a constitutive deficiency in the theory, reflecting the need to specify additional pieces of constitutive information through some kind of phenomenological modeling (see, for instance, Truskinovsky, 1987; Abeyaratne and Knowles, 1991). Here we take a different point of view and interpret the nonuniqueness as an indicator of essential interaction between macro and micro scales.

We recall that our wave equation represents a long wave approximation to the behavior of a structured media (atomic lattice, periodically layered composite, bar of finite thickness), and does not contain information about the processes at small scales which are effectively homogenized out. When the model at the microlevel is nonlinear, one expects essential interaction between different scales which in turn complicates any universal homogenization procedure. In this case, the macro model is often formulated on the basis of some phenomenological constitutive hypotheses; nonlinear elasticity with nonconvex energy is a theory of this type.

The well known phenomenon of a finite time blow up in nonlinear elastodynamics is a sign that the phenomenological equations are at least incomplete. In some cases (Dafermos, 1979), the detailed microlevel behavior turns out to be irrelevant and the closure can be achieved by prescribing a single inequality. This means, for instance, that the fine structure of a shock discontinuity does not affect the dynamics and that the localized perturbations in initial data die out instantly. The situation is more complex in the case of material with a generic nonconvex energy where in order to obtain a unique solution at the continuum (or macro) level, one must "de-homogenize" the model and introduce additional physical hypotheses about the behavior at the sub-continuum (micro) scale. It is important to remember that the physical picture at micro and macro levels can be quite different. For example, analysis of physically motivated discrete models show, that phase boundary motion at the micro scale requires overcoming a barrier which, as we show, is formally absent in a continuum picture (Slepyan and Trojankina, 1984); the same is true for the nucleation which is barrier-free in the classical elastodynamical setting. The regularization can also be achieved in numerical calculations because of the dissipation and dispersion which formal discretization brings into the model.

For the purpose of illustration, in this paper we use a viscosity-capillarity model (Truskinovsky, 1982; Slemrod, 1983) as an artificial "micromodel", and investigate how the information about the behavior of solutions at the microscale can be used to narrow the nonuniqueness at the macroscale. The viscosity-capillarity model contains a parameter $\sqrt{\epsilon}$ with a scale of length, and the nonlinear wave equation is viewed as a limit of this "micromodel" obtained when this parameter tends to zero. As we show, the localized perturbations of the form $\phi(x/\sqrt{\epsilon})$ can influence the choice of attractor; for this type of perturbation, support (but not amplitude) vanishes as the small parameter goes to zero. Another manifestation of this effect is the essential dependence of the limiting solution on the contributions of the type $\phi((x - Dt)/\sqrt{\epsilon})$, describing the structure of the jump discontinuity.

Since in this problem not only the limit but also the character of convergence matters we conclude that consistent homogenization of the micromodel should lead to a description in a broader functional space than is currently accepted. One interesting observation is that the concave part of the energy is relevant only in the region with zero measure where the singular, *measure valued* contribution to the solution is nontrivial (different from point mass). We remark that the situation is similar in fracture mechanics where a problem of closure at the continuum level can be addressed through the analysis of a discrete lattice (e.g. Truskinovsky, 1996).

METASTABILITY

Following Ericksen (1975), consider an elastic bar which occupies a segment $[0,1]$ in the reference state. Let $u(x)$ be a displacement field so that $x+u(x)$ is the deformed position of a material particle with the reference coordinate x . The stored elastic energy of the bar has a density $f(w)$ where $w = u_x$ is the longitudinal strain. We assume that $f(w)$ is not convex, in particular, $f''(w) > 0$ for $w < \alpha$ (phase 1) and $w > \beta$ (phase 2) and $f''(w) < 0$ for $\alpha < w < \beta$ (spinodal region) (see Fig. 1a). The corresponding stress-strain relation $\sigma = f'(w)$ is nonmonotone (see Fig. 1b), and one can formally define equilibrium stress σ_M , and equilibrium strains a and b in such a way that: $\sigma(a) = \sigma(b) = \sigma_M$, and $\int_a^b \sigma dw = \sigma_M(b - a)$ (Maxwell construction). Two regions $a < w < \alpha$ (in phase 1) and $\beta < w < b$ (in phase 2) are called *metastable*.

The concept of metastability in this elementary setting has exactly the same meaning as in the closely related case of van der Waals's fluid. Consider the simplest equilibrium treatment of a bar loaded by a constant stress σ_0 . The static problem reduces to the minimization of the functional

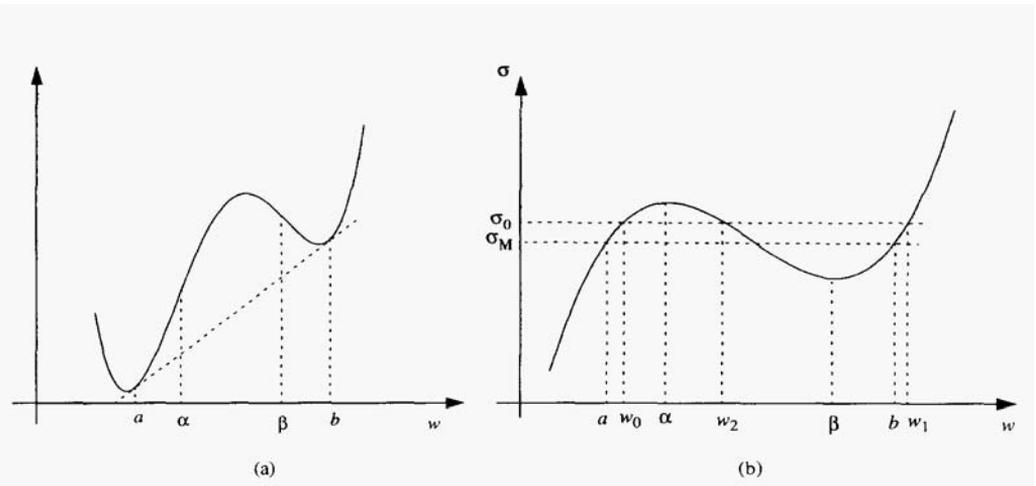


Figure 1. The free energy (a) and the corresponding stress-strain relation (b) for the elastic material supporting two phases.

$$G\{u\} = \int_0^1 g(w; \sigma_0) dx \tag{2.1}$$

where $g(w; \sigma_0) = f(w) - \sigma_0 w$ is the potential (Gibbs) energy. If we choose the value of stress from a metastable region, say $\sigma_0 \in (\sigma_M, \sigma(\alpha))$ as in Fig.1b, then the function $g(w; \sigma_0)$ has three extrema: two minima (at w_0 and w_1) and a maximum (at w_2) (see Fig.2).

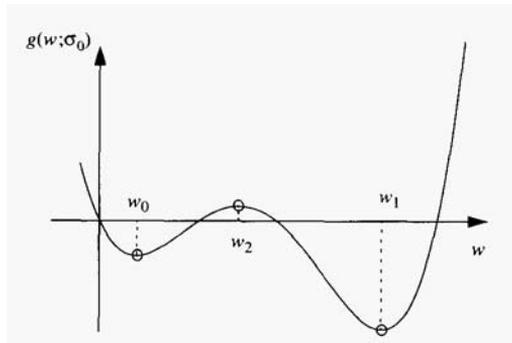


Figure 2. Potential (Gibbs) energy of the bar loaded by the constant stress $\sigma_0 \in (\sigma_M, \sigma(\alpha))$.

One can show (Ericksen, 1975) that the homogenous state $w(x) \equiv w_1$ corresponding to a deeper minimum of $g(w; \sigma_0)$ is the global minimizer of the functional (2.1); another homogenous configuration $w(x) = w_0$ (the metastable state), is only a weak local minimizer

which is not even isolated in the strong sense (in $W^{1,p}$). In other words, it is unstable in the class of piecewise smooth competitors: the "dangerous" perturbation is a "Weierstrass needle" a nucleus of state w_1 with an infinitesimal support. In the fully 3D case the situation is essentially similar, the only difference being that the metastable region begins with the failure of quasiconvexity rather than convexity, which is due to the nontrivial constraint of strain compatibility (see, for instance, Ball and James, 1996).

The absolute instability of the "metastable" states in the framework of classical elasticity manifests itself in dynamics as well. The associated elastodynamical problem reduces to a solution of the nonlinear wave equation $u_{tt} = \sigma'(u_x)u_{xx}$. It is convenient to rewrite it as a mixed type first order system

$$v_t = \sigma(w)_x, \quad w_t = v_x, \tag{2.2}$$

where we introduced particle velocity $v = u_t$. The elastodynamic problem with initial conditions $w(x,0) = w_0, \quad v(x,0) = 0$, corresponding to the metastable state, has a trivial solution $w(x,t) \equiv w_0, \quad v(x,t) \equiv 0$. To show that this solution is not unique, choose an arbitrary point $x = x_0$ inside the segment $[0,1]$ and prescribe the same initial data everywhere except for this point. Then, we obtain a (degenerate) Riemann problem with piecewise constant initial data and, at least locally, one expects to find a self-similar solution of the type $w = w(\zeta), \quad v = v(\zeta)$, where $\zeta = (x-x_0)/t$. The elastic field in this case must be a combination of constant states separated by jump discontinuities and/or centered Riemann waves. Classical conservation laws must be satisfied on the discontinuities which leads to the following Rankine Hugoniot jump conditions

$$D[v] + [\sigma] = 0, \quad D[w] + [v] = 0. \tag{2.3}$$

Here as usual $[A] = A_+ - A_-$ and D is the discontinuity speed. The entropy inequality yields

$$D([f] - \{\sigma\}[w]) \geq 0 \tag{2.4}$$

where $\{A\} = \frac{1}{2}(A_+ + A_-)$ the average value. As was first shown by James (1980), the nontrivial solution satisfying (2.2, 2.3) has the following form (see Fig.3)

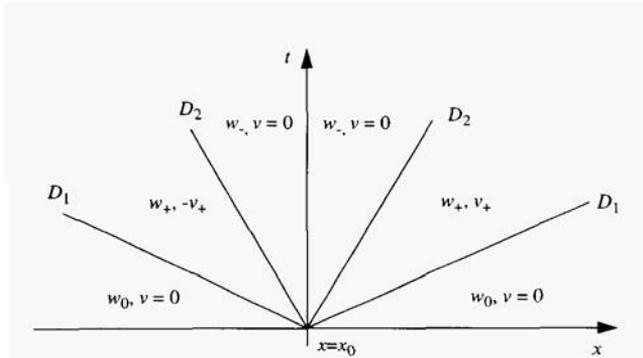


Figure 3. Nontrivial solution of a degenerate Riemann problem with initial data in the metastable area.

$$w(x,t), v(x,t) = \begin{cases} w_-, 0 & , \quad |x - x_0| < D_2 t \\ w_+ \pm v_+ & , \quad D_2 t < |x - x_0| < D_1 t \\ w_0, 0 & , \quad D_1 t < |x - x_0| \end{cases} \quad (2.5)$$

Solution (2.5) (see Fig. 4) describes the nucleation of a phase 2 ($w = w_-$) which is accompanied by a generation of shock wave precursors in phase 1 ($w = w_0$) and is satisfactory only until the first shock wave reaches the boundary of the segment $[0,1]$. The entropy inequality (2.4) is automatically satisfied for the precursors (moving with the speed D_1) and is satisfied for the phase boundaries (moving with the speed D_2) if the area A_1 in Fig. 4 is smaller than the area A_2 (phase boundary is dissipation free if $A_1 = A_2$).

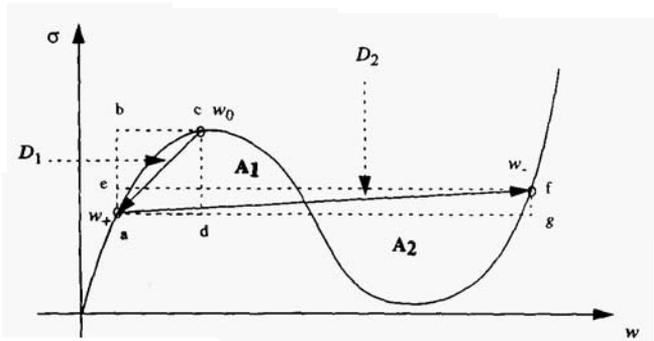


Figure 4. Nontrivial solution of a degenerate Riemann problem with initial data in the metastable area.

The only restriction imposed by the Rankine-Hugoniot conditions (2.3) is that the areas of the rectangles $abcd$ and $ae fg$ in Fig. 4 are equal. This shows that, the information contained in (2.3, 2.4) is not sufficient to find all the unknowns, since the balance equations impose only four restrictions on the five constants w_+, w_-, v_+, D_1, D_2 . Moreover, one obtains a two-parameter family of solutions since the nucleation point x_0 is also arbitrary. The two sources of nonuniqueness in this problem, and the necessity to make additional assumptions, have long been recognized by physicists who traditionally distinguished between the theories of *growth* and *nucleation*.

GROWTH

The only way to determine all five constants w_+, w_-, v_+, D_1, D_2 in the above problem is to supply an additional jump condition. This jump condition cannot be universal since, if applied at both discontinuities, it leads to an overdetermined system. We must therefore differentiate between the waves moving with the speeds D_1 and D_2 . Notice that only the first

one (with the speed D_1) satisfies the Lax condition (Lax, 1957) which means in this context that the wave is subsonic with respect to the state behind and supersonic with respect to the state ahead. We call this discontinuity a "shock". The second discontinuity (moving with the speed D_2) is subsonic with respect to the states both in front and behind; we refer to it as "kink" (Truskinovsky, 1993a). An elementary analysis of the configuration of the characteristic directions shows that it is the subsonic discontinuity (kink) which requires an additional jump condition (see Kulikovskiy (1976) for general background on "non-evolutionary" or "undercompressive" shocks).

There is a long history of phenomenological modeling of kinks - phase or domain boundaries - in physics (normal growth hypothesis in crystal growth, Hertz - Knudsen theory of condensation, etc.); in the framework of elasticity theory the phenomenological "kinetic relations" were recently reviewed by Gurtin (1993) and Lin and Pence (1996). Here instead of postulating the missing jump condition we shall focus on its *derivation* from a model for a fine structure of the interface. As shown in Truskinovsky (1993a) this method naturally distinguishes between shocks and kinks.

In order to describe the internal structure of a moving discontinuity, the classical balance equations are supplemented with an additional physical hypothesis regarding the material behavior in the transition region. The principal difference between shocks and kinks in terms of the relevant physical mechanisms can be understood as follows. Consider a generic discontinuity propagating with constant velocity $D > 0$ which transforms the state w_+ into the state w_- . Suppose that equations (2.2) and Rankine-Hugoniot conditions (2.3) are satisfied, in particular $D^2 = (\sigma_+ - \sigma_-) / (w_+ - w_-)$. Then the total energy release rate associated with the moving discontinuity can be written in the form $G dm$, where $dm = D dt$. One can show that $G(w_+, w_-) = f(w_+) - f(w_-) - \frac{1}{2}(\sigma_+ + \sigma_-)(w_+ - w_-)$, where G is a driving (or configurational) force (Knowles, 1979; Truskinovsky, 1987). To calculate the hypothetical "microscopic" variation of the rate of dissipation inside the discontinuity, suppose that the balance of mass and linear momentum is satisfied for every intermediate state between w_+ and w_- , which means that $D(w - w_+) + (v - v_+) = 0$ and $D(v - v_+) + (\sigma - \sigma_+) = 0$. Then the rate of dissipation $R = D(f(w_+) - f(w) + \frac{1}{2}(v_+^2 - v^2)) + (\sigma_+ v_+ - \sigma v)$ can be calculated explicitly as a function of w . Introduce $\Psi_{w_+}(w) = -R/D$, which may be viewed as a dynamic analog of the potential energy $g(w)$ from (2.1). The straightforward calculation gives

$$\Psi_{w_+}(w) = f(w) - f(w_+) - (w - w_+) \left(\sigma_+ + \frac{1}{2} \frac{\sigma_+ - \sigma_-}{w_+ - w_-} (w - w_+) \right), \quad (3.1)$$

in particular, $\Psi_{w_+}(w_-) = -G(w_+, w_-)$.

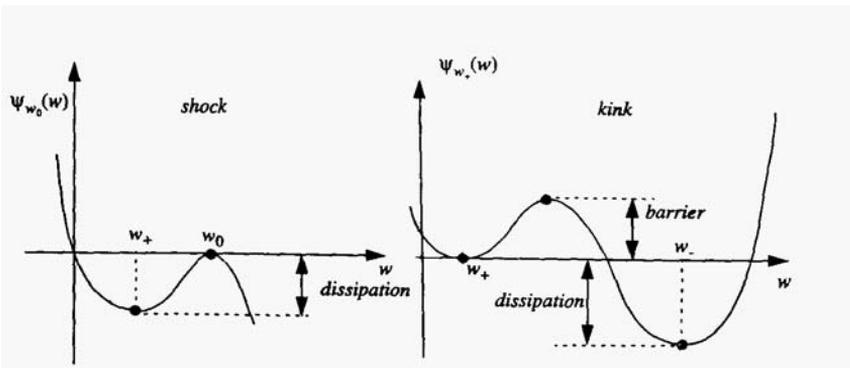


Figure 5. Dynamic driving force in the case of shocks and kinks.

Let us fix the state ahead of the discontinuity w_* and compare the behavior of the function $\psi_{w_*}(w)$ for shocks and kinks involved in solution (2.5). Two important conclusions can be drawn from the analysis of the graphs of $\psi_{w_0}(w)$ and $\psi_{w_*}(w)$ sketched in Fig.5. First, if $G(w_*, w_*) > 0$ (the opposite inequality is prohibited by the second law of thermodynamics) then one has to consider dissipation in the interphase region: for shocks introduction of the dissipation is usually sufficient to describe the structure of the discontinuity. Second, in case of kinks it is necessary to introduce an additional mechanism for crossing the *barrier*. The “no barrier” condition is implicit in the Oleinik (1959) criterion for shocks and the exclusively dissipative regularizations lead to the situation when kinks cannot move (Pego, 1987). On the other hand, in the absence of dissipation, the propagation of a kink can be viewed as an autocatalytic process which does not require extra energy after it is initiated. A process of this type is feasible in principle in dispersive media if group velocity for at least some wave lengths is greater than the speed of the kink. It is also clear that, contrary to the case of shocks, the velocity of the kink must be special to make this “tunneling” process possible.

One of the most interesting micromodels for the nonlinear wave equation is a discrete chain of atoms connected by nonlinear springs; such systems automatically exhibit “macroscopic” dissipation due to energy transfer between long and short waves. In discrete models, shocks are usually de-localized and classical discontinuous waves represent weak but not strong limits of highly oscillatory solutions (Lax et al., 1992)). Autocatalytic barrier crossing in bi-stable chains is also possible (Slepyan and Trojankina, 1984), however, here for simplicity we limit our consideration to mesoscopic continuum models exhibiting dispersion and dissipation.

There are several ways that dispersion (and the corresponding length scale) can be brought at the phenomenological level into the conservative part of the model. The two most well known examples of such theories are: gradient (or van der Waals) models with energy

$$f(u_x) + \frac{\epsilon}{2} u_{xx}^2$$

(e.g. Carr et al., 1984), and strongly nonlocal models with energy

$$f(u_x) + \int K(x-y) u_x(y) dy$$

(e.g. Fosdick and Mason, 1996). The nonlocal model can sometimes be reformulated as a local theory with an additional order parameter; an Ericksen-Timoshenko bar with energy

$$f(u_x) + \frac{\delta}{2} (u_x - \phi)^2 + \frac{\epsilon}{2} \phi_x^2$$

is one example (e.g. Rogers and Truskinovsky, 1996). More general phase field models with an energy of the type $f(u_x, \phi_x)$ have also been considered (e.g. Roshin and Truskinovsky, 1989; Fried and Gurtin, 1994)).

The simplest example of a theory which incorporates both dispersion and dissipation is the so called viscosity-capillarity model (Truskinovsky, 1982, Slemrod, 1983). It combines van der Waals correction to the energy with Kelvin viscoelasticity, which in the present context amounts to the following additional constitutive assumption

$$\eta w_t = \sigma - \sigma(w, w_x).$$

Here $\sigma(w, w_x)$ is the equilibrium stress and η is the effective viscosity coefficient prescribing a rate of interphase kinetics. One can also consider other phenomenological dissipation models like Maxwell viscoelasticity (e.g. Mihailescu-Suliciu and Suliciu, 1992), or internal order parameter relaxation (e.g. Truskinovsky, 1988). As is well known, the van der Waals model cannot be considered as a reasonable long wave description for the simple atomic lattice because of the “wrong” sign to the gradient term (e.g. Kunin, 1982). However, since the

group velocity is always larger than phase velocity, the dispersion is of the "right" type for the description of subsonic kinks.

With the introduction of the two new small parameters ε and η , the regularized wave equation takes the form

$$u_{tt} = \sigma'(u_x)u_{xx} + \eta u_{xxx} - \varepsilon u_{xxxx}. \quad (3.2)$$

Consider traveling wave solutions $u(x,t) = u(\xi)$, where $\xi = (x - Dt) / \sqrt{\varepsilon}$. The corresponding boundary value problem in the infinite domain takes the form

$$\begin{aligned} (\sigma(w) - D^2w - \mathbf{W}Dw' - w'')' &= 0; \\ w'(\pm\infty) &= 0, w(\pm\infty) = w_{\pm}; \end{aligned} \quad (3.3)$$

where $\mathbf{W} = \eta / \sqrt{\varepsilon}$. For the given state in front of the discontinuity, the set (spectrum) of admissible velocities D consists of two parts: *continuous*, corresponding to shocks (saddle-node (focus) trajectories) and *discrete*, corresponding to kinks (saddle-saddle trajectories). To be specific take $\sigma(w) = w(w-1)(w-1/2)$. Then an additional condition selecting kinks can be written explicitly (Truskinovsky, 1987, 1994)

$$3\left(1 - \frac{12}{\mathbf{W}^2}\right)(w_+ + w_- - 1)^2 + (w_- - w_+)^2 = 1 \quad (3.4)$$

We remark that the continuum spectrum does not contain all "supersonic" Lax discontinuities (Shearer and Yang, 1993; Truskinovsky, 1993b). The generic picture of the admissibility domain for both shocks and kinks is presented in Fig.6.

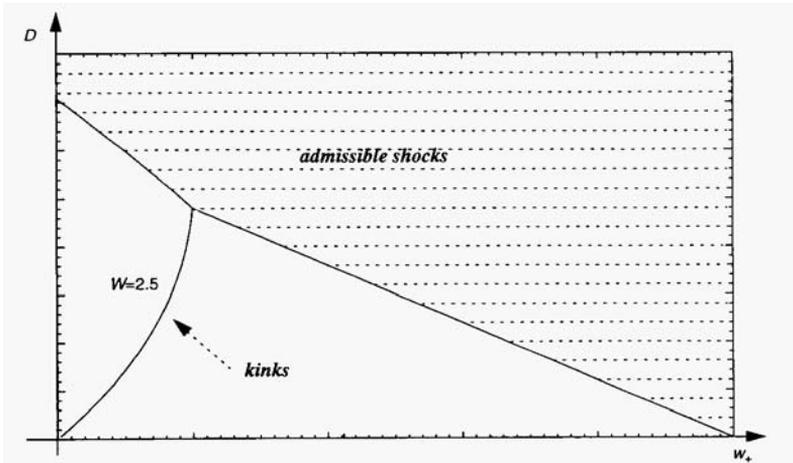


Figure 6. Set of jump discontinuities (kinks and shocks) compatible with the isothermal viscosity-capillarity model; $\mathbf{W}=2.5$.

Some interesting aspects of the interface kinetics appear only when temperature and latent heat are included into the model. If the process of heat conductivity is governed by a classical Fourier law, the entropy balance equation takes the form $Ts_t = T_{xx} + \eta w_t^2$ where $s = -\partial f / \partial T$. Suppose for simplicity that equilibrium stress is cubic in strain and linear in temperature and assume that specific heat at fixed strain is constant. Then in nondimensional variables the system of equations takes the form (see Ngan and Truskinovsky, 1996a)

$$\begin{aligned}
u_{tt} &= (\sigma(u_x, T))_x + \mathbf{W}_1 u_{xxx} - u_{xxxx} \\
Ts_t &= \mathbf{W}_2 T_{xx} + \mathbf{W}_1 u_{xt}^2 \\
\sigma &= 1 + \mathbf{W}_3 T + u_x(u_x - 1)(u_x - 1/2), \quad s = -\mathbf{W}_3 u_x + \ln T
\end{aligned}$$

where we introduced the following dimensionless numbers: $\mathbf{W}_1 = h / \sqrt{\varepsilon}$ - the ratio of viscosity to nonlocality, $\mathbf{W}_2 = \kappa / \sqrt{\varepsilon}$ - the ratio of heat conductivity to nonlocality and \mathbf{W}_3 - the measure the latent heat. A step-type traveling wave in this model describes an adiabatic shock or kink; the behavior of the corresponding heteroclinic trajectory in 3D phase space is similar to that for the 2D phase space of the isothermal system. Fig. 7 illustrates a numerical example of how the appropriate driving force

$$G = [f] - \{\sigma\}[w] + [T]\{s\}$$

(see Abeyaratne and Knowles, 1995) is then related to the speed of a kink D (i.e. a kinetic relation).

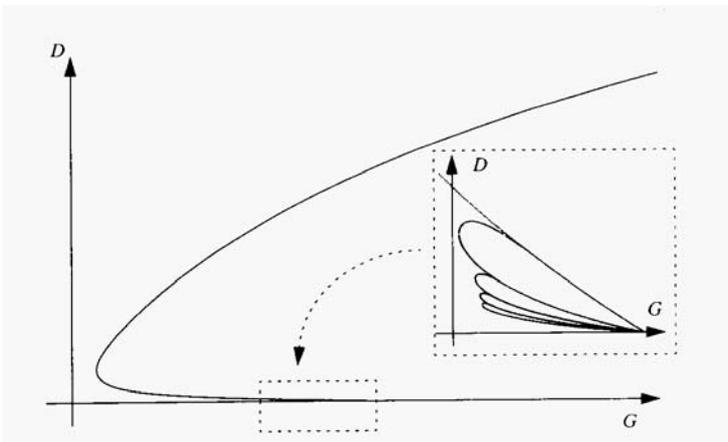


Figure 7. Multivalued kinetic relations for adiabatic kinks; $\mathbf{W}_1=1, \mathbf{W}_2=0.025, \mathbf{W}_3=0.03$.

Two important effects distinguish adiabatic kinks from isothermal ones. First, the kinetic curve does not originate from the point $G = 0$ due to the negative feedback provided by the latent heat (cf. Patashinskii and Chertkov, 1990 and Turteltaub, 1997). The second effect is the multivaluedness of the kinetic relation at small speeds, which has also been found in lattice models of fracture (Marder, 1995; Slepyan, 1996). Although most of the slow regimes are probably unstable, the general nonmonotonicity of the curve $G(D)$, can give rise to an interesting stick-slip behavior (Rosakis and Knowles, 1997). We also remark that the viscosity-capillarity model in the nonisothermal setting does not provide a kinetic relation of the form $G = G(D; \mathbf{W}_1, \mathbf{W}_2, \mathbf{W}_3)$ because of an implicit dependence on one additional parameter prescribed at infinity; this observation casts some doubts concerning the existence of the simple universal constitutive relations in a force-flux form for the configurational forces.

We conclude that the growth of a new phase is controlled by the rate of dissipation at a moving kink. This dissipation is taking place at the microlevel and must be prescribed in order for the macro-description to be complete. The incompleteness of the continuum model manifests itself through the sensitivity of the solution to the singular (measure-valued) contributions describing fine structure of the subsonic jump discontinuities (kinks).

NUCLEATION

We now turn to consider the other source of nonuniqueness in the breakdown of a metastable state, namely the ambiguity of the nucleation point(s) and the necessity for each point to select between the two solutions - trivial and nontrivial. The degenerate Riemann problem considered here is, of course, only the most elementary example where such a problem arises. For instance, similar nonuniqueness may be responsible for the instability of the moving phase boundary (Truskinovsky, 1993b). The phenomenological nucleation criterion suggested by Abeyaratne and Knowles (1991) selects a resolution based on the size of the static energy barrier shown in Fig.2. Here, again, we consider fine structure arguments for *deriving* a nucleation criterion.

In order to understand better what happens when a nucleation point, say $x = x_0$, is selected, let us focus on the small time behavior of the nontrivial self-similar solution. Consider a solution (2.5) at time $t = \Delta t$. It is convenient to parametrize the functions $w(x, \Delta t)$ and $v(x, \Delta t)$ by x and present them as a curve in the (w, v) plane. It is not hard to see that one then obtains a loop, beginning and ending in a point $(w_0, 0)$ (see Fig. 8b); the details of the loop depend, of course, on the fine internal structures of shocks and kinks (see Fig. 8a).

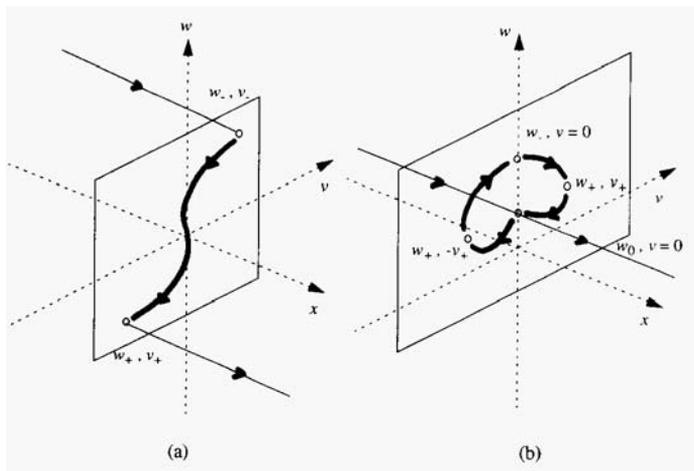


Figure 8. Schematic representation of the singular components of the solution and of the initial data: (a) - fine structure of the kink; (b) - fine structure of the nucleus.

In view of the self-similar character of the solution, the loop does not change as $\Delta t \rightarrow 0$ even though the strain and velocity fields converge to the constant initial data everywhere outside the point $x = x_0$. This means, that by selecting the point x_0 we have supplemented constant initial data with a singular part represented by a parametric measure (in the state space) located at $x = x_0$. We conclude that, contrary to the behavior of, say, genuinely nonlinear systems ($\sigma'(w) > 0$) (see Di Perna, 1985), the choice of a short time dynamic attractor in this problem (trivial solution vs. self similar dynamic regime (2.5)) is affected by a singular contribution to the initial data and may depend on the structure of the loop.

Since the energy of the nucleus is identically zero, the integral impact of this localized contribution to the initial data can be measured by the corresponding energy density which is finite. For our self-similar solution (2.5) one can equivalently calculate the rate of dissipation R (Dafermos, 1973)

$$R = D_1([f] - \{\sigma\}[w])_{shock} + D_2([f] - \{\sigma\}[w])_{kink}.$$

If the kinetic relation is known then the energy release rate R , which does not depend on t , can be calculated as a function of w_0 ; the fact that $R = 0$ at $t = 0$ means that the initial data with the superimposed loop are in fact instantly "dissipative". This observation, however, does not give insight into the associated barrier separating the uniform initial state and the state with the superimposed loop. As we have seen earlier such a barrier does not exist in the "homogenized" description. It can be calculated, however, in the framework of a regularized model which describes the initial stage of the transformation when internal length scales can not be neglected.

Suppose again that the isothermal viscosity-capillarity model (3.2) describes the "de-homogenized" structured material. Consider the initial value problem corresponding to a metastable state with the fixed strain w_0 and zero velocity but now add a finite perturbation with a small support. Numerical experiments based on the high-order accurate difference scheme developed by Cockburn and Gao (1996) show that sufficiently large perturbations evolve into a regime which closely resembles the self-similar dynamic solution (2.5), while small perturbations gradually decay (see Fig.9). This confirms the existence of the two dynamic attractors and makes it natural to relate the nucleation criterion to the size of the trivial regime's domain of attraction (basin).

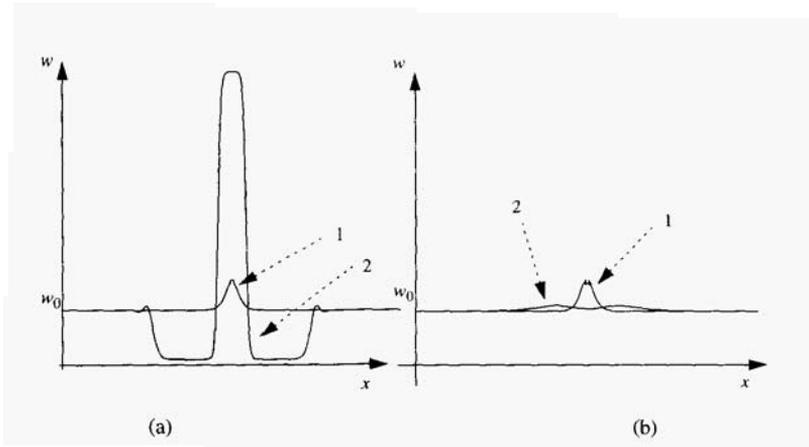


Figure 9. Two regimes of evolution for the initial data corresponding to slightly perturbed critical nucleus: (a) - perturbation leading to the growth of a new phase; (b) - perturbation which eventually decays; 1 - initial data; 2 - solution after finite time.

One representative point on the stability boundary is the so called *critical nucleus*, a saddle point (with a one dimensional unstable manifold) of the static energy functional

$$\int g(w) + \frac{\epsilon}{2} w_x^2 dx,$$

where

$$g(w) = f(w) - f(w_0) - \sigma_0(w - w_0).$$

The critical nucleus, which can be found explicitly, is described by a homoclinic trajectory of the Euler-Lagrange equation $\varepsilon w_{xx} = g'(w)$ (see, for instance Bates and Fife, 1993). The fact that this perturbation plays a role of a threshold is clear from Fig.9 which demonstrates extreme sensitivity of the problem to slight variations around the critical nucleus representing particular initial data (see Ngan and Truskinovsky (1996b) for details).

We note that both the energy of the critical nucleus and the size of its support are proportional to $\sqrt{\varepsilon}$. In the limit $\varepsilon \rightarrow 0$ the energy of this perturbation goes to zero, however the associated energy density

$$\bar{g}(w_0) = \lim_{\varepsilon \rightarrow 0} \varepsilon^{-1/2} \int (g(w) + \varepsilon/2 w_x^2) dx$$

is a function of w_0 (or applied stress) only. The limiting perturbation can therefore be described by a probability measure ν_{x_0} , which in turn suggests that the nucleation criterion should be formulated in terms of the intensity of the exterior, measure-valued "noise". We note that such noise is *invisible* at the continuum level.

CONCLUSIONS

Solids undergoing martensitic phase transformations are currently a subject of intense interest in mechanics. In spite of recent progress in understanding the absolute stability of elastic phases under applied loads, the presence of metastable configurations remains a major puzzle. In this overview we presented the simplest possible discussion of nucleation and growth phenomena in the framework of the dynamical theory of elastic rods. We argue that the resolution of an apparent nonuniqueness at the continuum level requires "de-homogenization" of the main system of equations and the detailed description of the processes at micro scale.

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REFERENCES

- Abeyaratne, R., and Knowles, J.K., 1991, Kinetic relations and the propagation of phase boundaries in solids, *Arch. Rat. Mech. Anal.* 114:119.
- Abeyaratne, R., and Knowles, J.K., 1995, Impact-induced phase transitions in thermoelastic solids, Caltech, Preprint.
- Ball, J.M., and James, R.D., 1996, Local minimizers and phase transformations, Preprint .
- Bates, P.W., and Fife, P.C., 1993, The dynamics of nucleation for the Cahn-Hilliard equation, *SIAM J. Appl. Math.* 53:90.
- Carr, J., Gurtin, M.E., and Slemrod, M., 1984, Structured phase transitions on a finite interval, *Arch. Rat. Mech. Anal.* 86:317.
- Cockburn, B., and Gao, H., 1996, A model numerical scheme for the propagation of phase transitions in solids, *SIAM J. Sci. Comput.* 17:1092.
- Dafermos, C.M., 1973, The entropy rate admissibility criterion for solutions of hyperbolic conservation laws, *J. Diff. Eq.*, 14:202.
- Dafermos, C.M., 1979, The second law of thermodynamics and stability, *Arch. Rat. Mech. Anal.* 70:167.
- Di Perna, R.J., 1985, Measure valued solutions to conservation laws, *Arch. Rat. Mech. Anal.* 88:223.
- Ericksen, J.L., 1975, Equilibrium of bars, *J. Elast.* 5:191.
- Fosdick, R.L., and Mason, D.E., 1996, Singular phase energy minimizers for materials with nonlocal spatial dependence, *Quart. Appl. Math.* 54:161.
- Fried, E., and Gurtin, M., 1994, Dynamic solid-solid transitions with phase characterized by an order parameter, *Physica D*, 72:287.

- Gurtin M., 1993, The dynamics of solid-solid phase transitions 1. Coherent interfaces, *Arch. Rat. Mech. Anal.* 123:305.
- James, R.D., 1980, The propagation of phase boundaries in elastic bars, *Arch. Rat. Mech. Anal.* 73:125.
- Knowles, J.K., 1979, On the dissipation associated with equilibrium shocks in finite elasticity, *J.Elast.* 9:131.
- Kulikovskiy, A.G., 1976, On the discontinuous solutions in mechanics of continuous media, in: *Theoretical and Applied Mechanics*, W.T. Koiter, ed., North Holland.
- Kunin, I.A., 1982, *Elastic Media With Microstructure 1 (One Dimensional Model)*, Springer.
- Lax, P.D., 1957, Hyperbolic systems of conservation laws II, *Com. Pure Appl. Math.* 10:537.
- Lax P.D., Levermore C.D., and Venakides S., 1992, The generation and propagation of oscillations in dispersive IVPs and their limiting behavior, in: *Important developments in soliton theory 1980-1990*, T. Fokas, V.E. Zakharov, ed., Springer-Verlag.
- Lin J., and Pence T.J., 1996, Wave attenuation by kinetically active phase boundary scattering during displacive phase transformations, Preprint.
- Marder, M., and Gross S., 1995, Origin of crack tip instabilities, *J.Mech.Phys.Solids* 43:1.
- Mihailescu-Suliciu, M., and Suliciu, I., 1992, On the method of characteristics in rate type viscoelasticity with non-monotone equilibrium curve, *ZAMM* 72:667.
- Ngan, S.C., and Truskinovsky, L., 1996a, kinetics of adiabatic phase boundaries. To be submitted.
- Ngan, S.C., and Truskinovsky, L., 1996b, Dynamics of nucleation in solids. To be submitted.
- Oleinik, O.A., 1959, Uniqueness and stability of the generalized solution of the Cauchy problem for a quasilinear equation, *Usp. Mat. Nauk* 14:165.
- Patashinskii, A.Z., and Chertkov, M.V., 1990, Motion of the front of a phase transition under strong supercooling conditions, *Sov.Phys.Solid State* 36:295.
- Pego, R., 1987, Phase transitions in a one dimensional nonlinear viscoelasticity: admissibility and stability, *Arch. Rat. Mech. Anal.* 97:353.
- Pitteri, M., and Zanzotto G., 1997, *Continuum Models for Phase Transitions and Twinning in Crystals*, Chapman and Hall .
- Rogers, R., and Truskinovsky, L., 1996, Discretization and hysteresis, *Physica D*. Submitted.
- Roshin, A. B., and Truskinovsky, L., 1989, Model of weakly Nonlocal Relaxing Compressible Media, *J. Appl. Math. Mech.*, (PMM) 53:904.
- Rosakis, P., and Knowles, J.K., 1997, Unstable kinetic relations and the dynamics of solid-solid phase transitions. In preparation.
- Shearer, M., and Y. Yang, 1993, The Riemann problem for a p-system of conservation laws of mixed type with cubic nonlinearity, *Proc.Roy.Soc. Edinburgh A* .
- Slemrod, M., 1983, Admissibility criteria for propagating phase boundaries in a van der Waals fluid, *Arch. Rat. Mech. Anal.* 81:301.
- Slepyan, L. I., 1996, Crack dynamics, in: *Fracture: A Topical Encyclopedia of Current Knowledge*, G. Cherepanov, ed., Krieger.
- Slepyan, L. I., and Trojankina, L. V., 1984, Fracture wave in a chain structure, *J. Appl. Mech. Techn. Phys.*, 25:921.
- Truskinovsky, L., 1982, Equilibrium phase boundaries, *Sov. Phys. Doklady*, 27:551.
- Truskinovsky, L., 1987, Dynamics of nonequilibrium phase boundaries in a heat conducting nonlinear elastic medium, *J.Appl. Math. and Mech. (PMM)* 51:777.
- Truskinovsky, L., 1988, Nonequilibrium phase boundaries, *Dokl. Akad. Nauk. SSSR*, 303:1337.
- Truskinovsky, L., 1993a, Kinks versus shocks, in: *Shock Induced Transitions and Phase Structures in General Media*, R. Fosdick, E.Dunn and M.Slemrod, ed., IMA 52, Springer-Verlag.
- Truskinovsky, L., 1993b, Transition to detonation in the dynamic phase changes, *Arch. Rat. Mech. Anal.* 125:375.
- Truskinovsky, L., 1994, About the normal growth approximation in the dynamical theory of phase transitions, *Cont. Mech. and Thermodyn.* 6:185.
- Truskinovsky, L., 1996, Fracture as a phase transformation, in: *Contemporary research in the mechanics and mathematics of materials* , R. C. Batra and M. F. Beatty, eds., CIMNE, Barcelona.
- Turteltaub, S. , 1997, Dynamics of phase transitions in thermoelastic solids, Ph.D.Thesis, Caltech.