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A phase field approach with a reaction pathways-based potential to model reconstructive martensitic transformations with a large number of variants

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ABSTRACT

A pathway tree is constructed by recursively duplicating a single reconstructive martensitic transformation path with respect to lattice symmetries and point-group rotations. An energy potential built on this pathway is implemented in a phase-field technique in large strain framework, with the transformational strain as the order parameter. A specific splitting between non-dissipative elastic behavior and the dissipative evolution of the order parameter allows for the modeling of acoustic waves during rapid transformations. A simple toy-model transition from hexa- to square-lattice successfully demonstrates the possibility to model reconstructive martensitic transformations for a large number of variants (more than one hundred). Pure traction applied to our toy-model shows that variants can nucleate into previously created variants, with a hierarchical nucleation of variants spanning over five levels of transformation.

1. Introduction

Martensitic transformations (MTs) are characterized by a very rapid evolution of crystal lattice that may occur at the microsecond scale (e.g., Kadau et al., 2002, 2005; Denoual et al., 2010), faster than any diffusion-driven transformations. For numerous MTs, a lattice distortion (spanning a zone larger by orders of magnitude than the average lattice spacing) is the only observable transformation process, accompanied by an instantaneous adaptation of the electronic structure. For these so-called "proper" MTs, a straightforward definition of a macroscopic scale free energy consists in averaging atomic energy, which is a function of local deformation only, through the Cauchy–Born rule. No dissipation has to be introduced at the macroscopic scale since most of the excess energy due to instabilities encountered between stable states are carried away by acoustic waves, which may be audible as a remarkable side effect of MTs. Thus, the instantaneous response of a "proper" MT could be modeled, at a microscopic scale, through a non-dissipative potential function of deformation only, in addition to the kinetic energy.

In contrast with molecular dynamics (MD) methods, for which phase stability depends on local atomic arrangements only, the modeling of MTs requires linking the deformation state and stable phases through local minima of a free energy potential. The definition of such potential is, however, complex for *reconstructive* MTs that are characterized by an evolving set of point-group symmetries, with some symmetries vanishing at the beginning of the transformation and new symmetries emerging when the transformation is complete. Taking the Bain transformation from body-centered cubic (BCC) to face-centered cubic (FCC) MTs as an example, one has to consider one stable state for the parent phase plus three additional

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Notations

$\boldsymbol{A}:\boldsymbol{B} = A_{ij}B_{ij}$ Scalar product

$|\boldsymbol{A}| = (\boldsymbol{A}:\boldsymbol{A})^{\frac{1}{2}}$ Frobenius norm

$\boldsymbol{P}$ 1st Piola–Kirchhoff stress

$\boldsymbol{S}$ 2nd Piola–Kirchhoff stress

$\mathbb{D}$ Elasticity tensor in reference frame

$\mathbb{B}$ Stress–strain tensor

$\boldsymbol{T}$ Distortion along a pathway

$\boldsymbol{F}$ Total distortion

$\boldsymbol{F}$t Transformational distortion

$\boldsymbol{F}$e Elastic distortion

$\boldsymbol{F}\mathrm{et} = \boldsymbol{F}\mathrm{e}\cdot\boldsymbol{F}\mathrm{t}$ Transformation and elastic distortion

$\boldsymbol{X}$ A vector in the initial frame

$\boldsymbol{x}$ A vector in the deformed frame

$\boldsymbol{D}$ Pathway direction

$\boldsymbol{N}$ Pathway normal

${}^{\mathrm{b}}_{\mathrm{a}}\boldsymbol{A}$, ${}^{\mathrm{b}}_{\mathrm{a}}\boldsymbol{A}^{\mathrm{T}}$, ${}^{\mathrm{b}}_{\mathrm{a}}\boldsymbol{A}^{-\mathrm{T}}$ Transformation to phase 'b' in the frame of phase 'a', its transposed and inverse transposed

${}^{\mathrm{a}}\boldsymbol{A}$ Transformational strain of a phase 'a' *in reference frame*

${}^{\mathrm{ab}}\boldsymbol{A}(s)$ Transformational strain between 'a' and 'b', i.e., along a pathway, with curvilinear abscissa *s in reference frame*

stable states for the FCC variants. The corresponding potential must have at least four energy wells, three for the Bain deformations plus the initial (parent) state. Since reversions from a variant also lead to additional stable phases (six additional stable BCC phases coming from the reversion of the three FCC variants), the energy landscape has an expanding set of variants for each transformation/reversion cycle, and is, in general, unbounded. In addition to the probable onset of plasticity during reconstructive phase transformations (as discussed in Bhattacharya et al., 2004), these transformations could lead to an irreversible fragmentation into grains of decreasing size. The definition of such a potential is therefore a key ingredient to model complex transformation sequences.

Pioneering works on MTs, using phase field techniques (e.g., Wang and Khachaturyan, 1997; Wang et al., 2013), have introduced transformational deformation as a source term in a fast-Fourier transform (FFT) method. Focusing on quasi-static evolution by construction and although limited to small strains, these methods are successfully used, e.g., by Wang and Khachaturyan (1997), to study the onset of platelets, the onset of martensite nuclei (e.g., Artemev et al., 2001), or by Zhang et al. (2007), the influence of dislocation on the structure of MT nuclei. The very limited set of variants involved in these studies allows for the representation of the chemical potential as a fourth-order polynomial, function of order parameters. Using the same formalism, an unlimited set of variants can also be represented by incorporating as many order parameters as stable phases, e.g., in a small strain formalism (Steinbach et al., 1996; Steinbach and Pezzolla, 1999; Levitas and Preston, 2002a,b; Levitas et al., 2003 and recently extended to large strains by Levitas et al., 2009; Levin et al., 2013; Levitas, 2014). To avoid the superposition of phases (i.e., the possibility to have more than one order parameter equal to one at the same location), the latter uses an additional energy that strongly penalizes this superposition for up to three phases, but allows for a linear evolution between two phases (see also Levitas and Roy, 2015). When a large number of variants have to be considered, the number of penalizing terms restricts, however, the capability of such methods and, so far, no modeling involving a large number of stable states has been proposed.

This work aims to represent an extended set of energy wells in the space of strain tensors in large strains. As noted by Finel et al. (2010), large strain formalism strongly modifies the microstructure stability, mainly because additional accommodation mechanisms involving rotations could take place for, e.g., interaction of macrotwins, and is a key feature for the understanding of complex microstructures. Following the method proposed in Denoual et al. (2010), we use pathways, defined as the set of strains linking two stable phases, to define a potential in a strain space. In this method, the so-called *Phase-Field based on Reaction Pathway* method, or PFRP, the choice of the transformational strain as state variable instead of multiple order parameters, as in Steinbach et al. (1996), Steinbach and Pezzolla (1999), Levitas and Preston (2002a,b), and Levitas et al. (2003), excludes, by construction, the possibility to superpose states, which therefore simplifies the expression for the potential. Hierarchical MTs encountered during cyclic loadings are easily represented through the topology of a pathway tree, as well as possible variant-to-variant transformations. In this paper, we consider a model reconstructive transformation to demonstrate the possibility to model more than one hundred variants.

Many MTs contain some atomistic displacements that are not linked to any overall homogeneous changes of lattice. In this case, called "improper" MTs, optical displacement modes that are silent at the macroscopic scale may strongly modify the energy landscape and the kinetics of the reaction to such an extent that they could be considered for some materials as a key mechanism that drives the transformation (see a discussion about 'improper' MT in Artemev et al., 2001). As an example, Fe-α (BCC) to Fe-ϵ (hexagonal close-packing lattice, HCP) MT at 13 GPa in iron involves a combination of shear deformation and shuffle in the (110) plane, described in Burgers (1934), Bassett and Huang (1987), and Wang et al. (2013). Ab initio calculations have shown that during this motion, a disorder of the shuffle possibly onsets (as proposed by Dupé et al., 2013), leading to the nonadiabaticity of the transformation (see a discussion in Johnson and Carter, 2008). The energy is no longer a function of the lattice distortion only, but is also a function of an internal variable evolving at a different timescale, and therefore with its own evolution law. Thus, and in opposition to previous instant respond of proper MTs, improper MTs need an internal variable to carry information on the progress of the transformation, at its own time scale.