A THERMODYNAMIC APPROACH TO MODELING OF STRESS-INDUCED PHASE-TRANSITION FRONT PROPAGATION IN SOLIDS

A. BEREZOVSKI, J. ENGELBRECHT
Department of Mechanics and Applied Mathematics
Institute of Cybernetics at Tallinn Technical University
Akadeemia tee 21, 12618 Tallinn, Estonia

AND

G.A. MAUGIN
Laboratoire de Modélisation en Mécanique
Université Pierre et Marie Curie
UMR 7607, Tour 66, 4 Place Jussieu, Case 162
75252, Paris Cédex 05, France

1. Introduction

A number of continual models for describing the dynamics of phase boundaries has been developed in order to understand evolving phase transitions (cf., for example, [1]). All these models take the basic balance laws of continuum mechanics as a starting point. However, the propagation speed of phase-transition fronts is not completely determined by the balance of momentum in the dynamic problems involving phase boundaries. As a result, an additional constitutive criterion is needed for the determination of the dynamics of phase boundaries. In the sharp-interface theory, phase boundaries are treated as discontinuity surfaces of zero thickness. The canonical formalism of continuum mechanics with a full exploitation of the balance of so called pseudo- or canonical momentum leads to the balance of "material" forces at the phase-transition front. The surface "balance" equation plays an essential role in the description of phase-transition front propagation. However, in all the theories, the constitutive relation for free energy is assumed to be able to describe the states in both sides of the phase-transition front simultaneously.

Here we consider a simpler situation, when each phase has its own prescribed classical constitutive equation for the thermoelastic free energy. In this case, the driving force and the entropy flux should be computed by means of the surface "balance" equation. However, for the computation of the phase-transition front propagation, the equations are not closed, because a criterion of the progress of the front is additionally needed. In this paper, a thermodynamic criterion is proposed, based on the stability conditions for complex thermodynamic systems. The conditions of the stability are derived and expressed in terms of contact quantities, which are introduced in the framework of the thermodynamics of discrete systems in order to describe the nonequilibrium states of discrete elements. The contact quantities at the phase boundary are determined by means of the above-mentioned balance of material forces at the interface and the jump relation for the entropy. As a result, an efficient and robust numerical method capable of solving dynamical phase transition problems is developed. As a first attempt, the numerical simulation of stress-induced austenitic-martensitic phase-transition front propagation in the one-dimensional case is performed. The analysis of the two-dimensional case is in progress.

2. Balance laws for linear thermoelasticity

We consider both two phases of the material as thermoelastic heat conductors. If geometrical nonlinearities are neglected, then the main *bulk* equations of inhomogeneous linear isotropic thermoelasticity (in the absence of body forces) can be written as the following three equations:

$$\rho_0(\mathbf{x})\frac{\partial v_i}{\partial t} - \frac{\partial \sigma_{ij}}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial \sigma_{ij}}{\partial t} = \lambda(\mathbf{x})\frac{\partial v_k}{\partial x_k}\delta_{ij} + \mu(\mathbf{x})\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial \theta}{\partial t}\delta_{ij}, \tag{2}$$

$$C(\mathbf{x})\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i}\left(k(\mathbf{x})\frac{\partial \theta}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial v_k}{\partial x_k}, \tag{3}$$

of which the second one is none other than the time derivative of the Duhamel-Neumann thermoelastic constitutive equation [2]. Here t is time, x_j are spatial coordinates, v_i are components of the velocity vector, σ_{ij} is the Cauchy stress tensor, ρ_0 is the density, θ is temperature, $C(\mathbf{x}) = \rho_0 c$, c is the specific heat at constant stress, k is the thermal conductivity. The *dilatation coefficient* α is related to the thermoelastic coefficient m, and the Lamé coefficients λ and μ by $m = -\alpha(3\lambda + 2\mu)$. The indicated explicit dependence on the point $\mathbf{x}$ means that the body is materially inhomogeneous in general.

The system of equations (1)-(3) is a system of hyperbolic conservation laws with source terms in a form that is suitable for a numerical solution. Well developed numerical methods exist for solving of this system of equations including the case of inhomogeneous media like, for example, the wave-propagation algorithm [3],[4]. However, in the case of moving phase transition fronts some additional considerations are needed.

3. Jump relations

In order 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 $\mathcal{S}$ across which some of the fields suffer finite discontinuity jumps. It is assumed that the phase transition fronts are *homothermal* (no jump in temperature) and *coherent* (they present no defects such as dislocations). Thus, we have the following continuity conditions [5]:

$$[\mathbf{V}] = \mathbf{0}, \qquad [\theta] = \mathbf{0} \qquad at \;\; \mathcal{S}. \tag{4}$$

Here $[A]$ denotes the jump of a discontinuous field A across $\mathcal{S}$.

The material velocity $\mathbf{V}$ is defined by means of the inverse mapping $\mathbf{X} = \chi^{-1}(\mathbf{x}, t)$, where $\mathbf{X}$ denotes the material points. Jump relations associated with the conservation laws in the bulk are formulated according to the theory of *weak solutions* of hyperbolic systems [6]-[7]

$$\tilde{V}_N [\rho_0 v_i] + N_j [\sigma_{ij}] = 0, \tag{5}$$

$$\tilde{V}_N [S] - N_i \left[\frac{k}{\theta} \frac{\partial \theta}{\partial x_i} \right] = \sigma_{\mathcal{S}} \geq 0. \tag{6}$$

where $\tilde{\mathbf{V}}$ is the material velocity of the geometrical points of $\mathcal{S}$, $\tilde{V}_N$ is the normal speed of the points of $\mathcal{S}$, N_i are components of the unit normal to $\mathcal{S}$, S is the entropy per unit volume, and $\sigma_{\mathcal{S}}$ is the entropy production at the interface. As it was shown in [5]-[7], the entropy production can be expressed in terms of the so-called "material" driving force $f_{\mathcal{S}}$

$$f_{\mathcal{S}} \tilde{V}_N = \theta_{\mathcal{S}} \sigma_{\mathcal{S}} \geq 0, \tag{7}$$

where $\theta_{\mathcal{S}}$ is the temperature at $\mathcal{S}$. In addition, the *balance of "material" forces* at the interface between phases should be satisfied [5]-[9]. In the considered case, this can be specified to the form

$$f_{\mathcal{S}} = -[W] + < \sigma_{ij} > [\varepsilon_{ij}] \, , \tag{8}$$

where W is the free energy per unit volume and $< A >$ denotes the mean value of a discontinuous field A. The surface "balance" equation (8) follows from the balance law for pseudomomentum [5]-[7] and generalizes the equilibrium conditions at the phase transition front [10] to the dynamical case. Usually, a relation of constitutive type between the values of driving force and material velocity at the front should be written for the computation of the phase transition. Instead of that we use a thermodynamic considerations based on the thermodynamics of discrete systems [11].

4. Thermodynamic consistency conditions for thermoelastic media

The thermodynamic consistency conditions for simple thermodynamic systems are expressed in terms of internal energy [12]

$$\left[\left(\frac{\partial \hat{E}+\hat{E}^{int}}{\partial V}\right)_\theta\right]=0, \qquad \left[\left(\frac{\partial \hat{E}+\hat{E}^{int}}{\partial V}\right)_p\right]=0, \tag{9}$$

in the homogeneous and heterogeneous case, respectively. Here $\hat{E}$ is the internal energy, V is volume, and E^{int} is the so-called *interaction energy*, which appears in the description of the interaction of non-equilibrium discrete elements [12]. It should be noted that the value of $\hat{E}^{int}$ is undetermined yet. In the *thermoelastic case*, the thermodynamic derivatives which should be exploited instead of $\left(\frac{\partial \hat{E}}{\partial V}\right)_\theta$ and $\left(\frac{\partial \hat{E}}{\partial V}\right)_p$ are the following [13] (i and j are fixed):

$$\left(\frac{\partial E}{\partial \varepsilon_{ij}}\right)_\theta=-\theta\left(\frac{\partial \sigma_{ij}}{\partial \theta}\right)_{\varepsilon_{ij}}+\sigma_{ij}, \quad \left(\frac{\partial E}{\partial \varepsilon_{ij}}\right)_{\sigma_{ij}}=\theta\left(\frac{\partial S}{\partial \varepsilon_{ij}}\right)_{\sigma_{ij}}+\sigma_{ij}. \tag{10}$$

Here E is the internal energy per unit volume.

For extending the concepts of the thermodynamics of discrete systems to the *thermoelastic case*, we divide the body into a *finite number of identical elements.* The state of each element is then identified with the thermodynamic state of a discrete system associated with that element; each element being assumed to be in local equilibrium. In thermoelasticity, in addition to the *contact temperature* Θ [11], which governs heat exchange, we must define a *contact dynamic stress tensor* Σ_{ij} since the state space includes the deformation. We have thus

$$\frac{\partial \varepsilon_{ij}}{\partial t}(\Sigma_{ij}-\sigma^*_{ij})\geq 0, \qquad (\dot{Q}=0). \tag{11}$$

Here σ^*_{ij} is the Cauchy stress tensor in the environment.

It is supposed that the introduced contact quantities are connected with the energy of interaction in the similar way as in Eqs (10), i.e.

$$\left(\frac{\partial E^{int}}{\partial \varepsilon_{ij}}\right)_\theta=-\Theta\left(\frac{\partial \Sigma_{ij}}{\partial \theta}\right)_{\varepsilon_{ij}}+\Sigma_{ij}, \left(\frac{\partial E^{int}}{\partial \varepsilon_{ij}}\right)_{\sigma_{ij}}=\Theta\left(\frac{\partial S^{int}}{\partial \varepsilon_{ij}}\right)_{\sigma_{ij}}+\Sigma_{ij}. \tag{12}$$

In fact, the latter two equations are the relations of a constitutive type for the introduced contact quantities. It should be noted that the interaction entropy S^{int} is still undetermined yet. Just these conditions will be applied to determine the values of the contact quantities at the phase boundary.

5. Contact quantities at the phase boundary

Suppose that the interface between two thermoelastic phases is placed between elements numbered $(p-1\,q)$ and (pq). We propose to apply the heterogeneous consistency conditions for the calculation of the contact stresses at the phase boundary. In the two-dimensional case, we can rewrite the heterogeneous consistency conditions in the form

$$[\sigma_{ij}] + \theta_{\mathcal{S}} \left[\left(\frac{\partial S^{int}}{\partial \varepsilon_{ij}} \right)_{\sigma} \right] + (\Sigma^{l}_{ij})_{pq} - (\Sigma^{r}_{ij})_{p-1\,q} = 0. \tag{13}$$

Further, we suppose that the jump of the entropy of interaction is equal to the jump of entropy at the phase boundary

$$[S^{int}] = [S]. \tag{14}$$

It is obvious that for zero entropy of interaction the heterogeneous consistency conditions can be reduced to those in homogeneous case and, therefore, no change is needed. However, the jump of entropy is nonzero at the phase boundary if phase transition occurs.

For the computation of the jump of entropy at the phase boundary we will exploit the jump relation corresponding to the balance of the entropy (6). In the two-dimensional homothermal case, we have

$$[S] = f_{\mathcal{S}}/\theta_{\mathcal{S}}, \tag{15}$$

where the driving force is determined by the balance of "material" forces (8) with the free energy in the two-dimensional thermoelastic case

$$W = \frac{1}{2}\left(\sigma_{ij}\varepsilon_{ij} - \frac{C}{\theta_0}(\theta-\theta_0)^2 - \alpha(3\lambda+2\mu)(\theta-\theta_0)(\varepsilon_{11}+\varepsilon_{22}) \right). \tag{16}$$

Thus, the jump of the entropy of interaction is determined completely. Remaining relations follow from the coherency conditions for the material velocity (4). Obtained conditions form a linear system of equations which can be solved exactly, and we can update the state of the elements adjacent to the phase boundary by means of the wave-propagation algorithm [12]. It should be noted that the proposed new procedure should be applied at the phase boundary instead of standard one only after the initiation of the phase transition process. The material velocity at the phase boundary can be determined by means of jump relation for linear momentum (5). At last, the direction of the front propagation is determined by the positivity of the entropy production

$$\sigma_{\mathcal{S}} = \frac{f_{\mathcal{S}} \tilde{V}_N}{\theta_{\mathcal{S}}} \geq 0. \tag{17}$$

Now all bulk quantities can be computed and the driving force and the material velocity at the phase boundary determined. However, these quantities manifest themselves only if the phase transition takes place.

6. A thermodynamic initiation criterion for the stress-induced phase transition

We propose to expect the initiation of the stress-induced phase transition if both heterogeneous and homogeneous consistency conditions are fulfilled at the phase boundary simultaneously. Let the heterogeneous consistency condition (13) be fulfilled. Then the homogeneous consistency condition can be represented at the phase boundary as follows

$$-\theta_{\mathcal{S}} \left[\left(\frac{\partial \sigma_{ij}}{\partial \theta} \right)_{\varepsilon} \right] - \theta_{\mathcal{S}} \left[\left(\frac{\partial S^{int}}{\partial \varepsilon_{ij}} \right)_{\sigma} \right] + \theta_{\mathcal{S}} \left[\left(\frac{\partial \Sigma_{ij}}{\partial \theta} \right)_{\varepsilon} \right] = 0. \tag{18}$$

It should be noted that the combined consistency condition (18) must be fulfilled at least for one component of the stress tensor, because only one additional condition to be satisfied in order to determine the initiation of the phase transition. In particular, for the shear component of the stress tensor σ_{12} we have a simple relation of continuity of the shear stress at the phase boundary

$$[\sigma_{12}] = 0. \tag{19}$$

The expression (19) is inconvenient for the determination of the initiation of the phase transition, because it is fulfilled even in the absence of phase transitions and any other perturbations. Just therefore the combined consistency condition (18) for the normal components of stress tensor should be also checked. The combined consistency condition (18) for the normal component of the stress tensor σ_{11} leads to the following expression for the driving force $f_{\mathcal{S}}$:

$$f_{critical} = -\frac{\theta_{\mathcal{S}}^2}{4} [\alpha(3\lambda + 2\mu)] \left\langle \frac{\alpha(3\lambda + 2\mu)}{\lambda + \mu} \right\rangle -$$

$$-\frac{\theta_{\mathcal{S}}}{8} [\sigma_{11}] \left\langle \frac{\alpha(3\lambda + 2\mu)}{\lambda + \mu} \right\rangle + \frac{\theta_{\mathcal{S}}}{2} [(\lambda + \mu)(\varepsilon_{11} + \varepsilon_{22})] \left\langle \frac{\alpha(3\lambda + 2\mu)}{\lambda + \mu} \right\rangle. \tag{20}$$

Therefore, the proposed criterion for the initiation of the stress-induced phase transition is the following:

$$|f_{\mathcal{S}}| \geq |f_{critical}|. \tag{21}$$

A similar condition can be obtained for the second normal component of the stress tensor.

7. Numerical results for stress-induced phase transition

As an example, an one-dimensional martensite-austenite phase-transition front propagation is simulated in a thermoelastic medium. The physical properties of the material correspond to the NiTi alloy [14].

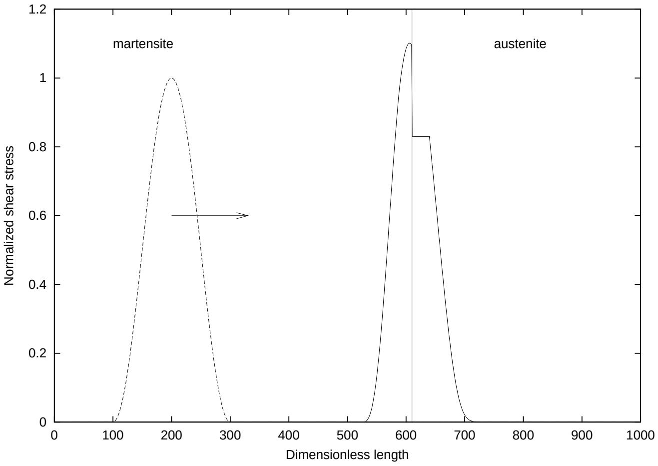

Figure 1. Interaction of shear wave with phase transition front.

It is supposed that the medium contains both martensitic and austenitic parts, which coexist at the temperature $\theta_{\mathcal{S}} = \theta = 300\,K$. An isothermal loading of shear stress is applied at the left boundary of the martensitic region. The form of the hump is shown in the left part of Fig. 1. The location of the phase boundary (initially $x = 600$) is marked by a vertical line.

If the amplitude of loading is sufficiently large to overcome the critical value of the driving force, we have the interaction of the shear wave with the phase-transition front (Fig. 1). As one can see, the value of the stress remains constant after the interaction, while the location of the phase boundary is displaced into the austenitic region.

It should be noted that the displacement of the front location depends nonlinearly on the amplitude of the loading, because of the nonlinearity in the computation of the driving force.

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References

1. Hou, T.Y, Rosakis, P. and LeFloch, P.: A level-set approach to the computation of twinning and phase-transition dynamics, *J. Comp. Physics* **150** (1999), 302-331.
2. Maugin, G.A. and Berezovski, A.: Material formulation of finite strain thermoelasticity and applications, *J. Thermal Stresses* **22** (1999), 421-449.
3. LeVeque, R.J.: Wave propagation algorithms for multidimensional hyperbolic systems, *J. Comp. Physics* **131** (1997), 327-353.
4. LeVeque, R.J.: Balancing source terms and flux gradients in high-resolution Godunov methods: the quasi-steady wave-propagation algorithm, *J. Comp. Physics* **148** (1998), 346-365.
5. Maugin, G.A.: On shock waves and phase-transition fronts in continua, *ARI* **50** (1998), 141-150.
6. Maugin, G.A.: Thermomechanics of inhomogeneous - heterogeneous systems: application to the irreversible progress of two- and three-dimensional defects, *ARI* **50** (1997), 41-56.
7. Maugin, G.A. and Trimarco, C.: Driving force on phase transition fronts in thermoelectroelastic crystals, *Math. Mech. Solids* **2** (1997), 199-214.
8. Abeyaratne, R. and Knowles, J.K.: On the driving traction acting on a surface of strain discontinuity in a continuum, *J. Mech. Phys. Solids* **38** (1990), 345-360.
9. Truskinovsky, L.: Dynamics of nonequilibrium phase boundaries in a heat conducting nonlinear elastic medium, *J. Appl. Math. Mech.* (PMM) **51** (1987), 777-784.
10. Grinfeld, M.A.: *Thermodynamic Methods in the Theory of Heterogeneous Systems*, Longman, London, 1991.
11. Muschik, W.: Fundamentals of non-equilibrium thermodynamics, in W. Muschik ed., *Non-Equilibrium Thermodynamics with Application to Solids*, Springer, Wien, 1993, pp. 1-63.
12. Berezovski,A., Engelbrecht, J. and Maugin, G.A.: Thermoelastic wave propagation in inhomogeneous media, *Arch. Appl. Mech.* **70** (2000), 694-706.
13. Callen, H.B. *Thermodynamics*, Wiley & Sons, New York, 1960.
14. Hodgson, D.E., Wu, M.H. and Biermann, R.J.: Shape memory alloys, in *Metals Handbook*, 10th Edition, **2**, ASM International, 1990, pp. 897-903.