Phase-field modelling of twinning and martensitic transformation at finite strain

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Abstract

We develop a micromechanical phase-field model that describes the transformation between the austenite and twinned martensites. The new model constrains the volume fractions of both parent and internally twinned phases such that the physically motivated bounds are not violated. As an application, we studied the twinned martensite and austenite-martensite interfaces in the cubic-to-orthorhombic transformation in a CuAlNi shape memory alloy and estimated the elastic part of the interfacial energy.

Keywords: phase-field modelling, martensitic phase transformation, shape memory alloys, interface structure

1. Introduction and description of the model

Shape memory alloys are materials with a complex response during deformation. The material can exist in different phases, usually called austenite (parent phase) and martensite (product phase). When being deformed, the material can undergo phase transformation and twinning, which is accompanied by storing energy in the interfaces and which often leads to formation of laminate microstructures. The microstructure is esentially multi-scaled, with characteristic dimension given by spacing of austenite and martensite plates and the twin spacing of two different variants of martensite.

We develop a finite-strain phase-field model of twinning and martensitic transformation in shape memory alloys. The model is based on the minimization of the total rate-potential which describes all processes in the material, namely it consists of the free energy, comprising the elastic and interfacial energy, and the dissipation potential. The interfacial energy describes the energy of diffuse interfaces of a chosen width (parameter of the model) which is a characteristic feature of phase-field modelling [4].

Compared to other phase-field models for twinning [1, 2] our model uses a different mixing of the corresponding transformation strains, so it could have been easily generalized to more variants of phases. Also it is important that our mixing is consistent with respect to the volume changes. Finally, the order parameter, that is in case of our model interpreted as the volume fraction, is restricted so that it does not exceed the physical range. This is implemented with the augmented Lagrangian method, see [7].

In order to model microstructure with the austenite and twinned martensite, we extended the model by introducing two hierarchical order parameters. The volume fraction of the austenite and the other differentiates between two variants of martensite are described. The free energies and dissipation potential are modified consistently. The resulting partial differential equations are solved using the finite element method.

As an application, we study the austenite-martensite interfaces in the cubic-to-orthorhombic transformation in a CuAlNi shape memory alloy. For this purpose we use anisotropic elastic energy with the elastic constants of single-crystalline austenite and martensite of CuAlNi taken from the literature.

Both presented problems are solved in a two-dimensional domain, however, three components of the unknown displacement field are considered. We choose a special 2D domain lying in the plane whose normal $\vec{n}$ is parallel with the vector $\vec{m} \times \vec{l}$, where $\vec{m}$ is the normal of the interface between austenite and twinned martensite obtained from the solution of habit plane equation and $\vec{l}$ is the normal of the interface between martensites from the twinning equation.

2. Shape of the austenite-martensite interface and the elastic microstrain energy factor

Using our model we find the shapes of the interface between austenite and twinned martensite for four different types of possible geometrical microstructures of CuAlNi. The problem is computed in the periodic domain Ω_{per} of the shape of parallelogram where the normal of lateral sides is equal to $\vec{l}$ and the normal of the top and bottom side is equal to $\vec{m}$.

For the order parameters the full periodicity is prescribed. For the displacement we prescribe a boundary condition with a periodic fluctuation, i.e. $\vec{u} = (\mathbf{F}-\mathbf{I})\vec{X}+\vec{\varphi}_{\mathrm{per}}$, where the deformation gradient $\mathbf{F}$ mixes the deformation gradients of austenite and both variants of martensite scaled by average volume fractions. The average volume fraction of austenite is the only prescribed value (one half is chosen in this problem), the average volume fraction of martensites are such that formation of a compatible interface between austenite and twinned martensite is enforced.

The four types of microstructures differ in the geometry and also in a size-independent energy factor Γ^e defined by

$$\Gamma^e = \frac{1}{hA_R} \int_{\Omega_{\mathrm{per}}} \psi_B \, \mathrm{d}X, \tag{1}$$

where ψ_B is the elastic bulk free energy, h is the twin spacing and A_R is the nominal area of the macroscopic austenite-martensite interfaces in the reference configuration.

Stupkiewicz et al. [5] studied the shapes and values of Γ^e for sharp interface between austenite and twinned martensite. They solved a purely elastic problem looking for such interface between austenite and twinned martensite which minimizes the elastic strain energy. In our case we use the phase-field model for dynamical simulation of the evolution of the material and in a steady solution we obtain shapes of the produced interfaces, which are similar to their results. Also the values of Γ^e com-

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puted by ourselves converge close to their values as the interface thickness goes to zero.

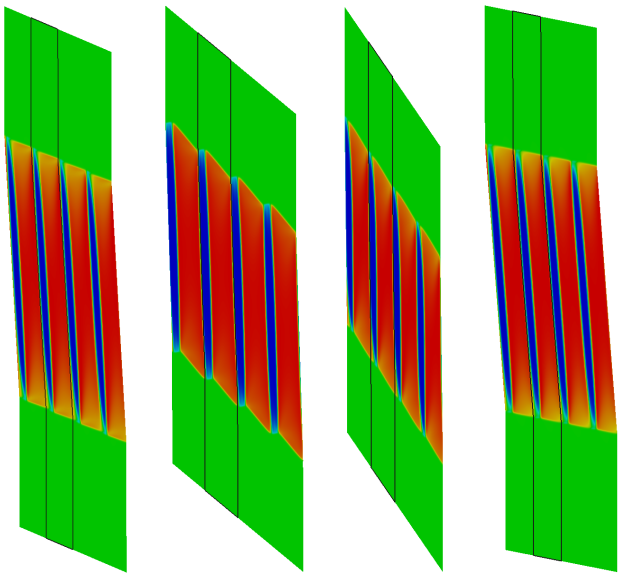

Figure 1: Shapes of interface between austenite and twinned martensite for four different types of microstructures. Austenite is depicted in green, one variant of martensite in red and the other in blue.

3. Full microstructure of the grain-like domain

In an other problem we compute the full microstructure for two variants of martensite and austenite in a circular grain-like domain with the fixed boundary condition for the displacement with the average volume fraction of austenite equal to 0.4.

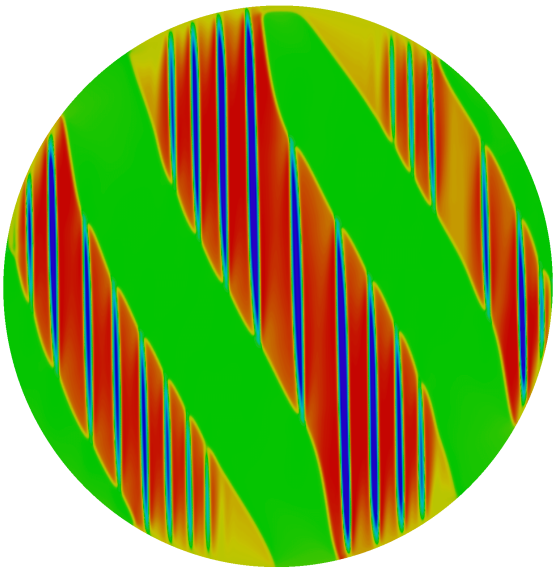

Figure 2: Full microstructure of the grain-like domain with the diameter 600 nm. Austenite is depicted in green, one variant of martensite in red and the other in blue.

The result for the circular domain with the diameter 600 nm is shown in Fig. 2. We study the dependence of the number of austenite-martensite interfaces on the diameter of the domain. By minimizing the energy accumulated on the rigid boundary, interfacial energy between the twins and interfacial energy between austenite and twinned martensite have been estimated by analytic formulae [3, 6]. That estimate is compared with the result obtained from the finite element computation in Fig. 3. The analytical result overestimates the result obtained from the phase-field model, however, the scaling law is correctly predicted.

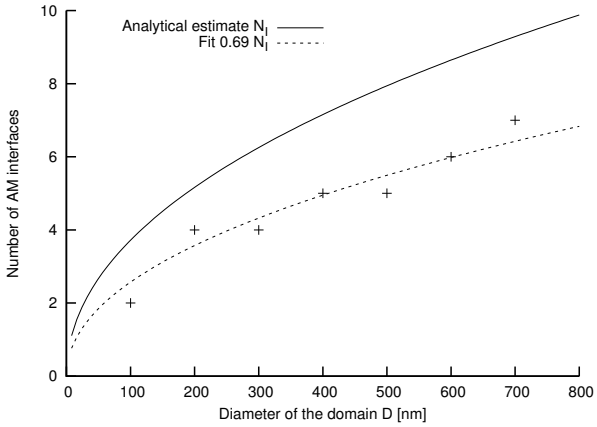

Figure 3: Dependency of number of austenite-martensite microstructure on the diameter, comparison of the analytical estimate and finite element computation

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