DYNAMICS OF IMPACT-INDUCED PHASE TRANSITION FRONTS

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Abstract. Most experiments in martensitic phase transformations are performed under quasi-static loading of a specimen. The only well-documented experimental investigation concerning the impact-induced austenite-martensite phase transformations was given by Escobar and Clifton ([1], [2]). As Escobar and Clifton noted, measured velocity profiles provide a difference between the particle velocity and the transverse component of the projectile velocity. This velocity difference, in the absence of any evidence of plastic deformation, is indicative of a stress induced phase transformation that propagates into the crystals from the impact face. We develop a thermomechanical approach to the modeling of phase-transition front propagation based on the balance laws of continuum mechanics in the reference configuration [3] and the thermodynamics of discrete systems [4]. It is shown that the developed model captures the experimentally observed particle velocity difference.

1. INTRODUCTION

Attempts of numerical simulations of moving phase boundaries in solids meet the problems with constitutive modeling of the nucleation criterion and kinetic relation at the phase boundary as well as with the construction of a proper numerical algorithm. It is found [5],[6] that the kinetic relation and the nucleation criterion together single out a unique solution from among infinitely many solutions that satisfy jump conditions at discontinuities. We propose to specify these additional constitutive notions by means of so-called thermodynamic consistency conditions [7]. In this case the construction of the algorithm is complemented by the development of a thermodynamic model of martensitic phase transformations. We consider the state of a material at a continuum point as either austenitic or martensitic but never both. We assume that each phase has its own material properties. We demand that jump conditions following from continuum mechanics are fulfilled at the interface between two phases. The thermodynamic consistency conditions are different for processes with and without entropy production. This gives us the possibility to apply distinct consistency conditions in the bulk and at the phase boundary (where
entropy is produced). The latter plays the role of a kinetic relation without its specification in an explicit form. A thermodynamic criterion of the initiation of phase transition process follows from the simultaneous satisfaction of both distinct thermodynamic consistency conditions at the phase boundary. The obtained model is completely discrete because the thermodynamic consistency conditions manifest themselves only on a discrete level of the description. At the same time, the model is completely thermomechanical, because it does not need any additional information about the phase transformation process.

2. UNIAXIAL MOTION OF A SLAB

Consider a slab, which in an unstressed reference configuration occupies the region $0 < x_1 < L$, $-\infty < x_2, x_3 < \infty$, and consider uniaxial motion of the form

$$u_i = u_i(x, t), \quad x = x_1,$$

where $t$ is time, $x_i$ are spatial coordinates, $u_i$ are components of the displacement vector. In this case, we have only three non-vanishing components of the strain tensor

$$\varepsilon_{11} = \frac{\partial u_1}{\partial x}, \quad \varepsilon_{12} = \varepsilon_{21} = \frac{1}{2} \frac{\partial u_2}{\partial x}, \quad \varepsilon_{13} = \varepsilon_{31} = \frac{1}{2} \frac{\partial u_3}{\partial x}.$$ (2)

Without loss of generality, we can set $\varepsilon_{13} = 0$. Then we obtain uncoupled systems of equation for longitudinal and shear components which express the balance of linear momentum and the time derivative of the Duhamel-Neumann thermoelastic constitutive equation, respectively. We focus our attention on the system of equations for shear components, because martensitic phase transformation is expected to be induced by shear:

$$\frac{\partial (\rho_0(x)v_2)}{\partial t} - \frac{\partial \sigma_{12}}{\partial x} = 0, \quad \frac{\partial}{\partial t} \left( \frac{\sigma_{12}}{\mu(x)} \right) - \frac{\partial v_2}{\partial x} = 0.$$ (3)

Here $\sigma_{12}$ is the shear component of the Cauchy stress tensor, $v_2$ is the transversal component of the velocity vector, $\rho_0$ is the density, $\mu$ is the Lamé coefficient. The indicated explicit dependence on the point $x$ means that the body is materially inhomogeneous in general.

To consider the possible irreversible transformation of a phase into another one, the separation between the two phases is idealized as a sharp, discontinuity surface $S$ across which most of the fields suffer finite discontinuity jumps.

Let $[A]$ and $< A >$ denote the jump and mean value of a discontinuous field $A$ across $S$, the unit normal to $S$ being oriented from the “minus” to the “plus” side. Let $V$ be the material velocity of the geometrical points of $S$. The material velocity $V$ is defined by means of the inverse mapping $X = \chi^{-1}(x, t)$, where $X$ denotes the material points [3]. For homothermal and coherent phase transition fronts we have the following continuity conditions [8]-[9]:

$$[V] = 0, \quad [\theta] = 0 \quad \text{at} \ S.$$ (4)
Jump relations are formulated according to the theory of weak solutions of hyperbolic systems. Those relations associated with the balance of linear momentum and balance of entropy read [8]-[9]

\[ V_N[\rho_0 v_2] + [\sigma_{12}] = 0, \quad V_N[S] + \left[ \frac{k}{\theta} \frac{\partial \theta}{\partial x} \right] = \sigma_S \geq 0, \quad (5) \]

where \( V_N = \dot{V} \) is the normal speed of the points of \( S \), and \( \sigma_S \) is the entropy production at the interface. As it was shown in [8]-[9], the entropy production can be expressed in terms of the so-called ”material” driving force \( f_S \)

\[ f_S V_N = \theta_S \sigma_S \geq 0, \quad f_S = -[W] + < \sigma_{ij} > [\varepsilon_{ij}], \quad (6) \]

where \( \theta_S \) is the temperature at \( S \) and \( W \) is the free energy per unit volume.

In a dynamic problem we shall seek piecewise smooth velocity and stress fields \( v_2(x, t), \sigma_{12}(x, t) \) for inhomogeneous thermoelastic materials, which conform the following initial and boundary conditions:

\[ \sigma_{12}(x, 0) = v_2(x, 0) = 0, \quad \text{for} \quad x > 0, \quad \text{(7)} \]

\[ v_2(0, t) = v_0(t), \quad \text{or} \quad \sigma_{12}(0, t) = \sigma_0(t) \quad \text{for} \quad t > 0, \quad \text{(8)} \]

and satisfy the field equations (3) and jump conditions (4)-(6).

The system of equations (3) is a system of conservation laws which is suitable for a numerical solution by the numerical algorithm described in [10].

3. NUMERICAL RESULTS

The only experimental investigation concerning impact-induced austenite-martensite phase transformations was given by Escobar and Clifton [1], [2]. In their experiments, Escobar and Clifton used thin plate-like specimens of Cu-14.44Al-4.19Ni shape-memory alloy single crystal. One face of this austenitic specimen was subjected to an oblique impact loading, generating both shear and compression. The conditions of the experiment were carefully designed so as to lead to plane wave propagation in the direction of the specimen surface normal and to activate only a single variant of martensite. The measurements are taken in the central part of the rear face of the specimen and were completed before the arrival of any release wave originating at the lateral faces of the slab. As Escobar and Clifton noted, a difference between the measured particle velocity and the transverse component of the projectile velocity is indicative of a stress induced phase transformation that propagates into the crystals from the impact face in the absence of any evidence of plastic deformation.

To compare the results of numerical simulation with experimental data by Escobar and Clifton [1], [2], we extract the properties of austenite phase of the Cu-14.44Al-4.19Ni shape-memory alloy from their paper: the density \( \rho = 7100 \text{ kg/m}^3 \), the elastic modulus \( E = 120 \text{ GPa} \), the shear wave velocity \( c_s = 2613.5 \text{ m/s} \), the dilatation coefficient \( \alpha = 6.75 \cdot 10^{-6} \text{ 1/K} \). For the martensitic phase we choose, respectively, \( E = 60 \text{ GPa}, \ c_s = 2128 \text{ m/s}, \) with the same density and dilatation coefficient as above.
To compare the results of modeling with experimental data by Escobar and Clifton, the calculations of the particle velocity were performed for different impact velocities.

a) b)

Figure 1: Particle velocity in the impact problem with phase transformation. a) Time-history; b) Particle velocity at phase boundary.

The results of the comparison are given in Fig. 1. The time-history of the particle velocity shows that at early times we have nothing because no waves reached the considered point. After the coming of a fastest elastic wave, the jump in the particle velocity is observed, but its amplitude is lower than the initial one. This amplitude is restored in the second jump, which is associated with phase transition front. The second part of the figure shows that the particle velocity at the phase boundary is practically independent of the impact velocity. This constant value of the particle velocity corresponds to the constant shear stress at the phase boundary. The corresponding value of the shear strain is equal to 0.0124, and can be associated with the transformation strain (c.f. [11], [12]).

References