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Front Dynamics in Inhomogeneous Solids

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Abstract. In the paper, results of thermomechanical modeling of moving discontinuities in heterogeneous solids are discussed. Attention is focused on the velocity of the discontinuity which cannot be calculated by means of standard thermomechanical conservation laws. The corresponding kinetic relations for phase transition fronts and straight through crack propagation are derived on the basis of the material description of continuum mechanics and the thermodynamics of discrete systems.

Key words: Moving discontinuities, Heterogeneous solids, Dynamics, Kinetic relation.

1. Introduction

Fronts are moving discontinuity surfaces (or lines) dividing the medium into distinct parts.

Conservation laws for mass, linear momentum, and energy are not sufficient for the description of moving discontinuities. Certain additional relations are requested for isolating a unique solution among the whole set of possible ones satisfied by given initial and boundary conditions.

The formal expression of the driving force acting on a singular set of material points (crack tip or phase-transition front) and of the accompanying dissipation in an irreversible progress of the set is independent of the precise material behavior at regular points [1]. As these sets appear to be displaced as a consequence of the general evolution of a field solution under the time dependent boundary conditions, driving forces acting on them are defined by duality with velocities of points of the sets. The power expended by the driving force can be written as the general bi-linear form

$$P(\mathbf{f}) = \mathbf{f} \cdot \mathbf{V}. \tag{1}$$

Here $\mathbf{f}$ is the driving force, and $\mathbf{V}$ is the material velocity [2].

In some cases, the observed motion of singular sets is thermodynamically irreversible, and the force $\mathbf{f}$ of a non-Newtonian nature acquires a physical meaning only through the power (Eq. (1)) it expends, as this is, in fact, its definition in a weak formulation on the material manifold. The irreversible progress of the singularity set is then governed by the second law of thermodynamics, that means (in terms of temperature $\theta_{\mathcal{S}}$ and entropy production $\sigma_{\mathcal{S}}$ at the singularity)

$$\mathbf{f} \cdot \mathbf{V} = \theta_{\mathcal{S}}\, \sigma_{\mathcal{S}} \geq 0, \tag{2}$$

and the closure of the full solution of the evolution problem requires the formulation of a kinetic law relating $\mathbf{f}$ and $\mathbf{V}$ or a hypothesis about entropy production at the singularity.

Consider a regular (simply connected) material body in which a straight through crack $C(t)$ expands with material velocity V_C at the crack tip. The extension of the crack is collinear to the crack. A material force f_C acting at the crack tip (sucking the crack in the body) is none other than the energy-release rate G (up to the velocity) [1]

$$G = f_C V_C = \theta_C\, \sigma_C \geq 0. \tag{3}$$

In quasi-statics and in the absence of thermal and intrinsic dissipations, the energy-release rate can be computed by means of the celebrated J-integral of fracture [3] that is known to be path-independent and, therefore, provides a very convenient estimation tool once the field solution is known. However, the velocity at the crack tip remains undetermined and requires additional consideration.

A similar situation holds for a displacive phase-transformation front propagation. A stress-induced martensitic phase transformation in a single crystal of a thermoelastic material occurs by the fast propagation of sharp interfaces through the material. Following the balance of pseudomomentum [2], one can determine the driving force acting on the interface between phases. However, as in the case of the crack tip, this is not enough to determine the velocity of the phase-transition front in crystalline solids.

Additional constitutive information is usually provided in the form of a kinetic relation between the driving force and the velocity of the phase boundary. The notion of kinetic relation is introduced by [4] following ideas from materials science. It is well understood [5] that the kinetic relation is required because of the non-equilibrium character of the phase transformation process. It is clear that the notion of kinetic relation cannot by itself solve the problem of the moving front propagation. The problem is transferred to another level, namely, to the derivation of this kinetic relation.

The macroscopic description of moving fronts in solids (such as phase-transition fronts or crack fronts) is based on the conventional local equilibrium approximation. This means that all the thermodynamic quantities, including temperature and entropy are defined following conventional methods [6]. However, both phase-transition and crack propagation are irreversible processes accompanied by entropy production at their moving front. Accordingly, it is clear that the local equilibrium approximation is not sufficient to describe such a behavior.

It is not an easy task to develop the non-equilibrium description, because even the notion of non-equilibrium temperature can be defined in different ways [7]. Fortunately, there is a rather nice similarity between the discrete representation of conservation laws [8] and the thermodynamics of discrete systems [9].

As shown by [10, 11], the Godunov-type numerical schemes can be reformulated in terms of excess quantities, which appear due to the interaction between discrete systems. The non-equilibrium jump relations at moving fronts, established by [12], are also formulated in terms of the excess quantities.

We have proposed to determine all the needed fluxes by means of the non-equilibrium jump relations [13]. The continuity of excess quantities across the

moving front is used for the closure of the model. This leads to the relation between the stress jump at the discontinuity and the corresponding driving force. From this even the velocity of a moving front can be determined [14]. As a consequence, we obtain a thermodynamically consistent numerical algorithm which can be applied to front propagation problems [13].

2. Velocity of moving front

2.1. Phase boundary

It is well known that the velocity of the phase boundary can be calculated by means of the jump relation corresponding to the balance of linear momentum [15] which can be represented in a one-dimensional case as

$$\bar{V}_N[\rho_0 v] + [\sigma] = 0, \tag{4}$$

where $\bar{V}_N$ is the material velocity of the front, ρ_0 is the density of a material, v is the particle velocity, and σ is the one-dimensional stress, rectangular brackets denote jumps across the front.

The only difficulty is that all fields should be determined in advance, accounting the unknown velocity of the front.

In the admitted non-equilibrium description [16], both stress and velocity are represented as the sum of averaged (local equilibrium) and excess parts:

$$\sigma = \bar{\sigma} + \Sigma, \quad v = \bar{v} + \mathcal{V}. \tag{5}$$

Here $\bar{\sigma}$ and $\bar{v}$ are averaged fields and Σ and $\mathcal{V}$ are the corresponding excess quantities.

At the phase boundary we apply the continuity of excess quantities [13]

$$[\Sigma] = 0, \quad [\mathcal{V}] = 0, \tag{6}$$

which leads to the jump relation for linear momentum in terms of averaged quantities

$$\bar{V}_N[\rho_0 \bar{v}] + [\bar{\sigma}] = 0, \tag{7}$$

and simultaneously determines the value of the jump of the averaged stress at the phase boundary for a thermoelastic body [14]

$$[\bar{\sigma}] = -2\theta_0 \left[\alpha(3\lambda + 2\mu)\right]. \tag{8}$$

Here θ_0 is the reference temperature, α is the coefficient of thermal expansion, λ and μ are Lamé coefficients.

Having the value of the stress jump, we can derive the relation for the determination of the velocity of the front in terms of the stress jump [17]

$$\rho_0 \bar{V}_N^2 = \frac{[\bar{\sigma}]}{A[\bar{\sigma}] - B}, \tag{9}$$

or in terms of the driving force

$$\rho_0 \bar{V}_N^2 = \frac{f_{\mathcal{S}}}{A f_{\mathcal{S}} - B/D}, \tag{10}$$

because the stress jump and the driving force are related (in the isothermal case) as follows [17]

$$f_{\mathcal{S}} \left[\frac{1}{\alpha(3\lambda + 2\mu)}\right] = \frac{\theta_0[\bar{\sigma}]}{2} \left[\frac{1}{\lambda + 2\mu}\right]. \tag{11}$$

Here $f_{\mathcal{S}}$ is the driving force, A, B and D are coefficients depending on material properties and transformation strain.

Eq. (11) is nothing else but the kinetic relation for the phase transition front propagation.

Thus, the supplementary constitutive information needed to avoid the non-uniqueness of the solution of the boundary-value problem is provided by means of non-equilibrium jump relations at the moving phase boundary, which are formulated in terms of excess quantities. The same excess quantities are used in the construction of a finite-volume numerical scheme [10, 11] that coincides with the conservative wave propagation algorithm in the absence of phase transformation. The continuity of the excess quantities at the phase boundary leads to the conservation of genuine jumps at the phase boundary. As a result, a closed system of governing equations and jump relations can be solved numerically [11].

Results of numerical simulations show that the proposed approach allows us to capture experimental observations while corresponding to theoretical predictions [13].

In the adiabatic formulation, the excess stresses needed for numerical calculations are determined in the same way as in the isothermal case. The non-equilibrium jump relations provide the possibility to establish a kinetic relation taking into account the temperature variation [17].

Numerical simulations of the phase-transition front propagation in Ni-Ti bar show that the entropy production at the moving phase boundary and latent heat release provide two different contributions in the temperature variation. The latter leads to distinct kinetic behaviors of the phase boundary depending on latent heat release [17].

2.2. Straight brittle crack

A similar procedure can be developed for the dynamics of a crack in mode I. The projection of the balance of linear momentum on the normal to the crack front leads to [18]

$$V_C\,[\rho_0(1+\bar{\varepsilon}_{11})V_C] - [\bar{\sigma}_{11}+\Sigma_{11}] = 0, \tag{12}$$

where V_C is the velocity of the crack front, $\bar{\sigma}_{11}$ is the component of the stress tensor normal to the crack front, $\bar{\varepsilon}_{11}$ is the corresponding strain tensor component, square brackets still denote jumps across the crack front.

Since we have no material behind the crack front, jumps are equal to values of quantities in front of the crack front from which we obtain

$$V_C^2 = \frac{\bar{\sigma}_{11}+\Sigma_{11}}{\rho_0(1+\bar{\varepsilon}_{11})}. \tag{13}$$

The stress at the crack front is related to the driving force f_C [18]

$$\bar{\sigma}_{11}+\Sigma_{11} = Af_C, \tag{14}$$

which is calculated by means of the J-integral as follows:

$$f_C = \frac{J}{l}, \tag{15}$$

where l is a scaling factor which has the dimension of a length.

Therefore, we will have different results for zero and non-zero excess stresses. Assuming zero excess stress at the crack front, we come to the well known relation for the crack velocity [19]. For non-zero values of the excess stress at the crack front, we arrive at more realistic expressions, as shown in [18].

We have applied the same formalism to a non-equilibrium description of the crack propagation process as in the case of phase-transition fronts. The non-equilibrium jump relation at the crack front allows us to establish a kinetic relation between the driving force and the velocity of a straight-through crack. This kinetic relation depends on the assumption concerning excess stress values at the crack front. It is shown that by zero values of the excess stress at the crack front, the obtained kinetic relation can be reduced to the prediction of the linear elasticity theory. However, the adopted approach provides new possibilities. In particular, a simple proportionality between excess and local equilibrium stresses leads to a limiting velocity which is different from the Rayleigh wave speed.

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