Stress-induced phase transition front propagation in thermoelastic solids

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Abstract

A simplest possible mathematical model of martensitic phase transition front propagation is considered in the paper. Martensite and austenite phases are treated as isotropic linear thermoelastic materials. The phase transition front is viewed as an ideal mathematical discontinuity surface. Only one variant of martensite is involved. The problem remains nonlinear even in this simplified description that supposes a numerical solution. A non-equilibrium description of the process is provided by means of non-equilibrium jump relations at the moving phase boundary, which are formulated in terms of contact quantities. The same contact quantities are used in the construction of a finite-volume numerical scheme. The additional constitutive information is introduced by a certain assumption about the entropy production at the phase boundary. Results of numerical simulations show that the proposed approach allows us to capture experimental observations while corresponding to theoretical predictions in spite of the idealization of the process.

Key words: martensitic phase transformations, moving phase boundary, finite volume methods, thermomechanical modelling

1 Introduction

Attention to stress-induced phase-transition front propagation in thermoelastic solids is due to the growing application potential of shape memory alloys,

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due to the complexity of martensitic transformations, and due to nonlinear mathematical and numerical problems arising in the presence of moving phase boundaries.

The propagation of phase interfaces in shape-memory alloys under applied stress is an experimentally observed phenomenon (Shaw and Kyriakydes, 1995, 1997). The description of this phenomenon is desirable both for material scientists, who are interested in understanding pseudoelasticity and shape memory, for physicists, because the general theory of phase transformations should include also the displacive martensitic transformations, for continuum mechanics researchers, who are dealing with inhomogeneous media, and for mathematicians, if they are interested in solutions of problems with moving discontinuities. While the two former directions are mainly related to the microscopic level of description, the two latter directions are based on the macroscopic conservation laws. In the latter case, the diffusionless stress-induced martensitic phase-transition front propagation can be viewed as an example of moving discontinuities in thermoelastic solids. From the mathematical point of view, such a problem is considered as a non-classical shock problem for conservation laws (Lefloch, 2002).

There are two distinct approaches to the macroscopic description of the stress-induced martensitic phase-transition front propagation. The first one stems from Ericksen’s analysis of the non-monotone behavior of stress-strain relation in an elastic bar (Ericksen, 1975). The second one represents the generalization of the constitutive modelling of shape-memory alloys behavior for the dynamic case.

Energy minimization naturally leads to distinct material regions with continuous strain that are separated from each other by strain discontinuity interfaces so as to avoid unstable stress-strain branches. Placing the distinct stable branches of the strain-stress curve into correspondence with distinct material phases provides the connection to stress-induced phase transformation. Avoidance of the unstable branches is then formally similar to spinodal decomposition.

The simplest possible formulation of the stress-induced phase-transition front propagation problem is given in (Abeyaratne, Bhattacharya, and Knowles, 2001) in the case of an isothermal uniaxial motion of a slab in small-strain approximation. The phase front is represented by a jump discontinuity separating the different austenite and martensite branches of the N-shaped stress-strain curve. A shift of the martensitic branch of the curve is provided by the incorporation of a transformation strain, which is considered as an experimentally determined material constant. Standard boundary value problem do not have a unique solution when phase boundaries are present. The uniqueness of the solution is provided by the introduction of two supplementary
constitutive relations: a kinetic law for a driving force that establishes the speed of the transformation front and a nucleation criterion (Abeyaratne and Knowles, 1990, 1991). The kinetic motion criteria can be extracted from more refined theories in which the phase boundaries are regarded as transition zones exhibiting additional physical effects (Truskinovsky, 1997; Ngan and Truskinovsky, 1999).

A similar problem was analyzed in (Chen and Lagoudas, 2000; Bekker et al., 2002; Lagoudas et al., 2003) on the basis of a constitutive model of the shape memory effect and pseudoelasticity of polycrystalline shape-memory alloy. The key feature of this approach is to introduce one or more internal variables (order parameters) describing the internal structure of the material. In the macroscopic modelling of shape-memory alloys, each point of the material represents a phase mixture. Local quantities are volume averaged macroscopic quantities that depend on the microstructure through some overall descriptor (usually the phase fraction). Solution of the problem is provided by prescribing two constitutive ingredients: the macroscopic free energy function and a set of kinetic rate equations for the microstructural descriptors. The free energy function is decomposed in elastic and inelastic parts (Helm and Haupt, 2003). The first part represents the energy storage in consequence of elastic deformations and temperature variations. The second part represents the energy storage due to internal stress fields (internal variables). The resulting equations for the macroscopic behavior fit into the framework of internal variable models (Bernardini, 2001). Several models fitting into this basic framework have been proposed although sometimes employing quite different formalisms (Fischer et al., 1994; Birman, 1997; Bernardini and Pence, 2002). All of them involve a constitutive information prescribed via state equations and kinetic equations for the internal variables. Differences involve the choice and interpretation of the internal variables and the form of kinetic equations.

The above mentioned approaches represent the best we can obtain both from the point of view of energy minimization (without introduction of internal variables) and from the point of view of the constitutive modelling of shape-memory alloys behavior based on the martensitic volume fraction as an internal variable in the framework of the thermomechanics of continua.

In spite of the differences of the above mentioned approaches, one assumption is common: both of them exploit the local equilibrium approximation though jump relations at the phase boundary may differ from the classical equilibrium jump relations. This means that all the fields including temperature and entropy are supposed to be well defined at any point as usual (Leo, Shield and Bruno, 1993; Kim and Abeyaratne, 1995; Shaw and Kyriakydes, 1997). At the same time, it is well understood that the martensitic phase transformation is a dissipative process, which involves entropy change. Moreover, to perform simulations of practical examples we need to move to a numerical
approximation. In this case, we face a non-equilibrium behavior of finite-size discrete elements or computational cells. The local equilibrium approximation is not sufficient to describe such a behavior.

Therefore, a consequent non-equilibrium description of the stress-induced phase-transition front propagation is preferable. To do this we need to choose an appropriate non-equilibrium theory. Our choice is influenced by numerical aspects of the modelling. This means that we need to have not only the non-equilibrium description of states of (finite volume) computational elements but also the description of their interactions. In our opinion, the best possibility is provided by the thermodynamics of discrete systems (Muschik, 1993). In this theory, in addition to usual local equilibrium quantities, so-called contact quantities are introduced to provide the description of interactions between the systems. Therefore, the thermodynamic state space is extended.

The employed constitutive modelling in some sense is in between the two above mentioned approaches: we suppose different free energy functions for austenitic and martensitic phases (like in (Abeyaratne, Bhattacharya, and Knowles, 2001)) but the free energy is decomposed into local equilibrium and excess parts (like in (Chen and Lagoudas, 2000)). The state equations for the contact quantities (related to the excess of free energy) are established in the same way as the state equations for the local equilibrium quantities based on the local equilibrium part of the free energy.

The next step is to establish the non-equilibrium jump conditions at the phase interface. Each model of the stress-induced martensitic phase-transition front propagation uses its own jump relations (Chen and Lagoudas, 2000; Bekker et al., 2002; Lagoudas et al., 2003; Shaw, 2002; Stoilov and Bhattacharyya, 2002). All of them one way or another differ from the classical equilibrium jump relations, which consist in the case of thermoelastic solids in the continuity of temperature and chemical potential and the continuity of the normal Cauchy traction at the phase boundary (Grinfeld, 1991; Cermelli and Sellers, 2000).

The equality of the products of velocity of the front and driving force, and temperature and entropy production at the phase boundary follows from the entropy balance at the phase boundary. The prescription of a kinetic relation between the velocity and the driving force (Abeyaratne, Bhattacharya, and Knowles, 2001) determines the entropy production at the interface. Otherwise, we can prescribe the entropy production at the phase boundary. In the latter case, the kinetic relation is introduced implicitly. Here we keep the latter point of view in the numerical simulations of stress-induced martensitic phase transition front propagation in thermoelastic solids.

We apply the non-equilibrium jump relations (Berezovski and Maugin, 2004), which should be fulfilled for each pair of adjacent discrete elements. Supple-
mentary constitutive information is introduced by means of certain assumptions about the entropy production at the phase boundary. It is shown (Berezovski and Maugin, 2001) that the final rules for the determination of averaged quantities following from the non-equilibrium jump relations and kinematic conditions can be reduced to those obtained from the solution of the Riemann problems at the interfaces between cells in the wave propagation algorithm (LeVeque, 1997) in the absence of phase transformation. As a result, we can derive a thermodynamically consistent algorithm for the numerical simulation of phase-transition front propagation.

The paper is organized in the following way. In the next part, basic equations of thermoelasticity and jump relations at the phase boundary are given. Discrete representations of these relations in terms of averaged and contact quantities for finite size computational elements are derived in the third part. The corresponding numerical algorithm is described in the fourth part on the example of an uniaxial motion of a slab. The initiation criterion for the martensitic phase transformation is also derived in this context. Results of numerical simulations of stress wave interaction with phase boundary and the comparison with experimental data are given in the fifth part. Main conclusions are presented in the last part of the paper.

2 Linear thermoelasticity

2.1 Local balance laws

The free energy per unit volume in linear isotropic thermoelasticity is given by (Maugin and Berezovski, 1999, e.g.)

\[ W(\varepsilon_{ij}, \theta; x) = \frac{1}{2} \left( \lambda(x) \varepsilon_{kk}^2 + 2\mu(x)\varepsilon_{ij}\varepsilon_{ij} \right) - C(x) \theta_0 \left( \theta - \theta_0 \right)^2 + m(x) \left( \theta - \theta_0 \right) \varepsilon_{kk}, \]

with the strain tensor in the small-strain approximation

\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \]

while \( u_i \) are the components of the elastic displacement, \( C(x) = \rho_0 c \), \( c \) is the specific heat at constant stress, \( \theta \) is temperature, \( \theta_0 \) is a spatially uniform reference temperature and only small deviations from it are envisaged. The dilatation coefficient \( \alpha \) is related to the thermoelastic coefficient \( m \), and the Lamé coefficients \( \lambda \) and \( \mu \) by \( m = -\alpha(3\lambda + 2\mu) \). The indicated explicit dependence on the point \( x \) means that the body is materially inhomogeneous in
general. In particular, we can apply different material parameters for distinct phases.

Neglecting geometrical nonlinearities, the main two equations of thermoelasticity are the local balance of momentum at each regular material point in the absence of body force (Nowacki, 1962):

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

and the heat propagation equation

$$\theta \frac{\partial S}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0,$$

where $t$ is time, $x_j$ are spatial coordinates, $v_i$ are components of the velocity vector, $\sigma_{ij}$ is the Cauchy stress tensor, $\rho_0$ is the density, $S$ is the entropy per unit volume, $q_i$ are components of the heat flux vector.

The entropy and the stress tensor can be expressed in terms of the free energy per unit volume $W = W(\varepsilon_{ij}, \theta; x)$ as follows

$$\sigma_{ij} = \frac{\partial W}{\partial \varepsilon_{ij}}, \quad S = -\frac{\partial W}{\partial \theta}.$$

Simultaneously, we assume the Fourier law of heat conduction

$$q_i = -k(x) \frac{\partial \theta}{\partial x_i},$$

where $k$ is the thermal conductivity.

We can then rewrite the relevant bulk equations of inhomogeneous linear isotropic thermoelasticity as the following three equations of which the second one is none other than the time derivative of the Duhamel-Neumann thermoelastic constitutive equation (Berezovski, Engelbrecht, and Maugin, 2000):

$$\rho_0(x) \frac{\partial v_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j},$$

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

$$C(x) \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left( k(x) \frac{\partial \theta}{\partial x_i} \right) + m(x) \frac{\partial v_k}{\partial x_k}.$$
The given form of governing equations is very convenient for numerical simulation.

### 2.2 Jump relations

The phase transformation is viewed as a deformable thermoelastic phase of a material growing at the expense of another deformable thermoelastic phase. 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 $N_i$ to $S$ being oriented from the “minus” to the “plus” side:

$$
[A] := A^+ - A^-, \quad <A> := \frac{1}{2}(A^+ + A^-). \quad (10)
$$

The phase transition fronts considered are homothermal (no jump in temperature; the two phases coexist at the same temperature) and coherent (they present no defects such as dislocations). Consequently, we have the following continuity conditions (Maugin, 1997, 1998):

$$
[V_j] = 0, \quad [\theta] = 0 \quad \text{at} \quad S, \quad (11)
$$

where the "material" velocity $V_j$ is connected with the physical velocity $v_i$ by (Maugin, 1993)

$$
v_i = -(\delta_{ij} + \frac{\partial u_i}{\partial x_j})V_j. \quad (12)
$$


$$
V_N[\rho_0v_i] + N_j[\sigma_{ij}] = 0, \quad (13)
$$

$$
V_N[S] + N_i \left[ \frac{k}{\theta} \frac{\partial \theta}{\partial x_i} \right] = \sigma_S \geq 0. \quad (14)
$$

where $V_N = V_i N_i$ is the normal speed of the points of $S$, and $\sigma_S$ is the entropy production at the interface.
As it is shown in (Truskinovsky, 1997; Maugin, 1997, 1998; Abeyaratne, Bhat-
tacharya, and Knowles, 2001), the entropy production can be expressed in
terms of the so-called "material" driving force $f_S$ such that

$$f_S V_N = \theta_S \sigma_S \geq 0,$$

(15)

where $\theta_S$ is the temperature at $S$.

The driving force at the interface between phases is determined by (Maugin,
1997; Maugin and Trimarco, 1995a,b):

$$f_S = -[W] + \sigma_{ij} \varepsilon_{ij}.$$  

(16)

It should be noted that the jump relations (13), (14) are useless until we
could determine the value of the velocity of the phase boundary. A possible
solution is the introduction of a supplementary constitutive relation between
the material velocity at the interface and the driving force in the form of
kinetic relation as it was proposed in (Abeyaratne and Knowles, 1990, 1991).
Additionally, the criterion of nucleation should also be prescribed as well as
the value of transformation strain and a hysteretic behavior in stress-strain
relation.

One way or another, the nonlinearity of the formulated problem due to the
moving phase boundary requires a numerical solution. Therefore we postpone
the introduction of the supplementary constitutive information to the num-
erical approximation.

3 Discrete representation

3.1 Integral balance laws for discrete elements

Following main ideas of finite volume numerical methods, we divide the body
in a finite number of identical elements of elementary volume $\Delta V$ and bound-
ary $\partial \Delta V$. Integration over the finite volume element of equations (7) - (9) and
of the definition of the strain rate yields the following set of integral forms:

$$\frac{\partial}{\partial t} \int_{\Delta V} \rho_0 v_i dV = \int_{\partial \Delta V} \sigma_{ij} n_j dA,$$  

(17)

$$\frac{\partial}{\partial t} \int_{\Delta V} \varepsilon_{ij} dV = \int_{\partial \Delta V} h_{ijk} n_k dA,$$  

(18)
\[
\frac{\partial}{\partial t} \int_{\Delta V} \sigma_{ij} dV = \int_{\Delta V} (2\mu h_{ijk}n_k + \lambda \delta_{ij} v_k n_k) dA + \varphi_{ij}, \quad (19)
\]
\[
\frac{\partial}{\partial t} \int_{\Delta V} C\theta dV = \int_{\Delta V} (kn_i \frac{\partial \theta}{\partial x_i} + mv_k n_k) dA + \varphi^{inh}, \quad (20)
\]

where \(h_{ijk} = 1/2(\delta_{ik}v_j + \delta_{jk}v_i)\), \(n_i\) is the unit outward normal to the boundary of a discrete element, and source terms due to material inhomogeneities (labelled "inh") and thermoelastic couplings (labelled "te") are given by

\[
\varphi_{ij} = \varphi_{ij}^{te} + \varphi_{ij}^{inh}, \quad \varphi_{ij}^{te} = \int_{\Delta V} m \delta_{ij} \frac{\partial \theta}{\partial t} dV,
\]
\[
\varphi_{ij}^{inh} = -\int_{\Delta V} \left(v_k \frac{\partial \lambda}{\partial x_k} \delta_{ij} + v_i \frac{\partial \mu}{\partial x_j} + v_j \frac{\partial \mu}{\partial x_i}\right) dV,
\]
\[
\varphi^{inh} = -\int_{\Delta V} v_k \frac{\partial m}{\partial x_k} dV.
\]

As \(m\) here does not depend on time the contribution \(\varphi_{ij}^{te}\) could possibly be rewritten as a time derivative and grouped with the left-hand side of the equation (19), leaving only terms originating from material inhomogeneities as source terms. However, we keep the above formalism in order to distinguish between the purely elastic and thermoelastic cases. The reason for this is that in "classical" thermoelasticity, the thermoelastic coupling in the equation (9) is usually considered small and hence negligible, leaving from (9) an equation determining temperature independently of other fields, even in inhomogeneous materials. In that thermal stress approximation (20) is reduced to

\[
\frac{\partial}{\partial t} \int_{\Delta V} C\theta dV = \int_{\Delta V} kn_i \frac{\partial \theta}{\partial x_i} dA. \quad (21)
\]

### 3.2 Averaged and contact quantities

Introducing averaged quantities at each time step

\[
\bar{v}_i = \frac{1}{\Delta V} \int_{\Delta V} v_i dV, \quad \bar{\varepsilon}_{ij} = \frac{1}{\Delta V} \int_{\Delta V} \varepsilon_{ij} dV, \quad (22)
\]
\[
\bar{\sigma}_{ij} = \frac{1}{\Delta V} \int_{\Delta V} \sigma_{ij} dV, \quad \bar{C}\bar{\theta} = \frac{1}{\Delta V} \int_{\Delta V} C\theta dV, \quad (23)
\]
and numerical fluxes at the boundaries of each element

\[ F_{ij} \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \sigma_{ij} \partial_{\Delta V} dt, \quad G_{ijk} \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} (2\mu h_{ij} + \lambda \delta_{ij} v_k) |\partial_{\Delta V} dt, \quad (24) \]

\[ J \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \theta |\partial_{\Delta V} dt, \quad (25) \]

we are able to write a finite-volume numerical scheme for equations (17), (19), (21) for a uniform grid \((n, m)\) in two dimensions in the form \((l\) denotes time steps\)

\[ (\bar{v})_{n,m}^{l+1} - (\bar{v})_{n,m}^{l} = \frac{\Delta t}{\rho_{nm} \Delta x_j} \left( (F_{ij}^{in})_{nm} + (F_{ij}^{out})_{nm} \right), \quad (26) \]

\[ (\bar{\sigma}_{ij})_{n,m}^{l+1} - (\bar{\sigma}_{ij})_{n,m}^{l} = \frac{\Delta t}{\Delta x_k} \left( (G_{ijk}^{in})_{nm} + (G_{ijk}^{out})_{nm} \right), \quad (27) \]

\[ (\bar{\theta})_{n,m}^{l+1} - (\bar{\theta})_{n,m}^{l} = \frac{k_{nm} \Delta t}{C_{nm} \Delta x_j \Delta x_k} \left( (J_{ij}^{in})_{nm} + (J_{ij}^{out})_{nm} \right), \quad (28) \]

where superscripts "in" and "out" denote inflow and outflow parts in the flux decomposition.

The main difficulty in the construction of a numerical scheme is the proper determination of the numerical fluxes (LeVeque, 2002). Here we should remember that our discrete elements are not in equilibrium, especially in the presence of phase transformation. Even if we can associate the averaged quantities with local equilibrium parameters, we still need to have a description of the non-equilibrium states of discrete elements. The most convenient non-equilibrium thermodynamic theory is the thermodynamics of discrete systems (Muschik, 1993), where the thermodynamic state space of non-equilibrium discrete systems is extended by means of so-called contact quantities (which correspond to the numerical fluxes) in addition to the local equilibrium fields (which correspond to the averaged quantities). Following the ideas of the thermodynamics of discrete systems, we decompose the free energy density in each finite volume element into two terms (Muschik and Berezovski, 2004)

\[ W = \bar{W} + W_{ex}, \quad (29) \]

where \(\bar{W}\) is the averaged (local equilibrium) free energy, and \(W_{ex}\) is the excess free energy. Such a decomposition looks like the decomposition of the free energy into elastic and anelastic parts in the constitutive modelling approach

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(Helm and Haupt, 2003), but the excess energy here characterizes both elastic and anelastic interactions between adjacent discrete elements. Continuing the consequent application of the thermodynamics of discrete systems, we introduce then a contact dynamic stress tensor and an excess entropy in addition to the contact temperature Θ

\[
\Sigma_{ij} = \frac{\partial W_{ex}}{\partial \varepsilon_{ij}}, \quad S_{ex} = -\frac{\partial W_{ex}}{\partial \theta},
\]  

(30)

which are determined similar to averaged (local equilibrium) stress and entropy

\[
\bar{\sigma}_{ij} = \frac{\partial \bar{W}}{\partial \varepsilon_{ij}}, \quad \bar{S} = -\frac{\partial \bar{W}}{\partial \theta}.
\]  

(31)

Following (Muschik and Domínguez-Cascante, 1996), we can consider the contact stress tensor \(\Sigma_{ij}\) as defined at the boundary \(\partial \Delta V\) of the discrete element of volume \(\Delta V\).

Now we can rewrite a finite-volume numerical scheme (26) - (28) by means of corresponding contact quantities instead of numerical fluxes:

\[
(\bar{v}_i)^{l+1}_{nm} - (\bar{v}_i)^{l}_{nm} = \frac{\Delta t}{\rho_n m \Delta x_j} \left( (\Sigma^+_{ij})^l_{nm} - (\Sigma^-_{ij})^l_{nm} \right),
\]  

(32)

\[
(\bar{\sigma}_{ij})^{l+1}_{nm} - (\bar{\sigma}_{ij})^l_{nm} = \frac{\Delta t}{\Delta x_k} \left( (2\mu H_{ijk}^+ + \lambda \delta_{ij} V^+_{k})^l_{nm} - (2\mu H_{ijk}^- + \lambda \delta_{ij} V^-_{k})^l_{nm} \right),
\]  

(33)

\[
(\bar{\theta})^{l+1}_{nm} - (\bar{\theta})^l_{nm} = \frac{k_n m \Delta t}{C_n m \Delta x_i \Delta x_k} \left( (\Theta^+)^l_{nm} - (\Theta^-)^l_{nm} \right),
\]  

(34)

where \(H_{ijk} = 1/2(\delta_{ik} V_j + \delta_{jk} V_i), V_i\) denotes, by duality, the contact deformation velocity at a boundary of a discrete element, where \(f^+ = f^{in}, f^- = -f^{out} \quad \forall \ f\).

What we need now is to determine the values of contact quantities. In the absence of phase transformations it can be done by means of a corresponding Riemann solver (LeVeque, 2002). However, our main goal is the phase-transition front propagation, where it is difficult even to formulate a Riemann problem at the moving phase boundary. Fortunately, we have a tool for such a determination. This is nothing else but the non-equilibrium jump relations (Berezovski and Maugin, 2004), which should be fulfilled for each pair of adjacent discrete elements. In linear thermoelasticity, these non-equilibrium jump
relations take on the following form

\[
\begin{bmatrix}
-\bar{\theta} \left( \frac{\partial \bar{\sigma}_{ij}}{\partial \theta} \right)_{\varepsilon_{ij}} + \bar{\sigma}_{ij} - \Theta \left( \frac{\partial \Sigma_{ij}}{\partial \theta} \right)_{\varepsilon_{ij}} + \Sigma_{ij} \right] N_j = 0, \quad (35)
\]

\[
\begin{bmatrix}
\bar{\theta} \left( \frac{\partial \bar{S}}{\partial \varepsilon_{ij}} \right)_{\sigma_{ij}} + \bar{\sigma}_{ij} + \Theta \left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right)_{\sigma_{ij}} + \Sigma_{ij} \right] N_j = 0. \quad (36)
\]

Just these conditions we will apply to determine the values of the contact quantities in the bulk and at the phase boundary.

4 Numerical procedure

To be as simple as possible, we demonstrate the key ideas in the one-dimensional setting. The generalization of the algorithm to the two-dimensional case can be found in (Berezovski and Maugin, 2001).

4.1 Uniaxial motion of a slab

Following (Abeyaratne, Bhattacharya, and Knowles, 2001), we consider the simplest possible formulation of the problem, namely, the 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

\[
u_i = u_i(x, t), \quad x = x_1. \quad (37)
\]

In this case, we have only three non-vanishing components of the strain tensor

\[
\varepsilon_{11} = \frac{\partial u_1}{\partial x}, \quad \varepsilon_{12} = \varepsilon_{21} = \frac{1}{2} \frac{\partial u_2}{\partial x}, \quad \varepsilon_{13} = \varepsilon_{31} = \frac{1}{2} \frac{\partial u_3}{\partial x}. \quad (38)
\]

Without loss in generality, we can set \(\varepsilon_{13} = 0\) due to zero initial and boundary conditions for this component. Then the expression for the free energy (1) is reduced to

\[
W = \frac{\lambda + 2\mu}{2} \varepsilon_{11}^2 + \mu \varepsilon_{12}^2 + \mu \varepsilon_{21}^2 - \frac{C(x)}{2\theta_0} (\theta - \theta_0)^2 + m(\theta - \theta_0)\varepsilon_{11}, \quad (39)
\]
and we obtain uncoupled systems of equations for longitudinal and shear components

\[ \rho_0(x) \frac{\partial v_1}{\partial t} = \frac{\partial \sigma_{11}}{\partial x}, \quad \frac{\partial \sigma_{11}}{\partial t} = (\lambda(x) + 2\mu(x)) \frac{\partial v_1}{\partial x} + m(x) \frac{\partial \theta}{\partial t}, \quad (40) \]

and

\[ \rho_0(x) \frac{\partial v_2}{\partial t} = \frac{\partial \sigma_{12}}{\partial x}, \quad \frac{\partial \sigma_{12}}{\partial t} = \mu(x) \frac{\partial v_2}{\partial x}, \quad (41) \]

which are complemented by the heat conduction equation

\[ C(x) \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left( k(x) \frac{\partial \theta}{\partial x} \right). \quad (42) \]

These systems of equations can be solved separately. We focus attention on the system of equations for shear components, because the martensitic phase transformation is expected to be induced by shear.

4.2 Dynamic problem

We seek piecewise smooth velocity and stress fields \( v_2(x, t), \sigma_{12}(x, t) \) in inhomogeneous thermoelastic materials subject to the following initial and boundary conditions:

\[ \sigma_{12}(x, 0) = v_2(x, 0) = 0, \quad \text{for} \quad 0 < x < L, \quad (43) \]

\[ v_2(0, t) = v_0(t), \quad \sigma_{12}(L, t) = 0, \quad \text{for} \quad t > 0, \quad (44) \]

where \( v_0 \) is given constant.

The unknown fields obey the field equations

\[ \frac{\partial (\rho_0(x)v_2)}{\partial t} - \frac{\partial \sigma_{12}}{\partial x} = 0, \quad \frac{\partial}{\partial t} \left( \frac{\sigma_{12}}{\mu(x)} \right) - \frac{\partial v_2}{\partial x} = 0, \quad (45) \]

and the jump relations at the moving phase boundary \( S \)

\[ V_N[\rho_0v_2] + [\sigma_{12}] = 0, \quad [V] = 0, \quad [\theta] = 0, \quad (46) \]

\[ f_S = -[W] + [\sigma_{ij}] > [\varepsilon_{ij}], \quad f_S V_N = \theta_S \sigma_S \geq 0. \quad (47) \]
To solve the formulated uniaxial dynamic problem (43)-(47) we reduce the finite-volume numerical scheme (32), (33) as follows

\[
(\bar{v}_2)^{l+1}_n - (\bar{v}_2)^l_n = \frac{\Delta t}{\Delta x} \frac{1}{\rho_n}(\Sigma_{12}^+)_n - (\Sigma_{12}^-)_n,
\]

(48)

\[
(\bar{\sigma}_{12})^{l+1}_n - (\bar{\sigma}_{12})^l_n = \frac{\Delta t}{\Delta x} \mu_n (\mathcal{V}^+_2)_n - (\mathcal{V}^-_2)_n.
\]

(49)

The contact quantities \(\Sigma_{12}\) and \(\mathcal{V}_2\) will be determined by means of the non-equilibrium jump relations (35), (36) in the next sections.

4.3 Contact quantities in the bulk

First we apply the non-equilibrium jump relation (35) to determine the values of the contact quantities in the absence of phase transformation. Since shear components of the stress tensor are independent of temperature, the non-equilibrium jump relation (35) reduces to

\[
[\sigma_{ij} + \Sigma_{ij}] = 0.
\]

(50)

In the uniaxial case we will have at the interface between elements \((n-1)\) and \(n\)

\[
(\Sigma_{12}^+)_n - (\Sigma_{12}^-)_n = (\bar{\sigma}_{12})_n - (\bar{\sigma}_{12})_{n-1}
\]

(51)

This relation should be complemented by the kinematic condition between material and physical velocity (Maugin, 1993) which can be rewritten in the small-strain approximation as follows

\[
[v + \mathcal{V}] = 0.
\]

(52)

Assuming that the jump of the contact velocity is determined by the second term of latter relation

\[
[\mathcal{V}] = [\mathcal{V}],
\]

(53)

we obtain in the uniaxial case

\[
(\mathcal{V}^+_2)_n - (\mathcal{V}^-_2)_n = (\bar{v}_2)_n - (\bar{v}_2)_{n-1}.
\]

(54)
The two relations (51) and (54) express together a characteristic property for the cell-centered numerical fluxes in the conservative wave-propagation algorithm (Bale et al., 2003). Moreover, as it is shown (Berezovski, Engelbrecht, and Maugin, 2003a) the final rules for the determination of the averaged quantities following from the non-equilibrium jump relation (50) and kinematic condition (52) are reduced to those obtained from the solution of the Riemann problems at the interfaces between cells in the conservative wave propagation algorithm (Bale et al., 2003) by means of the connection between contact stresses and contact velocities in the form

\[
\left( V_2^+ \right)_p = -\frac{\left( \Sigma_{12}^- \right)_p}{\rho_p c_p}, \quad \left( V_2^- \right)_{p-1} = -\frac{\left( \Sigma_{12}^+ \right)_{p-1}}{\rho_{p-1} c_{p-1}},
\]

where

\[
c = \sqrt{\frac{\mu}{\rho}}.
\]

This means that the introduced non-equilibrium jump relations are consistent with conservation laws. From another point of view, this means that the wave-propagation algorithm is thermodynamically consistent.

Examples of wave propagation simulations in thermoelastic media with rapidly-varying properties by means of the formulated algorithm can be found in (Berezovski and Maugin, 2001; Berezovski, Engelbrecht, and Maugin, 2000, 2003a,b). However, phase transitions are always accompanied by the production of entropy (Qidwai and Lagoudas, 2000). This is why we need to apply another consistency condition at the phase boundary.

### 4.4 Contact quantities at the phase boundary

Suppose that the boundary between two thermoelastic phases is placed between elements numbered \((p-1)\) and \(p\). For the shear wave, we have for the left element adjacent to the phase boundary

\[
(\bar{v}_2)^l+1_{p-1} - (\bar{v}_2)^l_{p-1} = \frac{\Delta t}{\Delta x} \frac{1}{\rho_{p-1}} \left( (\Sigma_{12}^+)^l_{p-1} - (\Sigma_{12}^-)^l_{p-1} \right),
\]

\[
(\bar{\sigma}_{12})^{l+1}_{p-1} - (\bar{\sigma}_{12})^l_{p-1} = \frac{\Delta t}{\Delta x} \mu_{p-1} \left( (V_2^+)^l_{p-1} - (V_2^-)^l_{p-1} \right).
\]

The contact quantities \((\Sigma_{12}^+)^l_{p-1}\) and \((V_2^-)^l_{p-1}\) are determined as usual. However, we need a more careful consideration for values of the contact quantities.
Similarly, for the right adjacent element, we have
\[
\begin{align*}
(\bar{v}_2)^{i+1}_p - (\bar{v}_2)^i_p &= \frac{\Delta t}{\Delta x} \frac{1}{\rho_p} \left((\Sigma_{12}^+)^i_p - (\Sigma_{12}^-)^i_p\right), \\
(\bar{\sigma}_{12})^{i+1}_p - (\bar{\sigma}_{12})^i_p &= \frac{\Delta t}{\Delta x} \mu_p \left((\bar{\nu}_2^+)^i_p - (\bar{\nu}_2^-)^i_p\right).
\end{align*}
\]

Here we need to determine the values of \((\Sigma_{12}^-)^i_p\) and \((\bar{\nu}_2^-)^i_p\).

The corresponding procedure is based on the non-equilibrium jump condition at the phase boundary (36) that is specified in the linear thermoelastic case to
\[
\left[\bar{\sigma}_{12} \left(\frac{\partial S}{\partial \varepsilon_{12}}\right) + \Theta \left(\frac{\partial S_{ex}}{\partial \varepsilon_{12}}\right) + \Sigma_{12}\right] = 0.
\]

We expect that the local equilibrium entropy remains unchanged. Therefore, the jump of contact stresses is determined by
\[
[\Sigma_{12}] = - \left[\bar{\sigma}_{12} + \Theta \left(\frac{\partial S_{ex}}{\partial \varepsilon_{12}}\right)\right].
\]

Now we should make certain assumption about the excess entropy. The simplest one is the following:
\[
[\bar{\sigma}_{12}] = - \left[\Theta \left(\frac{\partial S_{ex}}{\partial \varepsilon_{12}}\right)\right],
\]

which leads to the continuity of contact stresses at the phase boundary
\[
[\Sigma_{12}] = 0.
\]

The remaining relation follows from the coherency conditions for the material velocity (11) which can be expressed in the small-strain approximation as follows
\[
[\bar{\nu}_2] = 0.
\]
The contact velocities are still connected with contact stresses by the relations (55). Therefore, in terms of contact stresses, equation (64) yields

\[
\frac{(\Sigma_{ij})_{p-1}^+}{\rho_{p-1}c_{p-1}} + \frac{(\Sigma_{ij})_{p}^-}{\rho_{p}c_{p}} = 0. \tag{65}
\]

It follows from the conditions (63) and (65) that the values of contact stresses vanish at the phase boundary

\[
(\Sigma_{ij})_{p-1}^+ = (\Sigma_{ij})_{p}^- = 0. \tag{66}
\]

Now all the contact quantities at the phase boundary are determined, and we can update the state of the elements adjacent to the phase boundary.

However, the proposed procedure should be applied at the phase boundary only after the initiation of the phase transition process. The possible motion of the interface between phases should also be taken into account.

4.5 A thermodynamic initiation criterion for the stress-induced phase transition

Up to now we have used different non-equilibrium jump relations in the presence and in the absence of phase transformation. It is expected that at the beginning of the phase transformation process the non-equilibrium jump relations should be changed from one form to another. This means that at the initiation of the stress-induced phase transition both non-equilibrium jump relations are fulfilled at the phase boundary simultaneously:

\[
\left[ \bar{\theta} \left( \frac{\partial S}{\partial \varepsilon_{ij}} \right) + \bar{\sigma}_{ij} + \Theta \left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right) + \Sigma_{ij} \right] N_j = 0, \tag{67}
\]

\[
\left[ \bar{\sigma}_{ij} - \bar{\theta} \left( \frac{\partial \bar{\sigma}_{ij}}{\partial \theta} \right) + \Sigma_{ij} - \Theta \left( \frac{\partial \Sigma_{ij}}{\partial \theta} \right) \right] \varepsilon_j N_j = 0. \tag{68}
\]

Eliminating the jumps of stresses from the system of equations (67), (68), we obtain then

\[
\left[ \Theta \left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right) + \bar{\theta} \left( \frac{\partial \bar{\sigma}_{ij}}{\partial \theta} \right) + \Theta \left( \frac{\partial \Sigma_{ij}}{\partial \theta} \right) \right] N_j = 0. \tag{69}
\]
Remember, that we suppose that the equilibrium part of entropy is continuous across the phase boundary

\[ [S] = [S_{eq}] + [S_{ex}] = [S_{ex}], \quad (70) \]

Before the beginning of the phase transformation process, all the temperatures hold the initial values

\[ \bar{\theta}_{p-1} = \bar{\theta}_p = \Theta^+_p = \Theta^-_p = \theta_0. \quad (71) \]

We suppose that the temperature dependence for the contact stresses is the same as for averaged stresses

\[ \left( \frac{\partial \bar{\sigma}_{ij}}{\partial \theta} \right)_\varepsilon = \left( \frac{\partial \Sigma_{ij}}{\partial \theta} \right)_\varepsilon = m \delta_{ij}. \quad (72) \]

Therefore, the combined non-equilibrium jump relation (69) takes the form

\[ \left[ \theta_0 \left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right)_{\sigma} + 2\theta_0 m \delta_{ij} \right] N_j = 0. \quad (73) \]

Remembering the assumption of the entropy production at the phase boundary

\[ [\bar{\sigma}_{ij}] = - \left[ \Theta \left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right)_{\sigma} \right], \quad (74) \]

we will have finally

\[ [2\theta_0 m \delta_{ij} - \bar{\sigma}_{ij}] N_j = 0. \quad (75) \]

This is the desired criterion of the the initiation of phase transformation in terms of jump of the averaged stresses. Returning to the uniaxial problem, we see that the combined jump relation (75) leads to the continuity of the averaged shear stress component at the phase boundary

\[ [\bar{\sigma}_{12}] = 0. \quad (76) \]

Unfortunately, the latter relation can be fulfilled without any phase transformation (e.g., at rest). This is inconvenient for the criterion of the initiation of phase transformation process and we do not use it. Therefore, we still need a criterion for the initiation of the phase transformation process.
It should be noted that the combined consistency condition (75) must be fulfilled at least for one component of the stress tensor, because we need the satisfaction of only one additional condition to determine the beginning of the phase transition. For this purpose, we should check also the combined consistency condition (75) for the normal stress component. In the latter case we obtain

\[ [\bar{\sigma}_{11}] = 2\theta_0 [m]. \] (77)

It is more convenient to express the initiation criterion in terms of the driving force using the entropy production assumption (74). To be able to calculate the jumps of the derivatives of the excess entropy, we propose the following procedure. We exploit the jump relation corresponding to the balance of entropy (14) and the expression for the entropy production in terms of the driving force (15):

\[ V_N[S] + \left[ \frac{k}{\partial \bar{\theta}} \right] = \frac{f_S V_N}{\theta_S}, \] (78)

where the driving force takes the form

\[ f_S = -[\bar{W}] + <\bar{\sigma}_{ij}> [\bar{\varepsilon}_{ij}]. \] (79)

It follows from (70) and (78) that

\[ [S_{ex}] = \frac{f_S}{\theta_S} - \frac{1}{V_N} \left[ \frac{k}{\partial \bar{\theta}} \right]. \] (80)

Assuming for simplicity the continuity of heat flux at the phase boundary in the homothermal case, we have

\[ [S_{ex}] = \frac{f_S}{\theta_S}. \] (81)

Further we extend the definition of the excess entropy to every point of the body by similarity to (81):

\[ S_{ex} = \frac{f - f_0}{\theta}, \] (82)

where \( f \) is defined by analogy with (79)

\[ f - f_0 = -\bar{W} + <\bar{\sigma}_{ij}> [\bar{\varepsilon}_{ij}], \] (83)
with

\[
<\tilde{\sigma}_{ij}> = \frac{(\tilde{\sigma}_{ij})_p + (\tilde{\sigma}_{ij})_{p-1}}{2}, \quad [f_0] = 0. \tag{84}
\]

This supposes that at the point where (82) and (83) are defined, there exists in thought an oriented surface of unit normal \( n \). If there is no discontinuity across this surface, then \( f \) is a so-called generating function (the complementary energy changed of sign and up to a constant). If there does exist a discontinuity then the expression becomes meaningful only if the operator \([\cdots]\) is applied to it. Here no transformation strain is a priori included in equation (83).

Then we can compute the derivatives of the excess entropy with respect to thermodynamic variables \( \varepsilon_{ij} \) as usual

\[
\left( \frac{\partial S_{ex}}{\partial \varepsilon_{ij}} \right)_\sigma = \left( \frac{\partial}{\partial \varepsilon_{ij}} \left( \frac{f - f_0}{\theta} \right) \right)_\sigma. \tag{85}
\]

In the uniaxial case, we have for the driving force

\[
f - f_0 = -\frac{1}{2} \tilde{\sigma}_{11} \tilde{\varepsilon}_{11} - \tilde{\sigma}_{12} \tilde{\varepsilon}_{12} + \frac{1}{2} C \tilde{\theta}^{2} + \frac{1}{2} \alpha(3\lambda + 2\mu)(\tilde{\theta} - \theta_0)^2 + \frac{1}{2} \alpha(3\lambda + 2\mu)(\tilde{\theta} - \theta_0) \tilde{\varepsilon}_{11} + <\tilde{\sigma}_{11}> \tilde{\varepsilon}_{11} + 2 <\tilde{\sigma}_{12}> \tilde{\varepsilon}_{12}. \tag{86}
\]

Therefore, the derivative of \((f - f_0)\) with respect to the normal component is given by

\[
\left( \frac{\partial(f - f_0)}{\partial \varepsilon_{11}} \right)_\sigma = -\frac{1}{2} \tilde{\sigma}_{11} + \frac{1}{2} \alpha(3\lambda + 2\mu)(\tilde{\theta} - \theta_0) + <\tilde{\sigma}_{11} >. \tag{87}
\]

This means that the jump of normal component in the stress tensor at the phase boundary in the uniaxial case is determined as follows

\[
[\tilde{\sigma}_{11}] = - \left[ \frac{2(f - f_0)}{\theta_0} \frac{(\lambda + 2\mu)}{\alpha(3\lambda + 2\mu)} \right]. \tag{88}
\]

and we can specify the combined jump relation at the phase boundary (75) for the normal component of the stress tensor \( \sigma_{11} \) to the form

\[
\left[ \frac{2(f - f_0)}{\theta_0} \frac{(\lambda + 2\mu)}{\alpha(3\lambda + 2\mu)} \right] = \theta_0[\alpha(3\lambda + 2\mu)]. \tag{89}
\]
After rearranging, we will have

\[ [f - f_0] \left\langle \left( \frac{\lambda + 2\mu}{\alpha (3\lambda + 2\mu)} \right) \right\rangle + < f - f_0 > \left[ \frac{(\lambda + 2\mu)}{\alpha (3\lambda + 2\mu)} \right] = \theta_0^2 [\alpha (3\lambda + 2\mu)]. \tag{90} \]

Remember that the value of \( f_0 \) at the phase boundary is undetermined yet. We can choose this value in such a way that

\[ < f - f_0 >= 0. \tag{91} \]

Therefore, the combined jump relation at the phase boundary (90) determines the value of the driving force at the interface

\[ f_S = [f] = \theta_0^2 [\alpha (3\lambda + 2\mu)] \left\langle \frac{\alpha (3\lambda + 2\mu)}{(\lambda + 2\mu)} \right\rangle. \tag{92} \]

The right hand side of the latter relation can be interpreted as a critical value of the driving force in the uniaxial case. Therefore, the proposed criterion for the beginning of the stress-induced phase transition is the following one:

\[ |f_S| \geq |f_{\text{critical}}|, \tag{93} \]

where

\[ f_{\text{critical}} = \theta_0^2 [\alpha (3\lambda + 2\mu)] \left\langle \frac{\alpha (3\lambda + 2\mu)}{(\lambda + 2\mu)} \right\rangle = \frac{\theta_0^2 [m^2]}{2 < \lambda + 2\mu >}. \tag{94} \]

Note that (94) does not include the contribution of a transformation strain. Moreover, the critical value of the driving force should be equal to zero if the properties of the phases are identical.

As one can see, a phase transition which should involve essentially shear, is governed by the bulk and "longitudinal" properties. It relates to the fact that thermal effects are here active only through the bulk properties although we are primarily interested in shear waves. If we ignore the thermoelastic coupling, which is included only due to the temperature dependence of the normal component of stress tensor, we could not obtain any nontrivial expression for the critical value of the driving force at the phase boundary.

The material velocity at the interface is determined by means of the jump relation for linear momentum (13)

\[ V_2^2 = \frac{|\sigma_{12}|}{\rho_0 |\varepsilon_{12}|}, \tag{95} \]
The direction of the front propagation is determined by the positivity of the entropy production (15)

$$\sigma_S = \frac{f_S V_N}{\theta_S} \geq 0.$$  \hspace{1cm} (96)

The obtained relations at the phase boundary are used in the described numerical scheme for the simulation of phase-transition front propagation.

Fig. 1. Plane wave: geometry.

5 Numerical results

5.1 Algorithm description

As it was noted, the contact quantities are determined in the same way as the cell-centered numerical fluxes for the conservative wave-propagation algorithm (Bale et al., 2003). This means that we can exploit the advantages of the wave-propagation algorithm, including second-order corrections and transversal propagation terms (LeVeque, 1997). However, no limiters are used in the calculations. Suppressing of spurious oscillations is achieved by means of using a first-order Godunov step after each three second-order Lax-Wendroff steps. This idea of composition was invented by (Liska and Wendroff, 1998).

A procedure similar to a cellular automaton is applied to the phase-transition front tracking. At any time step, the values of the driving force are calculated
in cells adjacent to the phase boundary. If the value of the driving force at the phase boundary exceeds the critical one, the velocities of the phase front are computed by means of (95). Virtual displacements of the phase-transition front are calculated then for all possible phase boundaries adjacent to the cell. We keep the cell in the old phase state if the (algebraic) sum of the virtual displacements is less than the size of space step, and change it to another phase otherwise.

All the calculations are performed with Courant-Friedrichs-Levy number equal to 1.

![Normalized stress vs Time steps](image)

**Fig. 2. Loading time-history.**

### 5.2 Interaction of a plane wave with phase boundary

As the first example, we consider the interaction of a plane wave with a phase boundary to confirm the results of phase-transition front propagation in the one-dimensional case (Berezovski, Engelbrecht, and Maugin, 2003a; Berezovski and Maugin, 2002a,b; Berezovski, Engelbrecht, and Maugin, 2002).

The geometry of the problem is shown in Fig. 1. The wave is excited at the left boundary of the computation domain by prescribing a time variation of a component of the stress tensor. Upper and bottom boundaries are stress-free, the right boundary is assumed to be rigid. The time-history of loading is shown in Fig. 2. If the magnitude of the wave is high enough, the phase transformation process is activated at the phase boundary. The maximal value of the Gaussian pulse is chosen as 0.7 GPa. The considered situation is similar to that in experiments of Escobar and Clifton (1993), where a plane phase
transition front propagated in the normal direction to the plane of loading, and only one variant of martensite was activated.

Material properties correspond to Cu-14.44Al-4.19Ni shape-memory alloy (Escobar and Clifton, 1993) in austenitic phase: the density $\rho = 7100 \, kg/m^3$, the elastic modulus $E = 120 \, GPa$, the shear wave velocity $c_s = 1187 \, m/s$, the dilatation coefficient $\alpha = 6.75 \cdot 10^{-6} \, 1/K$. It was recently reported (Emel’yanov et al., 2000) that elastic properties of martensitic phase of Cu-Al-Ni shape-memory alloy after impact loading are very sensitive to the amplitude of loading. Therefore, for the martensitic phase we choose, respectively, $E = 60 \, GPa, c_s = 1055 \, m/s$, with the same density and dilatation coefficient as
above. As a first result of computations, the stress-strain relation is plotted in Fig. 3 at a fixed point inside the computational domain which was initially in the austenitic state. As we can see in Fig. 3, the stress-strain relation is

![Free energy at a fixed point.](image1)

**Fig. 5.** Free energy at a fixed point.

and

![Stress-strain relation.](image2)

**Fig. 6.** Stress-strain relation: comparison with experimental data from (Emel’yanov et al., 2000) (sample 1).

at first linear corresponding to elastic austenite. Then the strain value jumps along a constant stress line to its value in the martensitic state due to the phase transformation. After that both loading and unloading correspond to elastic martensite. The value of the strain jump between straight lines, the slope of which is prescribed by material properties of austenite and martensite, respectively, is determined by the value of stress that conforms to the
critical value of the driving force. This critical value of the driving force is also determined by the material properties (see eq. (94)). The critical value of the driving force should agree with the barrier of potential that we have to overcome to go from one phase to the other. Therefore, the stress value corresponding to the critical value of the driving force can be associated with the transformation stress, and the value of the strain jump is nothing else but the transformation strain.

Having the transformation strain, we can replot the stress-strain relations taking into account that martensite can exist only in the deformed state. This means that the martensitic line should start not from zero but from a non-zero value of the transformation strain. The result is shown in the Fig. 4, which looks very much like the stress-strain dependence given in (Abeyaratne, Bhattacharya, and Knowles, 2001).

This can be also represented in terms of free energy (Fig. 5), which has a typical two energy-wells structure like it is supposed in (Abeyaratne, Bhattacharya, and Knowles, 2001). The obtained stress-strain relation at any fixed point results in overall pseudoelastic response of a specimen. The overall stress-strain behavior can be compared with dynamic experiments provided in (Emel’yanov et al., 2000). The result of the comparison is given in Fig. 6. As one can see, numerical simulation captured the experimental observations in the phase transformation region. In this comparison, the shape and duration of the loading pulse were adjusted to fit the experimental data.
5.2.1 **Hysteretic behavior**

Up to now it was supposed that austenite is not recovered after unloading. If the value of reference temperature is above the onset of reverse transformation temperature, we should expect that the austenitic state will be recovered after unloading. The inverse phase transformation should occur immediately when the actual deformation of martensitic elements become less than the transformation strain. Since the inverse transformation is governed by another condition than the direct transformation, we obtain a hysteretic stress-strain behavior (Fig. 7).

Again, the overall stress-strain dependence can be compared with experimental data. Corresponding results are shown in Fig. 8, where the experimental data of a quasi-static loading of a similar material with relatively high applied loading rate (1 MPA/s) from the paper by Goo and Lexcellent (1997) are given. The shape and duration of the loading pulse again were adjusting parameters for the fitting the experimental data.

5.2.2 **Damping**

The obtained stress-strain behavior results in a specific interaction between a plane stress wave and the phase boundary. The result of the interaction is shown in Fig. 9 that represents the structure of the interaction of the incoming wave (from left) with the phase boundary. Here we return to the loading pulse shown in Fig. 2. We observe here that amplitudes of both transmitted and reflected waves are rejected, whereas the phase boundary has moved to
Fig. 9. Plane wave profile after interaction with moving phase boundary.

the austenitic region from its initial position shown in Fig. 1. Therefore, the martensitic phase transformation exhibits a property to be a filter for the amplitudes of incoming waves. The magnitude of the transmitted wave in Fig. 9 corresponds to the value of the transformation stress (see Figs. 3,4).

Fig. 10. Phase-transition front propagation under non-plane wave impact: solid line - initial phase boundary position, dashed line - phase boundary position after interaction, grid: 100x100 elements.
5.3 Interaction of a non-plane wave with phase boundary

The next example is similar to the previous one, but the excited stress wave is no more a plane wave. It is excited only at a part of the left boundary of the computational domain as shown in Fig. 10. Now the width along the transverse direction is finite. The problem becomes two-dimensional. We do not recall the 2D numerical scheme (cf. Berezovski and Maugin (2001)).

Material properties for both austenitic and martensitic phases are the same as previously as well as loading (compression) time-history in the middle of the left boundary of the computation domain. As the result of interaction between the stress wave and the phase boundary, the initially straight phase boundary is deformed to the form shown in Fig. 10. At this stage, we also compared the results of computation of the same problem by refining the mesh. The corresponding results are shown in Fig. 11. Here the longitudinal coordinate is zoomed to exhibit the differences more clearly. As one can see, the refining of the mesh leads to a finer description of the phase-transition front, but it does not change the overall shape significantly. The next example concerns the behavior of the phase-transition front under increasing of the loading magnitude. Corresponding results are shown in Fig. 12, where two distinct final shapes of the phase-transition front relate to magnitudes of loading equal to 0.7 and 1.4 GPa, respectively. The last Figure 13 shows the phase-transition front position in the case of an oblique impact of the stress wave on the phase boundary. The result exhibited is tantamount to the formation of fingers or dendrites.
Fig. 12. Phase transition front at 100 time steps: straight line - initial position, solid line corresponds to the maximum magnitude of the loading 0.7 GPa, dotted line - 1.4 GPa (400x400 elements grid).

Fig. 13. Oblique impact of the stress wave: solid line - initial position of the phase boundary, dashed line - phase-transition front at 100 time steps.

6 Conclusions

A simplest possible mathematical model of martensitic phase transition front propagation is considered in the paper. Martensite and austenite phases are treated as isotropic linear thermoelastic materials. The phase transition front is viewed as an ideal mathematical discontinuity surface. Only one variant
of martensite is involved. This means that the phenomenon is highly idealized but one of the essential features of martensitic transformation holds: the considered phase transformation is diffusionless. The problem remains non-linear even in this simplified description that supposes a numerical solution. Moreover, a supplementary constitutive information is needed to avoid the non-uniqueness of the solution of the boundary-value problem. One way or another such an information is connected to the entropy production at the phase transition front. The latter means that a non-equilibrium description of the process is needed, especially in view of numerical solution of the problem. The corresponding non-equilibrium description is provided by means of non-equilibrium jump relations at the moving phase boundary, which are formulated in terms of contact quantities. The same contact quantities are used in the construction of a finite-volume numerical scheme that coincides with the conservative wave propagation algorithm in the absence of phase transformation. The additional constitutive information is introduced by a certain assumption about the entropy production at the phase boundary. As a result, a closed system of equations and jump relations can be solved numerically.

The main distinction of the proposed model from existing ones consists in the way by which the supplementary constitutive information is introduced into the model. Kinetic relations in existing models are formulated in such a way as to reproduce the observed behavior of the two-phase material (pseudoelasticity, hysteresis) before the solution of the problem. The prediction of the entropy production at the phase boundary means that the behavior of the material can be analyzed only after the numerical simulation. Another distinction is the consistent non-equilibrium description of the martensitic phase transition front propagation.

Results of numerical simulations show that the proposed approach allows us to capture experimental observations while corresponding to theoretical predictions in spite of the idealization of the process.

Acknowledgments

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Figure captions

Fig 1. Plane wave: geometry.

Fig 2. Loading time-history.

Fig 3. Stress-strain behavior at a fixed point.

Fig 4. Stress-strain behavior at a fixed point.

Fig 5. Free energy at a fixed point.

Fig 6. Stress-strain relation: comparison with experimental data from (Emel’yanov et al., 2000) (sample 1).

Fig 7. Stress-strain behavior at a fixed point with full recovering of austenite.

Fig 8. Stress-strain relation at the phase boundary: comparison with experimental data from (Goo and Lexcellent, 1997).

Fig 9. Plane wave profile after interaction with moving phase boundary.

Fig 10. Phase-transition front propagation under non-plane wave impact: solid line - initial phase boundary position, dashed line - phase boundary position after interaction, grid: 100x100 elements.

Fig 11. Phase-transition front position under non-plane wave impact at 100 time steps: solid line - 100x100 elements grid, dashed line - 200x200 elements grid, dotted line - 400x400 elements grid.

Fig 12. Phase transition front at 100 time steps: straight line - initial position, solid line corresponds to the maximum magnitude of the loading 0.7 GPa, dotted line - 1.4 GPa (400x400 elements grid).

Fig 13. Oblique impact of the stress wave: solid line - initial position of the phase boundary, dashed line - phase-transition front at 100 time steps.
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Stress (GPa) vs. Strain (%)

0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1

Stress (GPa)
Strain (%)
Stress (GPa) vs. Strain (%) graph.