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A micromechanics-inspired constitutive model for shape-memory alloys that accounts for initiation and saturation of phase transformation

Alex Kelly^a, Aaron P. Stebner^b, Kaushik Bhattacharya^{a,*}^a Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA^b Mechanical Engineering, Colorado School of Mines, Golden, CO 80401, USA

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ABSTRACT

A constitutive model to describe macroscopic elastic and transformation behaviors of polycrystalline shape-memory alloys is formulated using an internal variable thermodynamic framework. In a departure from prior phenomenological models, the proposed model treats initiation, growth kinetics, and saturation of transformation distinctly, consistent with physics revealed by recent multi-scale experiments and theoretical studies. Specifically, the proposed approach captures the macroscopic manifestations of three micromechanical facts, even though microstructures are not explicitly modeled: (1) Individual grains with favorable orientations and stresses for transformation are the first to nucleate martensite, and the local nucleation strain is relatively large. (2) Then, transformation interfaces propagate according to growth kinetics to traverse networks of grains, while previously formed martensite may reorient. (3) Ultimately, transformation saturates prior to 100% completion as some unfavorably-oriented grains do not transform; thus the total transformation strain of a polycrystal is modest relative to the initial, local nucleation strain. The proposed formulation also accounts for tension–compression asymmetry, processing anisotropy, and the distinction between stress-induced and temperature-induced transformations. Consequently, the model describes thermoelastic responses of shape-memory alloys subject to complex, multi-axial thermo-mechanical loadings. These abilities are demonstrated through detailed comparisons of simulations with experiments.

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1. Introduction

Shape-memory alloys (SMAs) exhibit unusual macroscopic phenomena including superelasticity, the shape-memory effect, and actuation. Through these behaviors, inelastic strains on the order of several percent are recovered because they are accommodated through diffusionless, reversible microstructure rearrangement instead of slip, glide, climb, and other irrecoverable, plastic mechanisms. These remarkable phenomena are enabled by solid-to-solid phase transformation between a high symmetry *austenite* phase that is stable at high temperatures, and a low symmetry *martensite* phase that is stable at low temperatures. The symmetry disparity between the phases allows multiple *variants* of the martensite phase – martensite

* Corresponding author.

E-mail address: bhatta@caltech.edu (K. Bhattacharya).<http://dx.doi.org/10.1016/j.jmps.2016.02.007>

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structures that are identical up to their orientation – to form from each austenite structure during transformation. The ability to form variants or patterns of variants manifests an infinite number of possibilities for macroscopic strains, or shape changes, during transformation of a polycrystal. As for a liquid–solid or liquid–gas transformation, a Clausius–Clapeyron relation governs the solid-state phase transformation of SMAs. Thus, the transformation may be induced by changing temperature or stress. The state of thermo-mechanical loading during transformation will also dictate the shape change. Furthermore, while in the martensitic state, one variant may switch to another – *i.e.*, *reorient* – in response to applied forces, also resulting in macroscopic shape changes.

Regardless of whether a given martensite structure was formed directly during transformation or via post-transformation deformation, upon reverse transformation, all variants of martensite revert back to the same initial austenite structure, resulting in full shape recovery, or “shape-memory.” *Superelasticity* describes a constant ambient temperature event in which elastic and transformation strains induced by mechanical loading are completely recovered upon unloading. Analogously, via the *shape-memory effect*, a SMA mechanically deformed, then unloaded below the critical transformation temperature, while in the martensite phase, returns to its original shape upon heating to austenite. *Actuation* is achieved by maintaining an applied load while heating and cooling through transformation; the SMA recovers transformation strain against the load thereby producing mechanical work.

The unusual properties of SMAs have led to their use in a variety of engineering applications ranging from implantable medical devices to actuators. We refer the reader to [Otsuka and Wayman \(1998\)](#) for a detailed introduction. The increasingly sophisticated applications of these materials calls for a model that is capable of faithfully describing complex phenomena, while being simple enough to be used in the engineering design process. This demand has motivated a number of models. Some of these, like the widely used models of [Auricchio et al. \(1997\)](#), [Auricchio and Petrini \(2004\)](#) and [Lexcellent et al. \(2002\)](#), are phenomenological and adapt frameworks from other subjects like plasticity. Others, like the models of [Qidwai and Lagoudas \(2000\)](#), [Panico and Brinson \(2007\)](#), [Sadjadpour and Bhattacharya \(2007b,a\)](#), and [Chemisky et al. \(2011\)](#) introduce internal variables to incorporate some microscopic information. Yet other models like those of [Zaki and Mounni \(2007\)](#) focus on thermomechanical interactions and cyclic loadings. We refer the reader to [Chemisky et al. \(2011\)](#) for a comprehensive survey of the literature. Despite significant advances, a phenomenological model that accurately describes transformation initiation, growth, and saturation during multiaxial proportional and non-proportional loading remains a work in progress, and motivates the proposed model.

We now consider superelasticity in some detail to describe the ideas of the current model. To understand the underlying mechanisms behind this phenomenon, we first consider an ideal *single crystal* at a temperature just above its transformation temperature. At this temperature, austenite is the stable phase and martensite the metastable phase. As the crystal is subjected to stress, it initially responds elastically as in loading prior to point A in [Fig. 1a](#). However, at some critical stress, the martensite is stabilized ([Burkart and Read, 1953](#); [James, 1986](#)) and the material begins to transform from austenite to martensite. This event results in a macroscopic inelastic yield event that appears similar to perfect plasticity (A). Once the material is fully martensite, the martensite now responds elastically on further loading to some maximum load below the stress required for detwinning and/or plastic flow (B to C). Upon unloading, the martensite remains the stabilized phase as long as the stress remains high and unloads elastically (C–E). However, at some critical stress, it becomes unstable and begins to transform to the austenite, and this reverse transformation gives rise to the lower plateau (E to F). Once the transformation is complete, the austenite unloads elastically.

Hysteresis results from energy dissipated during transformation. For superelasticity, it is often characterized by the differences between the critical stresses for forward and reverse transformation. Single crystal transformation responses differ with differing loading directions due to crystallographic anisotropy ([Miyazaki et al., 1984](#); [Shield, 1995](#)). Specifically, a

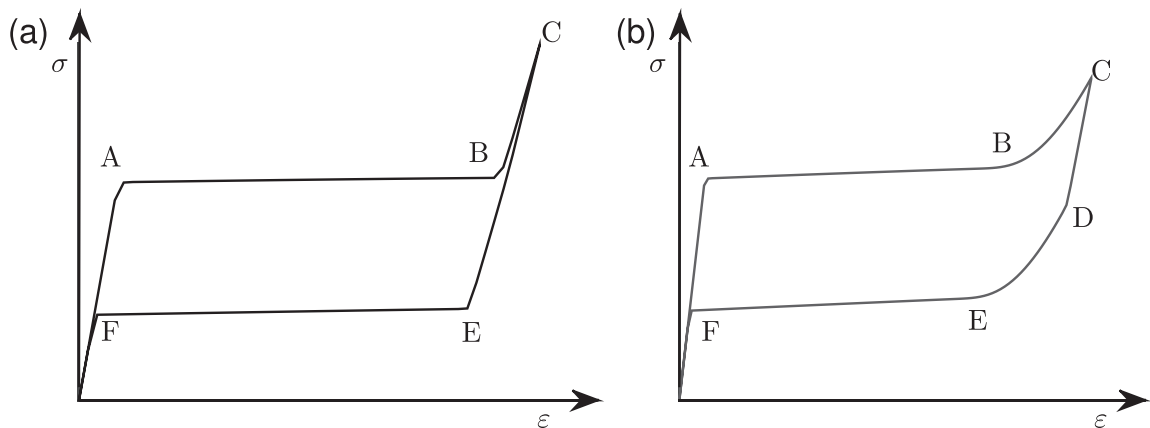


Fig. 1. A schematic representation of superelasticity in (a) single crystal and (a) polycrystalline specimens.

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