



A coupled kinetic Monte Carlo–finite element mesoscale model for thermoelastic martensitic phase transformations in shape memory alloys

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Abstract—A mesoscale modeling framework integrating thermodynamics, kinetic Monte Carlo (KMC) and finite element mechanics (FEM) is developed to simulate displacive thermoelastic transformations between austenite and martensite in shape memory alloys (SMAs). The model is based on a transition state approximation for the energy landscape of the two phases under loading or cooling, which leads to the activation energy and rate for transformation domains incorporating local stress states. The evolved stress state after each domain transformation event is calculated by FEM, and is subsequently used in the stochastic KMC algorithm to determine the next domain to transform. The model captures transformation stochasticity, and predicts internal phase and stress distributions and evolution throughout the entire incubation, nucleation and growth process. It also relates the critical transformation stresses or temperatures to internal activation energies. It therefore enables quantitative exploration of transformation dynamics and transformation–microstructure interactions. The model is used to simulate superelasticity (mechanically induced transformation) under both load control and strain control in single-crystal SMAs under uniaxial tension.

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1. Introduction

Thermoelastic shape memory alloys (SMAs) have broad applications in sensing, actuation, energy conversion and damping [1]. They can switch between their original shape and a notably different shape under thermal or mechanical cycling, and this process usually involves a temperature or stress hysteresis indicative of energy dissipation [2–4]. The shape memory and superelastic properties of SMAs are achieved by a reversible and diffusionless martensitic phase transformation that occurs mainly by a large, cooperative shear of atoms [5]. The transformation process (i.e. the nucleation and growth of thermoelastic martensite plates) involves extensive interactions with defects, including interfaces and surfaces. For example, martensite plates may preferentially nucleate at these defects [6,7], and may also interact with them at the transformation front [8]. The crystallographic shear by which martensite develops can lead to mechanical interactions across both phase and grain boundaries [9], as well as strain relief at free surfaces.

Transformation–microstructure interactions, however, are not well understood, and their effects on transformation kinematics have not been established quantitatively. The

need to gain a fundamental understanding of the roles of defects is further motivated by recent results showing size effects in small-scale SMAs. For example, grain size effects on transformation temperatures and stresses emerge below a critical size of about 100 μm in polycrystalline SMAs [10–13]. In single-crystalline SMA pillars with diameters below 20 μm , the pillar size clearly affects the transformation stresses [14–17]. In SMA microwires [18] and foams [19–21] with bamboo grain structures (i.e. with grain sizes equal to the wire diameter or strut thickness), the characteristics of transformation also depend on the sample size. These size effects have been attributed to the increasing relative density of grain boundaries or free surfaces at smaller scales, but their origins and microstructural mechanisms have just begun to be explored. Modeling martensitic transformation processes at the microstructural level can shed light onto the interplay between transformation processes and grain boundary or surface states, and perhaps eventually onto the microstructural design of SMAs.

The majority of existing models for SMAs are analytical and generally fall into the following categories.

- (1) Phenomenological theories of martensite crystallography, which examine the conversion pathways between two crystal structures in terms of distortion (or shearing) and rotation [22–25].

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- (2) Dislocation-based models of martensite interfaces, which use dislocation arrays to model interface structure and mobility based on the known properties, such as the stress fields of dislocations [26–31].
- (3) Thermodynamic models of martensitic nucleation [32–34] and transformation [35–38], which focus on the contribution to the free energy change from interface energy, elastic energy and dissipation mechanisms.
- (4) Constitutive micromechanical models for martensitic transformation, which determine macroscopic behaviors based on an assumed local stress–strain constitutive law and advance transformation by gradually changing a state variable such as martensite fraction [39–44].

These models provide profound understanding of martensitic transformation, mechanistically, thermodynamically and mechanically. In general, however, they neither involve a physical timescale nor address spatial phase distributions and evolution. Few of these models have been used to explore the effects of defects on transformation kinematics, and many are not suited for this purpose.

Computational models for reversible martensitic transformations in SMAs are relatively rare. There are relatively few atomistic studies, such as molecular dynamics (MD) of SMAs [45,46], and most of them deal with the binary NiTi system [47,48], since they rely on the availability of accurate inter-atomic potentials for complex SMAs. The limited length (e.g. 10–30 nm) and time (e.g. nanosecond) scales accessed by such MD studies are not directly comparable to those (e.g. hundreds of nanometers [49] to micrometers in size and milliseconds [17] to minutes in time) involved in existing experimental measurements of SMAs. There are also a number of finite element [50–55] and phase field [56–60] models for SMAs, which can incorporate much larger scales in the constitutive laws describing material energy during transformation. However, continuum models sometimes cannot predict reverse transformation, and more generally tend to lack connections between simulated scales and those intrinsic to martensitic transformation in SMAs, which are essential for understanding defect–transformation interactions.

All of the above points speak of the need for a physically based mesoscale model for thermoelastic martensitic transformation – one that can include a physical timescale for transformation and can specifically address issues of transformation kinematics in the presence of microstructure. Our purpose in this paper is to develop such a mesoscale modeling framework for SMAs by coupling the kinetic Monte Carlo (KMC) algorithm with the finite element method (FEM). FEM allows us to determine the mechanical state everywhere in the material, and to allow the local state to affect the transformation sequence. The onset and progression of the transformations are controlled by KMC using a transition-state rate equation characteristic of thermally activated phenomena, and the forward and reverse transformations are treated “symmetrically” in the model, i.e. they are both permitted at any time. In what follows we develop the framework for such a mesoscale model, and demonstrate its capabilities to simulate mechanically induced transformations under conditions of constant loading rate and constant strain rate.

2. Thermodynamic framework for thermoelastic reversible martensitic transformations

In this section, we examine the energetics governing austenite ↔ martensite transformations in SMAs. In Section 2.1, we determine the free energies of the two phases as functions of temperature and stress, as the difference between them is the driving force for transformation. In Section 2.2, we formulate the system energy evolution during transformations, which involves a variety of additional sources, such as interface energy, strain energy and dissipated energy. In Section 2.3, we propose an apparent equilibrium temperature/stress, and determine the transformation hysteresis incorporating coupled temperature–stress effects. In Section 2.4, we use an energy landscape approach to describe the above thermodynamic driving forces and energy penalties for transformations. Lastly, in Section 2.5, we present a new type of energy landscape map describing conversions between an initial state and a transformed state, which will lay the foundation for our subsequent KMC–finite element mesoscale modeling in Section 3. In the following, we use “A” and “M” to denote properties of austenite and martensite, respectively.

2.1. Free energy difference between austenite and martensite

The Gibbs free energies G_A and G_M per unit volume as a function of temperature T are illustrated in Fig. 1(a). When there is no external stress, $G_A = G_A^{ch}$ (red line) and $G_M = G_M^{ch}$ (bold blue line), where G_A^{ch} and G_M^{ch} are the chemical free energies. The slopes of these lines are the entropy S_A and S_M , respectively.

$$G_A^{ch} = H_A - TS_A \quad \text{and} \quad G_M^{ch} = H_M - TS_M \quad (1)$$

Let T_0 denote the equilibrium temperature at which $G_{A,0}^{ch} = G_{M,0}^{ch}$ and the transformation enthalpy $\Delta H_0 = H_{M,0} - H_{A,0} = T_0(S_{M,0} - S_{A,0}) = T_0\Delta S_0$, where $\Delta H_0 < 0$ and $\Delta S_0 < 0$. As $H_A = H_{A,0} + \rho C_p^A(T - T_0)$ and $H_M = H_{M,0} + \rho C_p^M(T - T_0)$, where ρ is the density and C_p is the specific heat capacity, the transformation enthalpy at T is

$$\Delta H = H_M - H_A = \Delta H_0 + \rho\Delta C_p(T - T_0) \quad (2)$$

with $\Delta C_p = C_p^M - C_p^A$. Meanwhile, $S_A = S_{A,0} + \rho C_p^A \ln(T/T_0)$ and $S_M = S_{M,0} + \rho C_p^M \ln(T/T_0)$, and therefore the transformation entropy at T is

$$\Delta S = S_M - S_A = \Delta S_0 + \rho\Delta C_p \ln(T/T_0) \quad (3)$$

where $S_M < S_A$ and $\Delta S < 0$. As a result, G_M^{ch} decreases with T more slowly than G_A^{ch} , as can be seen in Fig. 1(a). Eqs. (2) and (3) lead to the change in chemical free energy at T , $\Delta G^{ch} = G_M^{ch} - G_A^{ch} = \Delta H - T\Delta S$.

$$\Delta G^{ch} = -\Delta S_0(T - T_0) + \rho\Delta C_p[T - T_0 - T \ln(T/T_0)] \quad (4)$$

If the change in heat capacity is assumed insignificant and $\Delta C_p = 0$, Eq. (4) is reduced to

$$\Delta G^{ch} = (-\Delta S_0)(T - T_0) \quad (5)$$

When $T > T_0$, $\Delta G^{ch} > 0$, and austenite is preferred; when $T < T_0$, $\Delta G^{ch} < 0$, and martensite is preferred.

Upon application of an external stress that leads to a resolved shear stress τ on the habit plane (in the elastic regime before yielding), G_A changes little while G_M is

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