

Interfacial energy and grain-size effect in micromechanical modelling of shape memory alloys

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Abstract

A multiscale approach is presented that is aimed at the modelling of evolution of martensitic microstructures in shape memory alloys with account for the interfacial energy effects. The total Holmholz free energy and the dissipated energy are split into bulk and interfacial contributions, the latter are further split into parts corresponding to specific scales of the microstructure. Microstructure evolution is determined by the incremental energy minimization. Numerical examples are provided to illustrate the predicted grain-size effect in pseudoelastic shape memory alloys.

Keywords: interface problems, laminates, microstructures, multiscale problems, smart materials

1. Introduction

Martensitic phase transformation is the basic mechanism responsible for the effects, such as pseudoelasticity and shape memory effect, which are observed in shape memory alloys (SMA). The martensitic transformation proceeds through evolution of martensitic microstructures, and this is associated with formation and evolution of interfaces at multiple scales. As each interface carries some energy (the interfacial energy), the microstructure evolution and the macroscopic behaviour of the material are significantly influenced by the interfacial energy. The paper presents the approach [1, 2] aimed at including the effects of interfacial energies present at different scales of martensitic microstructures into micromechanical models of SMA polycrystals.

2. Modelling framework

The approach is based on the following minimization problem [3]

$$\Delta E \rightarrow \min \quad \text{subject to kinematical constraints,} \quad (1)$$

where ΔE is the incremental energy supplied to the thermodynamic system under consideration. Assuming kinematic control, the incremental energy is in the present context equal to

$$\Delta E = \Delta \Phi + \Delta \mathcal{D}, \quad (2)$$

where Φ is the total Helmholtz free energy and $\Delta \mathcal{D}$ is the increment of dissipated energy, both per unit representative volume. The process is assumed here to be isothermal and quasi-static at the time scale associated with slowly varying external loading.

The total free energy Φ is expressed as a sum of a size-independent bulk energy contribution Φ_v and several size-dependent interfacial energy contributions Φ_k , each corresponding to a specific scale,

$$\Phi = \Phi_v + \Phi_i, \quad \Phi_i = \sum_k \Phi_k. \quad (3)$$

Similarly, the dissipation is also assumed to comprise a size-independent bulk contribution $\Delta \mathcal{D}_v$ and size-dependent interfa-

cial contributions $\Delta \mathcal{D}_k$,

$$\Delta \mathcal{D} = \Delta \mathcal{D}_v + \Delta \mathcal{D}_i, \quad \Delta \mathcal{D}_i = \sum_k \Delta \mathcal{D}_k. \quad (4)$$

It is further assumed that the negative increments of interfacial energy, typically associated with annihilation of interfaces, can hardly be reverted into the bulk free energy and thus contribute to (size-dependent) dissipation. Accordingly, we have

$$\Delta \mathcal{D}_k = \kappa_k (-\Delta \Phi_k)_+, \quad 0 \leq \kappa_k \leq 1, \quad (5)$$

where κ_k is rather close to unity, and $(\psi)_+ = \psi$ if $\psi > 0$ and $(\psi)_+ = 0$ otherwise.

3. Interfacial energy

In accord with experimental observations, the microstructure formed within a grain of a polycrystalline aggregate is assumed to be composed of domains (sub-grains) of austenite-martensite laminates formed by parallel internally twinned martensitic plates within the austenite matrix. Accordingly, interfaces at three spatial scales are considered: at the twin boundaries within internally twinned martensitic plates, at the austenite-martensite interfaces, and at grain or domain boundaries.

An atomic-scale interfacial energy is accounted for at the twin boundaries and at the direct austenite-martensite boundaries. The atomic-scale interfacial energy is taken from the materials science literature.

There is also another source of interfacial energy, namely the energy of elastic micro-strains. These strains result from local incompatibility of transformation strains (eigenstrains) at the austenite-twinned martensite interfaces and at the grain or domain boundaries attained by parallel plates of martensite. The elastic micro-strain energy is a bulk energy on a sufficiently fine scale, but upon averaging it is interpreted as an interfacial energy at a higher scale. It follows from dimensional analysis, that the interfacial energy γ_k^e of elastic micro-strains is proportional to the spacing h_k of the laminate terminating at the interface,

$$\gamma_k^e = \Gamma_k^e h_k, \quad (6)$$

where Γ_k^e is a size-independent energy factor. The energy factor Γ_{am}^e corresponding to the austenite-twinned martensite interfaces

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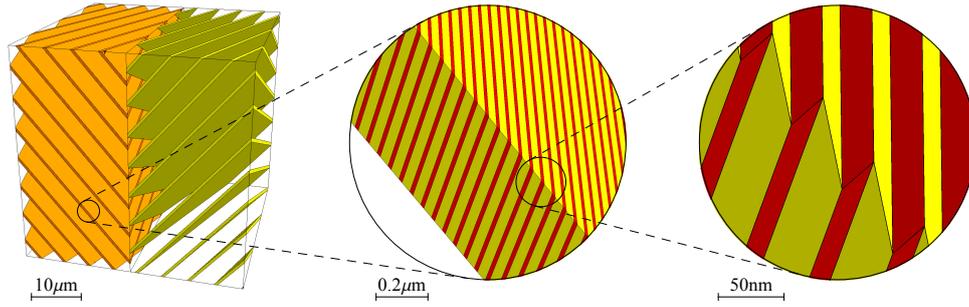


Figure 1: Microstructure of an idealized SMA polycrystal (rank-three laminate) during stress-induced transformation (Petryk et al. [1]). The austenite is transparent. Note the scale markers.

can be determined using the approach developed in [4], which employs finite element computations, shape sensitivity analysis and gradient-based minimization. The energy factor Γ_{gb}^e corresponding to grain or domain boundaries is estimated using a simplified approach proposed in [1, 2].

The interfacial energy contribution Φ_k corresponding to a specific scale is finally determined as a product of the interfacial energy at this scale and the total area of the interfaces within a representative volume element. In the case of simplified microstructures, this can be done in a closed form so that the total interfacial energy Φ_1 explicitly depends on the microstructural parameters describing the characteristic dimensions of the microstructure, cf. [1, 2].

4. Selected results

Selected results are presented in Figs. 1–3. Minimization of incremental energy ΔE includes the size-dependent interfacial energy contribution so that the characteristic dimensions of the microstructure are obtained as a result of minimization. Figure 1 shows a sample microstructure (shown to scale) of an idealized SMA polycrystal (CuAlNi alloy) during stress-induced transformation. Size-dependent dissipation and initial thickness of martensite plates predicted for two values of twin boundary energy γ_{tw}^a are shown in Fig. 2 (NiTi alloy). Finally, the effect of grain size on the macroscopic pseudoelastic hysteresis loop is shown in Fig. 3. Here, the response of a NiTi polycrystal has been determined using the bi-crystal aggregate model developed in [5].

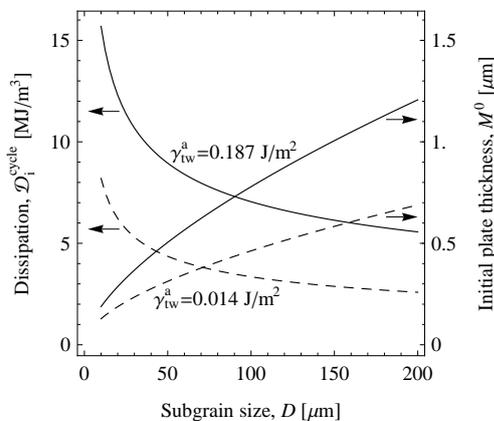


Figure 2: Initial martensite plate thickness M^0 and the dissipated interfacial energy D_i^{cycle} in a complete forward-reverse transformation cycle, as a function of the subgrain diameter D (Stupkiewicz and Petryk [2]).

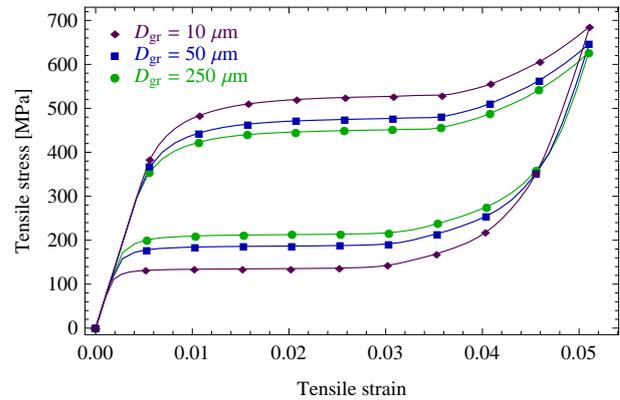


Figure 3: Macroscopic stress-strain diagrams (uniaxial tension of NiTi SMA polycrystal) for selected grain diameters D_{gr} (Stupkiewicz and Petryk [2]).

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