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DYNAMICS OF SOLID-SOLID PHASE INTERFACES VIA A LEVEL SET APPROACH

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Abstract

The so-called sharp interface model for solid-solid phase boundaries describes the dynamics of interfaces in solid materials undergoing phase transformations of the austenite-martensite type. Antiplane shear deformations are modeled by the conservation laws of linear elastodynamics supplemented with a two-well internal energy function together with a *kinetic relation,* driving the propagation of the phase interfaces. In this paper we introduce a new level set formulation adapted to this problem. The phase interfaces are viewed as the zero-level set of a function that evolves in time according to an Hamilton-Jacobi equation. The propagation speed in the latter is determined by suitably extending to the whole computational domain the interfacial propagation speed known on the interface only via the kinetic relation.

A numerical algorithm using centered differencing for the displacement and upwind differencing for the level set function is proposed. We demonstrate the interest of the method on antiplane shear deformations in crystals. The scheme allows complex topological changes of the interfaces and twin splitting.

1. Introduction

This paper, based on a joint work in preparation with T. Hou and P. Rosakis [17], presents a new numerical method for computing propagating interfaces in solid materials undergoing phase transformations such as the austenite-martensite transformation in metallic alloys. Displacive phase boundaries propagate in crystalline structures at subsonic speeds that can not be determined solely

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from the macroscopic stored-energy function and the time-dependent conservation laws of continuum mechanics. This makes difficult the use of standard computational techniques which, therefore, need be adapted.

For a material admitting two distinct phases, the energy function is taken to be a two-well function, each well being a preferred deformation state of the material. The static and quasi-static problems have been formulated and extensively studied in the last two decades. As one tries to minimize the energy functional, the deformation-gradient jumps from one well to the other and a typical observed behavior is the formation of *microstructures*, i.e. fine-scale mixtures of two (or more) phases of the material (Ball-James [5], James [18, 19], Kohn [21], Luskin [26], Nicolaides-Walkington [27]). Regarding the dynamics, a large literature on the physical modeling of the processes of phase transformations, as well as recent experimental work in laboratories on their growth rate, have become available. The emergence of complex patterns such as dendritic structures forming from planar interfaces has been observed experimentally. This research activity motivates the development of computational methods for phase boundaries propagating in martensitic crystals. Computational studies may contribute to the development of new technologies that depend on material properties such as shape-memory, magnetostriction, etc.

We restrict attention here to a continuum model based on the fundamental conservation laws of continuum mechanics. A macroscopic description of the phenomena of phase propagation is sought, rather than a detailed understanding of the highly complex processes taking place in the neighborhood of the interface. A two-well, stored-energy function is used and the system of P.D.E.'s under study is hyperbolic in the neighborhood of each of the two wells, but is elliptic away from them, so that the system is of mixed type. A phase boundary, by definition, connects a state close to one of the wells to a state close to the other. Due to the existence of the elliptic region, the propagation of the interface is not determined uniquely at this level of the modeling. To fully describe the dynamics, several strategies have been developed:

(1) *Higher order diffusion effects* are added to the equations, in order for the model to carry an internal structure for the material discontinuities. In this setting, the important issue of the formation of microstructures as time increases was addressed (Ball et al. [4] and Swart-Holmes [36]). A one-dimensional model including viscosity and capillarity effects was studied by Slemrod in the mathematically equivalent context of the dynamics of liquid-vapor phase boundaries in a van der Waals fluid. (See, for a review, Fan-Slemrod [8].)

(2) *Phase field models* include an internal parameter which explicitly describes the location of the interface. The internal variable satisfies a Ginzburg-Landau type equation involving a two-well potential. (See, for instance, Caginalp [6], Fried-Gurtin [11], and Gurtin [13]).

(3) Finally, in the *sharp interface theory*, an interface kinetics is explicitly introduced along the interface, providing its *driving traction* (i.e. the mechanical entropy dissipation) as a function of its propagation speed. (See Abeyaratne-Knowles [1]-[3] and Truskinovsky [37]-[39]).

The present paper focuses on the third approach which we briefly review in Section 2 below. The interfaces are assumed to be infinitely thin and have no internal structure. Using the set of conservation laws, Rankine-Hugoniot jump relations can be derived along an interface. The Clausius-Duhem inequality from the thermodynamics yields an inequality for the mechanical dissipation along each interface. The jump conditions and the entropy inequality do not determine uniquely the propagation of a phase interface. James [18] has established the existence of a *one-parameter family* of solutions, satisfying all the natural requirements, for the evolution of an initial discontinuity in a one-dimensional elastic bar (the so-called Riemann problem).

Phase boundaries behave very differently from classical shock waves arising in fluid dynamics. Such waves that require additional constitutive information derived from physics are called *undercompressive* in the mathematical field of

systems of conservation laws (Liu-Zumbrun [25] and the references therein). They are referred to as kink waves by Truskinovsky [37]-[39]) and as nonclassical shocks by Hayes-LeFloch [14]-[16]. They arise in a variety of problems of continuum mechanics, especially when dissipative and dispersive effects are in competition.

Following Abeyaratne-Knowles [3], we add an additional jump relation along the interface, called a *kinetic relation*. It determines the interfacial speed as a function of the mechanical dissipation or *driving traction*. The free parameter in James' one-parameter family of solutions to the Riemann problem is uniquely determined by the kinetic relation. For one-dimensional elastic bars, Abeyaratne-Knowles [2] established the well-posedness of the Riemann problem; more general initial data are treated in LeFloch [23]. In those results, additional constitutive information –a nucleation criterion– is also required for the possible occurence of new phase boundaries. For other interesting results on the one-dimensional problem, see Pence [29]-[30] and Shearer [35].

Developing computational algorithms for propagating phase interfaces is an important challenge. Standard numerical methods, such as shock capturing schemes and finite element methods, cannot be applied directly to the sharp interface model. Undercompressive waves such as phase interfaces turn out to be very sensitive to numerical dissipation, regularization, mesh refinements, etc, as is demonstrated in Hayes-LeFloch [16].

For classical fluid dynamics problems, it is known (by Lax-Wendroff's theorem) that difference schemes that are consistent with the conservation form of the equations converge to weak (discontinuous) solutions of the PDE's. This result is not pertinent for phase transition problems which admit multi-parameter families of solutions.

The challenge is therefore to design numerical schemes that are consistent with a given interfacial kinetic relation, so that, when the mesh size diminishes, there is convergence of the numerical solution to the solution of the sharp interface model. The interface should be driven by the given kinetic relation rather than by unphysical, numerical dissipation.

A numerical algorithm sharing the following requirements was proposed in Zhong-Hou-LeFloch [41]. Therein phase boundaries were *tracked* and other discontinuities *captured* by a high order Godunov-type scheme. This method is fully satisfactory for one-dimensional problems and in presence of a limited number of interfaces. Front tracking strategies is one of the few strategies that apply to phase boundary propagation. For multidimensional problems the techniques developed for computational fluid dynamics by LeVeque-Shyue [24] and Glimm et al. [12] could also be adapted. However tracking wave fronts for multidimensional problems and/or complex interface geometry is delicate. Some of the difficulties are avoided in the method we propose, which additionally captures certain aspects of the formation of dendritic structures in crystals.

For definiteness we focus attention on a two-dimensional problem describing antiplane shear deformations. The model is relevant for twinning processes in body-centered cubic crystals. For background on the physical modeling, we refer to Rosakis-Tsai [33] for the statics and to [34, 40] for the dynamics.

The concept of the level set formulation for moving curves or surfaces was introduced by Osher-Sethian [28] to compute various problems of curvature-driven interfaces. The principal advantage of this class of numerical methods is that they easily deal with self-intersection, topological changes, and the formation of complex interface geometry, with no additional computational cost or complexity. In particular the merging and, possibly, the nucleation of interfaces are treated automatically.

Numerical works on interface problems and their level set formulations focus primarily on curvature-driven interfaces; the evolution of the interface depends on its curvature which is determined solely from the interface. More recently the strategy was applied to cases where the flow on each side of the interface drives the interface in a way or another. For instance, in the generalized Stefan problem, the interface couples two heat diffusion equations and a nonlinear interface relation is imposed. For incompressible and immiscible fluid flows, we refer to Chang-Hou-Merriman-Osher [7]. The problem studied in this paper is of a different nature; it takes the form of an interface coupling two hyperbolic

systems of equations. This problem suffers from a higher lack of uniqueness than the problems treated in previous works.

In Section 3, we reformulate the problem under consideration by introducing a level set function, ϕ, and viewing the interface as the zero-level set of ϕ. This function evolves in time according to an Hamilton-Jacobi equation whose propagation speed is determined by extending to the whole computational domain the interfacial speed provided by the kinetic relation. Observe that the evolution of the level sets $\{\phi = k\}$ for $k \neq 0$ is irrelevant for the evolution of the interface itself. The extension of the wave speed is based on an averaged stored-energy function and a regularization parameter, ε. In the level set formulation, the interface has a finite width of order ε and the propagation speed is determined from the averaged stored-energy function.

In Section 4, the algorithm based on the level set formulation and high-order shock capturing techniques is presented.

Our formulation has some analogy in spirit with the phase field models described in Fried-Gurtin [11]. The level set function is analogous with an order parameter. The level set formulation however mimics qualitatively, but not quantitatively, the behavior of the phase field model nearby the interface. The sharp interface theory does not include explicitly interfacial and exchange energies as it is done in [11].

2. Review on the Sharp Interface Model

In this section we recall a general setting suitable to describe propagating phase boundaries in solids undergoing phase transformations. We adopt a now classical theory referred to as the *sharp interface theory* after Abeyaratne-Knowles [1].

We describe the propagation of phase interfaces in a two-phases material in a two-dimensional setting. The focus is on antiplane shear deformations of a two-dimensional plate: the displacement is supposed to be normal to the plate. In the reference configuration, the solid body under consideration occupies an

open and bounded domain $\Omega \subset \mathbb{R}^2$ with smooth boundary $\partial\Omega$. The exterior unit normal along $\partial\Omega$ is denoted by n. The domain is decomposed into two time-dependent subdomains, i.e. $\overline{\Omega} = \overline{\Omega_+(t)} \cup \overline{\Omega_-(t)}$, with the property that, at each time $t \geq 0$, the material is in its phase 1 in the domain $\Omega_+(t)$ and in its phase 2 in $\Omega_-(t)$. The interface, by definition $\Gamma(t) = \overline{\Omega_+(t)} \cap \overline{\Omega_-(t)}$, is a parametrized curve

$$\Gamma(t) = \Big\{ y(s,t) = \big(y_1(s,t), y_2(s,t)\big) \,/\, s \in I(t) \Big\}, \tag{2.1}$$

where $y(.,.)$ is a Lipschitz continuous parametrization by arc length of the (possibly several) connected components of the interface and $I(t)$ is a union of bounded and closed intervals of $\mathbb{R}$. The unit normal along $\Gamma(t)$, directed into the interior of $\Omega_-(t)$, is denoted by $n(s,t)$. Since the parameter s is the arc-length along the interface, $n(s,t) = (\partial_s y_2(s,t), -\partial_s y_1(s,t))$.

The material is described by a Lipschitz continuous displacement field $u(x,t) \in \mathbb{R}$, the out-of-plane displacement field, defined on the reference configuration Ω. For every $t \geq 0$, the restrictions of the function $u(t)$ to the domains $\Omega_\pm(t)$ is of class $\mathcal{C}^2$. The strain function ∇u in general has a jump along the interfaces $\Gamma(t)$. We set $\gamma = \nabla u \in \mathbb{R}^2$ and $v = \partial_t u \in \mathbb{R}$. The material properties are described by a stored energy function and the basic conservation principles of continuum mechanics.

The *strain energy function* provides the material energy W as a function of ∇u. Two-phase transformations can be modeled by a two-well function. We assume that W is a smooth function satisfying

$$W(\gamma) \geq W(0) = W(\xi) \qquad \text{for all } \gamma \in \mathbb{R}^2, \tag{2.2}$$

where 0 and ξ in $\mathbb{R}^2$ are two given values of strain. Moreover there exist two *disjoint* regions of strain S_i, $i = 1, 2$, such that for all $\gamma \in \mathbb{R}^2$

$$W(\gamma) = \begin{cases} W_1(\gamma) & \text{for } \gamma \in S_1, \\ W_2(\gamma) & \text{for } \gamma \in S_2, \end{cases} \tag{2.3}$$

where W_1 and W_2 are globally defined and strictly convex functions achieving their minimum point at $0 \in S_1$ and $\xi \in S_2$, respectively. Each of the two

regions S_i correspond to different material phases. The stress tensor $\sigma(\gamma) \in \mathbb{R}^2$ is classically computed by

$$\sigma_\alpha(\gamma) = \frac{\partial W}{\partial \gamma_\alpha}(\gamma), \qquad \alpha = 1, 2. \tag{2.4}$$

We also use the notation σ_i for the stress tensor associated with W_i.

If the linear elasticity theory is applicable to each phase, each W_i is a quadratic function:

$$W_1(\gamma) = \frac{\mu}{2} |\gamma|^2, \qquad W_2(\gamma) = \frac{\mu}{2} |\gamma - \xi|^2, \tag{2.5}$$

where μ a positive coefficient. Define the sound speed c by the relation $c^2 = \mu/\rho$. The stress tensors take the form $\sigma_1(\gamma) = \mu\gamma$ and $\sigma_2(\gamma) = \mu(\gamma - \xi)$. We refer to this case as the *quadratic energy model*.

The interfaces are supposed be be infinitely thin with no internal structure and the flow on both sides of the interfaces is described by a linear (or nonlinear) second-order wave equation. The compatibility relations

$$\partial_t \gamma - \nabla_x v = 0 \tag{2.6}$$

express the fact that γ is a gradient field. The conservation law of total momentum reads

$$\rho\, \partial_t v - \operatorname{div} \sigma(\gamma) = 0. \tag{2.7}$$

Differentiation is understood in the sense of distributions. According to the Clausius-Duhem's principle of thermodynamics, admissible solutions should satisfy

$$\partial_t \Big(W(\gamma) + \rho\, v^2/2 \Big) - \operatorname{div} \big(\sigma(\gamma) v \big) \leq 0. \tag{2.8}$$

The initial location of the interface,

$$\Gamma(0) = \Gamma_0, \tag{2.9}$$

and the initial conditions for the unknown fields,

$$\gamma(0) = \gamma_0, \qquad v(0) = v_0, \tag{2.10}$$

are given, with Γ_0 being a union of parametrized curves and $\gamma_0 : \Omega \to \mathbb{R}^2$ and $v_0 : \Omega \to \mathbb{R}$. Let $\partial\Omega = \partial\Omega' \cup \partial\Omega''$ be a partition of the boundary of the body. A Dirichlet boundary condition for v is imposed on $\partial\Omega'$ and a Neumann boundary condition for the stress on $\partial\Omega''$:

$$v = v_b \quad \text{on } \partial\Omega', \qquad \nabla\sigma(\gamma) \cdot n = \nabla\sigma_b \cdot n \quad \text{on } \partial\Omega''. \tag{2.11}$$

The functions v_b and σ_b are possibly time-dependent.

The solutions we are seeking are discontinuous along the interface $\Gamma(t)$, and the equations must be understood in the sense of distributions. It will be convenient to use the strain $\gamma \in \mathbb{R}^2$ and the velocity $v \in \mathbb{R}$ as the main variables. Those functions are expected to be discontinuous along $\Gamma(t)$; the traces of γ and v along Γ will be denoted by $\gamma_\pm$ and $v_\pm$, respectively. When the functions W_i are not quadratic, discontinuities in the regions $\Omega_\pm$ may also form. Provided suitable compatibility are imposed on the data γ_0, v_0, $\Omega_\pm(0)$, etc, the solution (γ, v) to the problem (2.6)–(2.11) will remain smooth, locally in time, in each domain $\Omega_\pm(t)$. In the case of the quadratic energies, the solution will remain smooth on either side of the interface $\Omega_\pm(t)$ for all times.

In a way similar to what is done in the theory of shock waves, jump relations for an interface are now deduced from the conservative form of the equations. Additionally the entropy inequality (2.8) is imposed as an attempt to select the physically correct interfaces. A propagating interface is not uniquely determined by the jump relation and the Clausius-Duhem inequality. The *mechanical dissipation* must be imposed as well, in order to determine the propagating interface in a unique way.

This non-uniqueness is explained from several standpoints. It is checked that the interface is not stable in the sense of the linearized analysis unless additional relations along the interface are imposed. The information carried on the interface by the characteristics is incomplete in order to determine the propagation of the interface. This is in contrast with the classical shock waves which obey the Lax entropy inequalities. Such underdetermined waves are called *undercompressive shocks* in the terminology of systems of conservation laws.

Assume that (γ, v) is smooth on both sides of $\Gamma(t)$. In $\Omega_\pm(t)$, the equations (2.6)-(2.7) are satisfied in a classical sense, and the inequality (2.8) is an equality. The following jump relations and entropy inequality hold along the interface, where V represents the *normal speed* of propagation,

$$V\,[\gamma \cdot n] + [v] = 0, \tag{2.12}$$

$$\rho\, V\,[v] + [\sigma(\gamma) \cdot n] = 0, \tag{2.13}$$

and

$$-V\Big[W(\gamma) + \rho\,\frac{v^2}{2}\Big] - [n \cdot \sigma(\gamma) v] \leq 0. \tag{2.14}$$

Here we denote by $[q] = q_+ - q_-$ the jump of a quantity q along the interface $\Gamma(t)$ limiting $\Omega_+(t)$ and $\Omega_-(t)$. According to our notation, the speed is $V(s,t) = \partial_t y(s,t) \cdot n(s,t)$.

Denote by f the left hand side of the inequality (2.14) divided by the velocity V. This term depends on the traces of (γ, v) on both sides of the interfaces. Based on the relations (2.12)-(2.13), it is easy to rewrite f as a function of $\gamma_\pm$ only:

$$\begin{aligned} f &= -\Big[W(\gamma) + \rho\,\tfrac{v^2}{2}\Big] - \tfrac{1}{V}[n \cdot \sigma(\gamma) v] \\ &= -[W(\gamma)] + \tfrac{1}{2}(\sigma_+ + \sigma_-) \cdot [\gamma]. \end{aligned} \tag{2.15}$$

For the quadratic energy model, the driving traction reads

$$2\,f = \mu\,\gamma_- \cdot \gamma_+ - (\gamma_+ - \xi) \cdot (\gamma_- - \xi) = \xi \cdot (\sigma_+ + \sigma_-). \tag{2.16}$$

We write $f = f(s,t)$ to emphasize that f is defined along the interfaces $\Gamma(t)$. This function is called the *driving traction* or entropy dissipation of the interface. Observe that f can be equivalently defined by the formula

$$\partial_t\Big(W(\gamma) + \rho\,\frac{v^2}{2}\Big) - \operatorname{div}\big(\sigma(\gamma) v\big) = f\,V\,\delta_{\Gamma(t)}. \tag{2.17}$$

Here, for every $t \geq 0$, $\delta_{\Gamma(t)}$ is the Dirac measure concentrated on the curve $\Gamma(t)$. By definition, if $\theta : \Omega \to \mathbb{R}$ is a smooth function, one has

$$< \delta_{\Gamma(t)}, \theta > \equiv \int_{\Gamma(t)} \theta(y(s,t))\, ds. \tag{2.18}$$

So (2.17) is an equality between bounded Radon measures, where the left hand side is defined in the sense of distributions and the right hand side is understood in the sense of Radon measures on $\Omega \times \mathbb{R}_+$.

We can now complete the formulation (2.6)–(2.8) with the so-called *kinetic relation* for $\Gamma(t)$, which provides an explicit relation between the driving traction and the propagation speed:

$$V(s,t) = g(f(s,t), n) \tag{2.19}$$

for all (s,t), where the response kinetic function $g(f,n)$ depends on the properties of the material under study and satisfies the restriction

$$f\, g(f,n) \leq 0. \tag{2.20}$$

When g is smooth enough, the latter implies

$$g(0,n) = 0 \qquad \text{and} \qquad \frac{\partial g}{\partial f}(0,n) \geq 0. \tag{2.21}$$

In particular one may take choice

$$g(f,n) = M_1\, f + M_2 |n_1|\, f, \tag{2.22}$$

where $M_1 \geq 0$ and $M_2 \geq 0$ are material constants. Observe that (2.22) is anisotropic: for an interface to move, this kinetic relation requires a higher driving traction for interface moving in the x_2 direction than in the x_1's. In other words, interfaces move more easily in the x_1 direction.

The linear stability of an interface under small perturbations is studied by Fried [10] and Pego (unpublished work). Fried establishes that the property $\partial_f g(f_0, n_0) > 0$ is a necessary and sufficient condition for an interface with unit normal n_0 and driving traction f_0 to be stable under small perturbations. His analysis is based on computing the Fourier amplification factor of a linearized version of the system of PDE's, the jump relations, and the kinetic relation. In particular the steady (i.e. $V = 0$) interfaces are stable when the kinetic function is smooth. The nonlinear stability of the interface does not follow from the theory of shock fronts to nonlinear hyperbolic systems, since the geometric Lax shock inequalities do not hold here.

3. Level Set Formulation

In this section, we introduce a new, level set formulation adapted to the sharp interface model described in Section 2. The level function φ determines the the location of the interfaces. Our formulation uses a regularized version of the two-well stored energy function.

Let $\varepsilon \in (0,1)$ be a given small parameter, roughly representing a characteristic width. The interface is searched as the zero set of a function $\varphi_\varepsilon : \mathbb{R}_+ \to \mathbb{R}$, i.e.,

$$\Gamma(t) = \Big\{ x \in \Omega \,/\, \varphi_\varepsilon(x,t) = 0 \Big\}$$

with the condition

$$\varphi_\varepsilon > 0 \quad \text{on } \Omega_+ \quad \text{and} \quad \varphi_\varepsilon < 0 \quad \text{on } \Omega_-.$$

The main difficulty is to write an equation for φ_ε that is consistent with the kinetic relation (2.19). As is classical in moving interface problems, φ_ε solves an Hamilton-Jacobi equation,

$$\partial_t \varphi_\varepsilon + V_\varepsilon \Big| \nabla \varphi_\varepsilon \Big| = 0. \tag{3.1}$$

The normal speed of propagation, $V_\varepsilon = V_\varepsilon(x,t) \in \mathbb{R}$, will be determined from the kinetic relation. First of all, (2.19) can not be used directly since it involves the traces of the variable (γ, v) from both sides of the interface. (See (2.15) or (2.16) for the definition of f.) The latter would be difficult to evaluate numerically, especially since we intend to capture the interface rather than track it. For that reason, a suitable regularization of (2.19) is necessary.

Suppose that we are given a function $\hat{W}(\gamma, h)$ for $h \in [0,1]$ that "connects" the two energy functions W_i, in the sense that, at the points $h = 0$ and $h = 1$ we have

$$\hat{W}(\gamma, 0) = W_1(\gamma) \quad \text{and} \quad \hat{W}(\gamma, 1) = W_2(\gamma).$$

Using this energy function with an "internal variable" h, we define a regularized strain energy function W_ε, in the following fashion. For each $\varepsilon > 0$, let H_ε be a regularized version of the Heaviside function H defined by $H(y) = 0$ for $y < 0$

and $H(y) = 1$ for $y > 0$. The functions H_ε should converge to H in an averaged sense. It is convenient to assume that

$$H_\varepsilon \text{ is a monotonically increasing function,}$$
$$H_\varepsilon(y) = \begin{cases} 0 & \text{if} \quad y < -\varepsilon, \\ 1 & \text{if} \quad y > \varepsilon. \end{cases} \tag{3.2}$$

Observe that the Dirac measure $\delta = dH/dy$ is correspondingly approximated by the regularized Dirac function δ_ε:

$$\delta_\varepsilon = \frac{dH_\varepsilon}{dy}. \tag{3.3}$$

The regularized energy is defined by

$$W_\varepsilon(\gamma, y) = \hat{W}(\gamma, H_\varepsilon(y)). \tag{3.4}$$

The function $\hat{W}$ should be defined by suitably averaging the energies of the two phases. Two approaches to defining $\hat{W}$ will be considered.

Model I: For arbitrary energy functions, one may use a linear combination (with respect to the parameter h) of the two energies

$$\hat{W}(\gamma, h) = W_1(\gamma) + h\Big(W_2(\gamma) - W_1(\gamma)\Big),$$

so that

$$W_\varepsilon(\gamma, y) = W_1(\gamma) + H_\varepsilon(y)\Big(W_2(\gamma) - W_1(\gamma)\Big). \tag{3.5}$$

Model II: In the special case that the two energies coincide up to a translation, one may linearly interpolate between the two wells, i.e. assuming that there exists $\xi \in \mathbb{R}^2$ such that

$$W_2(\gamma) = W_1(\gamma - \xi),$$

one defines $\hat{W}$ by

$$\hat{W}(\gamma, h) = W_1(\gamma - h\,\xi).$$

The regularized energy function is given by

$$W_\varepsilon(\gamma, y) = W_1(\gamma - H_\varepsilon(y)\,\xi). \tag{3.6}$$

The regularized problem is determined by the equations (2.6)-(2.7) with the energy function $W(\gamma)$ replaced by $W_\varepsilon(\gamma, \varphi)$. The regularized stress tensor is $\sigma_\varepsilon = \partial W_\varepsilon / \partial \gamma$. The equations (2.6)-(2.7) together with the Hamilton-Jacobi equation (3.1) form a complete set of equations for the unknowns $\gamma_\varepsilon \in \mathbb{R}^2$, $v_\varepsilon \in \mathbb{R}$, and $\varphi_\varepsilon \in \mathbb{R}$, *provided* the propagation speed V_ε in (3.1) is known. To that purpose, based on (2.6)-(2.7) (with σ replaced with σ_ε) and (3.3)-(3.4), it is an easy calculation to check that the entropy dissipation balance takes now the form

$$\partial_t \Big(W_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon) + \rho \frac{v_\varepsilon^2}{2} \Big) - \operatorname{div} \big(\sigma_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon) v_\varepsilon \big) = f_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon)\, V_\varepsilon \left| \nabla \varphi_\varepsilon \right| \delta_\varepsilon(\varphi_\varepsilon), \quad (3.7)$$

where

$$f_\varepsilon \equiv - \frac{\partial \hat{W}}{\partial h} \big(\gamma_\varepsilon, H_\varepsilon(\varphi_\varepsilon) \big) \quad (3.8)$$

will be referred to as the *regularized driving traction*.

The driving traction f was defined along the phase interface only, while f_ε is defined at *every point* of Ω. A natural extension, $n_\varepsilon(x)$, of the unit normal to the interface is defined globally (i.e. for all $x \in \Omega$) by

$$n_\varepsilon = \frac{\nabla \varphi_\varepsilon}{\left| \nabla \varphi_\varepsilon \right|}. \quad (3.9)$$

The vector field n_ε coincides with the unit normal to the interface when restricted to points $x = y(s,t)$.

The formula (3.8) for the regularized driving traction should be compared to the one we had in the $\varepsilon = 0$ case, say (2.15). To this end we rewrite the right handside of (2.17) in a form similar to the right handside of (3.7). Following [7], we have

$$\delta_\Gamma = \left| \nabla \varphi_\varepsilon \right| \delta(\varphi_\varepsilon), \quad (3.10)$$

in the sense that

$$\int_{\Gamma(t)} \theta(y(s,t))\, ds = \int_\Omega \left| \nabla \varphi_\varepsilon(x,t) \right| \theta(\varphi_\varepsilon(x,t))\, dx \quad (3.11)$$

for every smooth function $\theta : \Omega \to \mathbb{R}$. The function y by definition is the arc-length parametrization of the interface. The term $\delta(\varphi_\varepsilon)$ is classically defined

as a Radon measure on Ω. Since θ and $\nabla\varphi$ are continuous (at least), the right hand side of (3.11) has a classical meaning.

Fix a time t, which for simplicity is omitted in the notation. Introduce a (conformal) change of variables

$$x = (x_1, x_2) \to x^\star = (x_1^\star, x_2^\star) = \Big(\varphi_\varepsilon(x), \psi_\varepsilon(x)\Big), \tag{3.12}$$

where ψ_ε satisfies

$$\nabla\varphi_\varepsilon \cdot \nabla\psi_\varepsilon = 0, \qquad \Big|\nabla\psi_\varepsilon\Big| = 1.$$

The Jacobian of the transformation is

$$\begin{aligned}
\tfrac{Dx^\star}{Dx} &= \Big|\partial_{x_1}\varphi_\varepsilon\, \partial_{x_2}\psi_\varepsilon - \partial_{x_2}\varphi_\varepsilon\, \partial_{x_1}\psi_\varepsilon\Big| \\
&= \Big(\partial_{x_1}\psi_\varepsilon, \partial_{x_2}\psi_\varepsilon\Big) \cdot \Big(\partial_{x_2}\varphi_\varepsilon, -\partial_{x_1}\varphi_\varepsilon\Big) \\
&= \Big|\nabla\varphi_\varepsilon\Big|\,\Big|\nabla\psi_\varepsilon\Big| \\
&= \Big|\nabla\varphi_\varepsilon\Big|,
\end{aligned}$$

since $\Big(\partial_{x_1}\psi_\varepsilon, \partial_{x_2}\psi_\varepsilon\Big)$ and $\Big(\partial_{x_2}\varphi_\varepsilon, -\partial_{x_1}\varphi_\varepsilon\Big)$ are parallel vectors in $\mathbb{R}^2$. One may need to change ψ into $-\psi$ to get the correct sign in the latter two equalities. The function ψ exists in a neighborhood of the interface, at least, which is sufficient for our purpose.

Using (3.12), we arrive at

$$\begin{aligned}
\int_\Omega \delta(\varphi_\varepsilon(x))\theta(x)\Big|\nabla\varphi_\varepsilon(x)\Big|\,dx &= \int_{\Omega^\star} \delta(x_1^\star)\,\theta^\star(x^\star)\,dx^\star \\
&= \int_{\{x_1^\star = 0\}} \theta^\star(0, x_2^\star)\,dx_2^\star
\end{aligned} \tag{3.13}$$

with the obvious notation for $\Omega^\star$ and $\theta^\star(x^\star) = \theta(x)$. Note that $\Big\{x_1^\star = 0\Big\}$ is the equation of the interface $\Big\{y(s) = 0\Big\}$, so the right handside of (3.13) and the left handside of (3.11) are both an integral of the test function along the interface. But $\varphi_\varepsilon(y(s)) = 0$ implies $\nabla\varphi_\varepsilon \cdot \partial_s y = 0$, so the vectors $\nabla\varphi_\varepsilon$ and $\partial_s y$ are orthogonal. Since $\psi_\varepsilon(y(s)) = x_2^\star$, we obtain by differentiation

$$dx_2^\star = \Big|\nabla\psi_\varepsilon \cdot \partial_s y\Big|\,ds = ds,$$

since $\Big|\nabla\psi_\varepsilon\Big| = |\partial_s y| = 1$ and $\nabla\psi_\varepsilon$ and $\partial_s y$ are both orthogonal to $\nabla\varphi_\varepsilon$.

Comparing (3.7)-(3.10) and (2.17)-(2.19), we propose to define V_ε by the kinetic relation (2.19), the driving traction f being replaced with f_ε. At this stage, we are implicitly replacing the "exact" Dirac mass in (3.10) by its regularization introduced in (3.3).

In other words, we define V_ε by

$$V_\varepsilon = g\Big(f_\varepsilon, \frac{\nabla\varphi_\varepsilon}{\big|\nabla\varphi_\varepsilon\big|}\Big). \tag{3.14}$$

For future reference, we summarize the level formulation:

$$\partial_t\gamma_\varepsilon - \nabla_x v_\varepsilon = 0, \tag{3.15}$$

$$\rho\,\partial_t v_\varepsilon - \operatorname{div}\sigma_\varepsilon(\gamma_\varepsilon,\varphi_\varepsilon) = 0, \tag{3.16}$$

and

$$\partial_t\varphi_\varepsilon + g\Big(f_\varepsilon, \frac{\nabla\varphi_\varepsilon}{\big|\nabla\varphi_\varepsilon\big|}\Big)\big|\nabla\varphi_\varepsilon\big| = 0, \tag{3.17}$$

Besides the initial and boundary conditions (2.10)-(2.11) for γ_ε and v_ε, we need an initial and boundary condition for φ_ε:

$$\varphi_\varepsilon(0) = \varphi_0 \quad \text{in } \Omega, \qquad \varphi_\varepsilon = \varphi_b \quad \text{on } \partial\Omega, \tag{3.18}$$

where φ_0 and φ_b are given data.

Several observations should be made. First of all, the jump relations (2.12)-(2.13) and the kinetic relation (2.19) do not explicitly appear in the level set formulation. However it is checked [17] that, as expected, the jump relations and the kinetic relation are recovered as $\varepsilon \to 0$. Including the kinetic relation in the formulation comes however at the expense of introducing a small parameter, ε, which must be handled with care in the numerics. Our level set formulation is formally analogous to a phase field model, introduced by Fried-Gurtin [11] for the phase dynamics in solids and by Caginalp [6] for the Stefan problem for fluids.

Restricting now attention to one-dimensional elastic bars. We consider solutions that only depend upon x_1 and such that $\gamma_2 = 0$. For simplicity, set

$x = x_1$, so now $x \in \mathbb{R}$ and $\Omega = \mathbb{R}$. In this setting, the level set model takes the form :

$$\begin{aligned} &\partial_t \gamma_\varepsilon - \partial_x v_\varepsilon = 0, \\ &\rho\, \partial_t v_\varepsilon - \partial_x \sigma_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon) = 0, \\ &\partial_t \varphi_\varepsilon + g\Big(f_\varepsilon\Big)\Big|\partial_x \varphi_\varepsilon\Big| = 0. \end{aligned} \tag{3.19}$$

For Model I, the regularized energy function is

$$\hat{W}(\gamma, h) = \frac{\mu}{2}\Big((1-h)\gamma^2 + h(\gamma - \xi)^2\Big) = \frac{\mu}{2}\Big(\gamma^2 + h\,\xi^2 - 2\,\xi\, h\gamma\Big).$$

The regularized stress is

$$\sigma_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon) = \mu(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\,\xi),$$

and the regularized driving traction is

$$f_\varepsilon = \mu\,\xi\,\Big(\gamma_\varepsilon - \frac{\xi}{2}\Big) = \xi\,\sigma_\varepsilon + \xi^2\Big(H_\varepsilon(\varphi_\varepsilon) - 1/2\Big).$$

Using a linear kinetic relation

$$g(f) = Mf$$

and setting $c = (\mu/\rho)^{1/2}$ and $N = M\mu\,\xi$, Model I reads

$$\text{Model I}: \quad \left\{ \begin{array}{l} \partial_t \gamma_\varepsilon - \partial_x v_\varepsilon = 0, \\ \partial_t v_\varepsilon - c^2 \partial_x\Big(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\,\xi\Big) = 0, \\ \partial_t \varphi_\varepsilon + N\,\Big(\gamma_\varepsilon - \frac{\xi}{2}\Big)\,|\partial_x \varphi_\varepsilon| = 0. \end{array} \right. \tag{3.20}$$

For Model II, the regularized energy function is

$$\hat{W}(\gamma, h) = \frac{\mu}{2}(\gamma - h\,\xi)^2.$$

So we get

$$\sigma_\varepsilon(\gamma_\varepsilon, \varphi_\varepsilon) = \frac{\partial \hat{W}}{\partial \gamma}\Big(\gamma_\varepsilon, H_\varepsilon(\varphi_\varepsilon)\Big) = \mu\Big(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\,\xi\Big)$$

and

$$f_\varepsilon = -\frac{\partial \hat{W}}{\partial h}\Big(\gamma_\varepsilon, H_\varepsilon(\varphi_\varepsilon)\Big) = \mu\,\xi\Big(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\,\xi\Big) = \xi\,\sigma_\varepsilon.$$

The regularized stress is the same in Models I and II, but the driving tractions are different. Model II takes the form :

$$\text{Model II}: \quad \begin{cases} \partial_t \gamma_\varepsilon - \partial_x v_\varepsilon = 0, \\ \partial_t v_\varepsilon - c^2 \partial_x \Big(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\, \xi \Big) = 0, \\ \partial_t \varphi_\varepsilon + N \left(\gamma_\varepsilon - H_\varepsilon(\varphi_\varepsilon)\, \xi \right) |\partial_x \varphi_\varepsilon| = 0. \end{cases} \tag{3.21}$$

For both models, the corresponding sharp interface model is

$$\text{Limiting Model}: \quad \begin{cases} \partial_t \gamma - \partial_x v = 0, \\ \partial_t v - c^2 \partial_x \Big(\gamma - \xi H(\varphi) \Big) = 0, \end{cases} \tag{3.22}$$

where $\varphi = 1$ in the phase 1 and $\varphi = 0$ in the phase 2.

4. Numerical Algorithm

A numerical algorithm based on the level set formulation introduced in Section 3 is developed in [17], based on modern higher-order, shock-capturing techniques. Consider a square domain Ω and a regular cartesian mesh with mesh size Δx and Δt. Since we use explicit differencing and the problem under study is hyperbolic, the mesh parameters are restricted by the CFL stability condition. It is numerically convenient to compute directly the displacement u rather than the two variables γ and v.

The computation was performed with the quadractic model and the averaged energy of Model II, which has been found to be more effective numerically. The regularized energy is given by

$$W_\varepsilon(\gamma, y) = (1 - H_\varepsilon(y)) \frac{\mu}{2} \left| \gamma \right|^2 + H_\varepsilon(y) \frac{\mu}{2} \left| \gamma - \xi \right|^2. \tag{4.1}$$

We also assume that the well for the phase 2 has the form $\xi = (0, k)$. The regularized stress reads:

$$\sigma_\varepsilon(\gamma, y) = \mu \left(\gamma - H_\varepsilon(y)\, \xi \right). \tag{4.2}$$

The kinetic relation is taken to be

$$g(f, n) = M_1\, f + M_2\, |n_1| f, \tag{4.3}$$

with suitably chosen values of the parameters M_1 and M_2.

The system to be solved numerically reads

$$\begin{aligned} &\tfrac{1}{c^2}\,\partial_{tt}u - \Delta u = -k\,\partial_{x_2} H_\varepsilon(\varphi), \\ &\partial_t\varphi - \xi_2\,\mu\Big(\partial_{x_2}u - k\,H_\varepsilon(\varphi)\Big)\Big(M_1\,|\nabla\varphi| + M_2\,|\partial_{x_1}\varphi|\Big) \;=\; 0. \end{aligned} \tag{4.5}$$

The numerical experiments are performed with an ellipsoidal region made of a material in the phase 1 surrounded by the phase 2 of the material. In our calculations, $\xi_2 = c = \mu = 1$ and we solve the coupled equations for u and φ,

$$\partial_{tt}u = \Delta u - \delta_\varepsilon(\varphi)\,\partial_{x_2}\varphi,$$

$$\partial_t\varphi - (\partial_{x_2}u - k\,H_\varepsilon(\varphi))(M_1\,|\nabla\varphi| + M_2\,|\partial_{x_1}\varphi|) = 0.$$

The numerical algorithm is as follows:

Initialization: At the initial time $t = 0$, the level set function is defined to be the signed distance-function to the interface.

Step 1: Evolution-step.

The displacement and the level set function are evolved according to (4.5), using finite differences. A higher-order centered scheme is used for the displacement. The Hamilton-Jacobi type equation is discretized by using a second order ENO (essentially nonoscillatory) upwinding scheme.

Step 2: Re-initialization.

The level set function is re-initialized to be the signed distance-function to the new interface.

The computation of phase interfaces proves to be very challenging. We review some of the difficulties that we had to cope with:

The extension of the interface velocity nearby the phase boundary is discontinuous at the interface. This produces a discontinuous level set function in the time evolution. We overcome this difficulty by introducing a re-initialization procedure every time step to enforce the level set function to coincide with the

signed distance function for all times. This also ensures that the thickness of the smoothed interface layer remains small for all times.

In the numerics, the driving traction and therefore the speed of propagation in the Hamilton-Jacobi equation admits a large numerical gradient near the interface. This tends to produce numerical oscillations at the phase boundary which may give rise to incorrect phase velocity. It is important that the mesh size h remains much smaller than the regularization parameter: $h << \varepsilon$. (In pratice we used $5\,h \leq \epsilon \leq 10\,h$.) The re-initialization is motivated by the results in Section 4: this is necessary in order for the function ϕ to remain continuous.

We observed sensitivity of the method with respect to the mesh. This is to be expected in view of previous numerical experiments on similar problems, for instance on incompressible fluid dynamics problems. The choice of the averaged energy function is important to prevent formation of spurious spikes in the driving traction near the interface. Model II turned out to behave much better in this respect.

The boundary condition for u is $u = 0$ on the top and bottom boundaries, and $u_n = k$ at the left and right boundaries. With such boundary conditions, the steady state solution should be a configuration with volume fraction equal to k. We used one sided boundary condition for φ at the solid wall boundary condition. For most of the time, this is just the upwinding boundary condition.

Formation of cusp singularities and complex topological changes in the phase boundary can be captured naturally without explicit tracking of the phase boundary. We have tested our model for several kinetic relations. These results give qualitative agreement with the sharp interface theory. The level set formulation can also compute beyond the time where the sharp interface formulation fails.

See Figure 4.1 and 4.2 for numerical results obtained with a square mesh having 256 points in each space directions, $\varepsilon = 0.01$ and $M_1 = 0$, $M_2 = 3$ in the formula (4.3). The initial data is a small ellipse with main axis having length $a = 0.3$ and $b = 0.15$. Figure 4.1 displays the phase boundary at different times. In Figure 4.1a, the larger phase boundary is reached at time $t = 0.2$. The

asymptotic state is reached at time $t = 10$ in Figure 4.1e. Figure 4.2 shows that the total energy decays in time, as the solution reaches an asymptotic state. We refer to [17] for extensive numerical results.

5. Concluding Remarks

We presented in this paper a numerical algorithm to capture moving phase boundaries in solid materials. The solutions to the sharp interface model can be computed accurately and efficiently.

Further investigations of this model and other models including more detailed physics of phase transformations are desirable. A more realistic model should take into account thermal effects, which are important for phase transformations. A three-dimensional setting including a nonlinear geometry of the equilibrium wells could also be considered.

In order to make quantitative predictions with the sharp interface model, the kinetic response function should be determined from laboratory experiments. It would be also interesting to investigate whether a criterion for the *nucleation* of new phase boundaries may be incorporated in the level set formulation. Another avenue of research is to incorporate in the numerical algorithm an asymptotic model describing the behavior of the interface near a spike or a cusp.

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