THE EFFECT OF TWIN SPACING ON THE MORPHOLOGY OF AUSTENITE-TWINNED MARTENSITE INTERFACE

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1. Introduction and description of the model

The shape memory effect or pseudoelasticity observed in shape memory alloys (SMA) is associated with martensitic phase transformation. SMA can exist in different phases, usually called austenite (parent phase) and martensite (product phase), the latter in different variants. During the phase transformation, interfaces are created and a part of the energy is stored in them.

In most of the materials the transformation strain of a single variant of martensite is usually incompatible with the transformation strain of austenite, and thus the martensitic plates are usually internally twinned. At the macroscale, classical crystallographic theory predicts a planar interface between the austenite and the twinned martensite, but it says nothing about the morphology of the transition layer at the microscale.

A recently developed finite-strain phase-field model for martensitic transformation in shape memory alloys [4] is used to study the size-dependent microstructure of the interface between austenite and twinned martensite. The model is based on the minimization of the total rate-potential which consists of the elastic and interfacial energy and of the dissipation potential. The interfacial energy corresponds to the energy of diffuse interfaces of a width described by the thickness parameter ℓ , which is usual in the phase-field modelling [2].

Two hierarchical order parameters are introduced to model a microstructure composed of the austenite and twinned martensite. They are interpreted as volume fractions: one describes the volume fraction of the austenite and the other distinguishes between two variants of martensite. The order parameters are non-conserved but restricted to lie within the physical range from zero to unity. The respective unilaterial constraints are implemented in the model by using the augmented Lagrangian method, see [3].

2. Results

In order to study the properties of the austenite-twinned martensite interface, a steady solution for the phase-field model is computed. The problem is studied in a plane orthogonal to the twinning plane and to the habit plane known from the classical crystallographic theory of martensite. It is assumed that the microstructure is periodic and two dimensional, but with three components of the displacement field. The phase-field model is implemented in a finite element code AceGen/AceFEM. The computations are performed for CuAlNi shape memory alloy undergoing the cubic-to-orthorhombic transformation. The crystallographic theory predicts 96 austenite-twinned martensite microstructures but only four of them are crystallographically distinct (denoted M1 to M4).

Specifically, we study how the morphology of the interface layer as well as the related interfacial and elastic micro-strain energy contributions depend on the twin spacing h_{tw} and thickness parameter ℓ . It turns out that the elastic micro-strain energy can be reduced by two mechanisms.

For microstructure M2, a formation a non-planar zigzag-like interface (see Figure 1) is a result of a competition between the interfacial energy of austenite-martensite interfaces and the energy of elastic micro-strains that accommodate local incompatibility of the phases. With increasing twin spacing h_{tw} the angle θ is sharper, see Figure 2, which is in a good agreement with the sharp interface model [1].



Figure 1. Microstructure M2: dependence of the microstructure on the twin spacing $h_{\rm tw}$ for $\ell = 0.4$ nm. Austenite is marked by green and the two variants of martensite are marked by blue and red.

All other microstructures M1, M3 and M4 exhibit a tendency to form twin branches which is illustrated for microstructure M3 in Figure 3. With increasing twin spacing h_{tw} , the microstructure is locally refined forming thin needle-like plates of one martensite variant within the other one. This decreases the effective twin spacing and reduces the elastic strain energy.



 $h_{\rm tw} = 10\,\rm nm$ $h_{\rm tw} = 20\,\rm nm$ $h_{\rm tw} = 30\,{\rm nm}$ $h_{\rm tw} = 40\,\rm nm$

the sharp-interface model [1].

Figure 2. Microstructure M2: dependence of the an- Figure 3. Microstructure M3: dependence of the migle θ on $h_{\rm tw}$ and ℓ . Dashed line depicts prediction of crostructure on the twin spacing $h_{\rm tw}$ for $\ell = 0.4$ nm. Austenite is marked by green and the two variants of martensite are marked by blue and red.

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4. References

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