STRESS-INDUCED MARTENSITIC PHASE TRANSITION FRONT PROPAGATION

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Summary A non-equilibrium description of states of computational elements and their interaction is proposed for the numerical simulation of stress-induced martensitic phase transition front propagation in thermoelastic solids. This description is based on the generalization of the thermodynamics of discrete systems to the thermoelastic case. A finite-volume numerical scheme is then constructed by means of corresponding contact quantities. Additional constitutive information is introduced by means of certain assumptions about the entropy production at the phase boundary. Results of numerical simulations capture experimental observations.

BACKGROUND

The propagation of phase interfaces in shape-memory alloys under applied stress is an experimentally observed phenomenon. At the macroscopic level of description, 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.

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. The second one represents the generalization of the constitutive modelling of shape-memory alloys behavior for the dynamic case.

Energy minimization [1] naturally leads to distinct material regions with continuous strain, that are separated from each other by strain discontinuity interfaces so as to avoid unstable 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. Standard boundary value problems do not have a unique solution when phase boundaries are present. The crucial assumption in the model is the application of a kinetic law relating the front propagation speed and the driving force. Additionally, a nucleation criterion is also introduced. Theoretical prediction of possible forms of the kinetic law can be extracted from more refined theories in which the phase boundaries are regarded as transition zones exhibiting additional physical effects [2].

The problem of stress-induced phase transformation was also considered on the basis of a constitutive model of the shape memory effect and pseudoelasticity of polycrystalline shape-memory alloy [3]. The key feature of this approach is to introduce one or more internal variables describing the internal structure of the material. Several models fitting into this basic framework have been proposed although sometimes employing quite different formalisms [4]. They involve a constitutive information prescribed via state equations and kinetic equations for the internal variables. Macroscopic free energy function is decomposed into elastic and inelastic parts. The first part represents the energy storage in consequence of elastic deformations and temperature. The second part represents the energy storage due to internal stress fields (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 SMA behavior based on the martensitic volume fraction as an internal variable in the framework of the thermomechanics of continua.

In spite of the differences between the above mentioned approaches, one assumption is common: both of them exploit the local equilibrium approximation. However, to perform simulations of practical examples we need to move to numerical approximation. In this case we meet with a non-equilibrium behavior of finite-size discrete elements or computational cells accompanied by entropy production at the moving phase boundary. The local equilibrium approximation is not sufficient to describe such a behavior.

NON-EQUILIBRIUM DESCRIPTION AND NUMERICAL APPROXIMATION

A consistent non-equilibrium description of the process means that we need to have both the non-equilibrium description of states of computational elements and their interactions. The best possibility is provided by the thermodynamics of discrete systems [5]. In this theory, in addition to usual local equilibrium quantities, so-called contact quantities are introduced which provide the description of interaction between the systems. The constitutive modelling in some sense is in between above mentioned approaches: we suppose different free energy functions for austenitic and martensitic phases (like in [1]) but the free energy is decomposed into a local equilibrium and an excess part (like in [3]). 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 free energy. A finite-volume numerical scheme is then constructed by means of corresponding contact quantities.
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. 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. We apply the *non-equilibrium jump relations* [6], which should be fulfilled for each pair of adjacent discrete elements. Additional constitutive information is introduced by means of certain assumptions about the entropy production at the phase boundary. It is shown [7] that the final rules for the determination of the averaged quantities following from the non-equilibrium jump relation and kinematic condition fully coincide with those obtained from the solution of the Riemann problems at the interfaces between cells in the wave propagation algorithm in the absence of phase transformation.

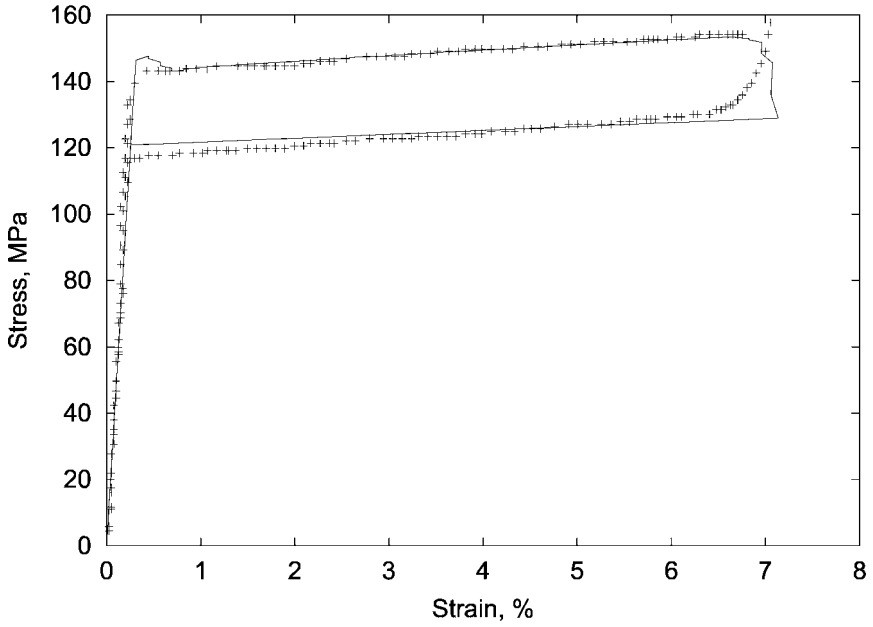

Fig.1. Stress-strain relation at the phase boundary: comparison with experimental data.

NUMERICAL RESULTS

To show the capability of the algorithm, we compare the results of computation for the stress-strain relation in single crystalline CuZnAl shape-memory alloy with the experimental data [8]. The comparison of the stress-strain relation in the case of the full recovering of austenite after unloading is shown in Fig. 1. Here the solid line corresponds to computations, and crosses denote the experimental data.

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