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Finite element simulations of microstructure evolution in stress-induced martensitic transformations



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ABSTRACT

Microstructure evolution in single crystal and polycrystal shape memory alloys under uniaxial tension and compression is investigated using the finite element method. To determine stress-strain diagrams and evolution of martensitic microstructure during external loading, a micromechanics based thermo-mechanical material model is used. The results reveal the significant difference between the local and global material behavior when defects are present. It is shown that defects act as nucleation sites and result in transformation localization, which in turn causes a sudden drop in the stress-strain diagram followed by a stress plateau. Moreover, it is found that some regions undergo reverse transformation although the elastic moduli of the phases are equal and the loading is monotonic. Increase in athermal friction, which is the resistance to interface propagation, is found to delay the phase transformation and different magnitudes of hysteresis are obtained at different friction values. The model predicts the tension-compression asymmetry observed in shape memory alloys. The simulation results are in qualitative agreement with several experimental studies.

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1. Introduction

Martensitic phase transformations (PTs) are observed in several materials such as metals, ceramics, alloys and biological systems. The main deformation mechanism of shape memory alloys (SMA) is based on martensitic PTs. Physical and mechanical properties of the material is determined by the formed microstructure. SMAs have complex and non-linear stress-strain behavior under thermomechanical loadings. They exhibit unique material behavior such as shape memory effect and superelasticity. An understanding of these properties and the governing deformation mechanism is important for material design and industrial applications.

There are various phenomenological (Abeyaratne and Kim, 1997; Arghavani et al., 2010; Auricchio et al., 1997; Bo and Lagoudas, 1999; Brinson, 1993; Lagoudas et al., 2012; Lexcellent et al., 2000; Liang and Rogers, 1990; Panico and Brinson, 2007; Saleeb et al., 2011; Zaki and Moumni, 2007) and micromechanics based (Gao et al., 2000; Heinen et al., 2009; Levitas and Ozsoy, 2009a, 2009b; Lexcellent et al., 1996; Pan et al., 2007; Patoor et al., 1996; Thamburaja and Anand, 2001; Thamburaja et al., 2009; Yu et al., 2013) models developed for the description of the behavior of materials that undergo martensitic phase transformations. The phenomenological models aim to determine the macroscopic behavior of SMA using homogenization techniques. In order to fit the material behavior observed in experiments to the calculations, they use several parameters that are measurable macroscopically in these experiments. On the other hand, the microstructure of the SMA, which is paid less importance in phenomenological models, is used to determine both the microscopic and macroscopic behavior of the SMAs in micromechanics based models. The macroscopic behavior of the material is usually captured by using finite element method (FEM) for a finite sample. Microstructure evolution can be determined by FEM based on extremum principles of thermodynamics for elastic and elastoplastic materials (Idesman et al., 1999; Levitas et al., 1998; Reisner et al., 1998) or kinetic extremum principles (Idesman et al., 2000; Levitas, 2000a; 2000b).

At the nanoscale, phase field approach is used to model multivariant microstructure evolution in a single crystal and polycrystal materials (Artemev et al., 2001; Jin et al., 2001) which is generalized in dynamic problems (Cho et al., 2012; Idesman et al., 2008) and large strains (Levin et al., 2013; Levitas, 2013; Levitas et al., 2013). Due to necessity to resolve few nanometer size interface, this approach is limited to nanosize samples. Also, athermal threshold was missing in the phase field approach, which was resolved in Levitas and Lee (2007), Levitas et al. (2010).

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Recently, we developed a micromechanics based model for the description of martensitic PT at small and large deformations and derived the universal (i.e. independent of constitutive equations) thermodynamic driving force for interface orientation (Levitas and Ozsoy, 2009a, 2009b; Levitas et al., 2007). Considering a representative volume element (RVE) consisting of austenite and two martensitic variants, each separated by plane interfaces, the complete system of equations that describes the evolution of martensitic microstructure is derived. The model incorporates athermal interface friction, which is the resistance to interface motion caused by the interactions between the corresponding interface and the long-range stress fields of defects (point defects, dislocations, grain and subgrain boundaries), the Peierls barrier and acoustic emission. The value of this parameter varies by preliminary plastic deformation or thermomechanical treatment, and can be determined by cyclic loading experiments. We presented several examples of microstructure evolution in the RVE (local material behavior) under complex loading with different athermal frictions. A small artificial martensitic nucleus is assumed to be present in the RVE to calculate the equilibrium crystallographic parameters for stress- and temperature-induced transformations. Macroscopic stress for the RVE is found to decrease (strain softening) monotonically during a direct PT with an increase in applied strain under uniaxial tension which is due to the internal stresses caused by incompatible transformation strain. Although this is valid for local material response, such material instability causes localization of transformation strain in the solution of a boundary-value problem for bulk material and results in formation of discrete martensitic microstructure (Levitas et al., 2004; Idesman et al., 2005). Thus, the stress-strain diagram for a finite sample which can either be a single crystal or polycrystal would be different than the local one. In addition, when the material is a single crystal, the presence of nucleation sites results in totally different behavior of the material since such real nuclei create internal stresses in the surrounding matrix, which in turn yields more material to transform into martensite instantly. Therefore, these constitutive equations should be used for a finite sample to determine the macroscopic behavior of the material, which is the motivation of the current study.

In this paper, we investigate the evolution of martensitic microstructure in single crystal and polycrystal finite samples of SMA under uniaxial load using the finite element method, which is missing in our previous studies (Levitas and Ozsoy, 2009a, 2009b; Levitas et al., 2007). A numerical scheme is implemented into the finite element analysis software ABAQUS via user-defined material subroutine (UMAT). The following aspects of the stress-induced martensitic PT in elastic materials are studied:

- (a) the effect of crystal orientation on the material behavior of single crystal SMA,
- (b) the propagation of phase transformation in an austenitic SMA which has several martensitic nuclei,
- (c) the material behavior of polycrystal SMA,
- (d) the effect of athermal friction on the material behavior and hysteresis.

The paper is organized as follows: Section 2 describes the thermomechanical model that we used in our calculations. The model incorporates driving forces for both interface propagation and rotation based on a RVE that consists of a parent phase (austenite) and a product phase (fine mixture of two martensitic variants). In Section 3, the finite element model of PT for single crystal and polycrystal SMA in elastic range is described and explanation for solution of the constitutive equations is presented. Several simulation results for single and polycrystal plates with or without nucleation sites are also given in this section.



Fig. 1. Cubic representative volume element *V* used in the model. RVE consists of austenite phase (A) and a fine mixture of two martensitic variants (M_1 , M_2). Vectors *a* and *a*₁ represent the jumps in the strain across the A–M interface and M_1 – M_2 interfaces; *n* and *n*₁ are the normal vectors to the interfaces between A-M interface and M_1 – M_2 interfaces, respectively.

2. Description of the model

A cubic RVE of volume V consisting of austenite and fine mixture of two martensitic variants, as shown in Fig. 1, is considered in the model (Levitas and Ozsoy, 2009a, 2009b; Levitas et al., 2007). The letters and subscripts A, M, 1 and 2 represent austenite, martensite and first and second martensitic variants, respectively, c represents the volume fraction of the corresponding phase or martensitic variant. The jump in the strain across the A-M interface and M_1-M_2 interfaces are designated by **a** and **a**₁, respectively. All interfaces between A-M and martensitic variants (M₁-M₂) are planes and parallel to each other. The position of the A-M interface is determined by the normal vector \boldsymbol{n} to the A-M interface and the volume fraction of A, c_A . Similarly, the normal vector \mathbf{n}_1 to the interface between martensitic variants and the volume fraction of one of the variants determine the geometry of the martensitic mixture. As the position of these interfaces change, phase transformation occurs from one phase to the other. The main assumption is that stresses and all strains (total, elastic and transformational) are homogeneous in each phase and martensitic variant. Let the strain tensor $m{arepsilon}$ averaged over the volume V is prescribed as a function of time and the orientation of the crystal lattice of A, transformation strains $\boldsymbol{\varepsilon}_{ti}$ for all symmetry-related martensitic variants, and the elastic properties of single crystals of A and M are given. In this problem, the two M variants among all possible in the system, the evolution of strains and stresses in A and each M variant, the stress σ averaged over the volume V, and the evolution of all microstructural parameters (n, n_1 , c_A , and c_1) have to be found. These are all determined by the system of equations given below. Although the model developed in Levitas and Ozsoy (2009a, 2009b) has several different and sophisticated versions, we use the most basic one for simplicity and computational efficiency.

Homogenization: A simple homogenization rule based on the volume fractions is considered as given in Eqs. (1) and (2) where the relationship between volume fractions are given in Eq. (3). Here, σ and ε are the stress and strain tensors averaged over the RVE and σ_M and ε_M are the ones averaged over the martensitic volume in the RVE.

$$\boldsymbol{\varepsilon} = c_1 \boldsymbol{\varepsilon}_1 + c_2 \boldsymbol{\varepsilon}_2 + c_A \boldsymbol{\varepsilon}_A; \quad \boldsymbol{\varepsilon}_M = \frac{c_1}{c_M} \boldsymbol{\varepsilon}_1 + \frac{c_2}{c_M} \boldsymbol{\varepsilon}_2, \tag{1}$$

$$\boldsymbol{\sigma} = c_1 \boldsymbol{\sigma}_1 + c_2 \boldsymbol{\sigma}_2 + c_A \boldsymbol{\sigma}_A; \quad \boldsymbol{\sigma}_M = \frac{c_1}{c_M} \boldsymbol{\sigma}_1 + \frac{c_2}{c_M} \boldsymbol{\sigma}_2.$$
(2)

$$c_A + c_M = 1, \quad c_M = c_1 + c_2,$$
 (3)

Kinematic decomposition: In Eq. (4), the strain is decomposed into its elastic and transformational parts, represented by the subscripts *e* and *t*, respectively. Note that e_A does not have a

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