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Nanoscale multiphase phase field approach for stress- and temperature-induced martensitic phase transformations with interfacial stresses at finite strains

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ABSTRACT

A thermodynamically consistent, novel multiphase phase field approach for stress- and temperature-induced martensitic phase transformations at finite strains and with interfacial stresses has been developed. The model considers a single order parameter to describe the austenite↔martensitic transformations, and another N order parameters describing N variants and constrained to a plane in an N-dimensional order parameter space. In the free energy model coexistence of three or more phases at a single material point (multiphase junction), and deviation of each variant-variant transformation path from a straight line have been penalized. Some shortcomings of the existing models are resolved. Three different kinematic models (KMs) for the transformation deformation gradient tensors are assumed: (i) In KM-I the transformation deformation gradient tensor is a is a linear function of the Bain tensors for the variants. (ii) In KM-II the natural logarithms of the transformation deformation gradient is taken as a linear combination of the natural logarithm of the Bain tensors multiplied with the interpolation functions. (iii) In KM-III it is derived using the twinning equation from the crystallographic theory. The instability criteria for all the phase transformations have been derived for all the kinematic models, and their comparative study is presented. A large strain finite element procedure has been developed and used for studying the evolution of some complex microstructures in nanoscale samples under various loading conditions. Also, the stresses within variant-variant boundaries, the sample size effect, effect of penalizing the triple junctions, and twinned microstructures have been studied. The present approach can be extended for studying grain growth, solidifications, para↔ferro electric transformations, and diffusive phase transformations.

1. Introduction

Multivariant martensitic transformations (*crystallographic theory*). Martensitic phase transformation (PT) plays the central role in exhibiting some important phenomena, such as shape memory effect, pseudoelasticity, and pseudoplasticity (Bhattacharya, 2004; Pitteri and Zanzotto, 2003). Such transformations usually result in complex microstructures, including austenite-twinned martensites, wedge, twins within twins etc. (Ball and James, 1987; Bhattacharya, 2004; Pitteri and Zanzotto, 2003; Schryvers, 1993; Wayman, 1964). In this paper we denote the austenite phase (parent phase) by A, the

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martensite (product phase) by M, and the N variants of martensites by M_1, M_2, ..., M_i, M_j, ..., M_N. In actual microstructures we seldom see interface between A and a single martensite variant, as the lattices of stress-free A and a single M_i are not geometrically compatible in the sense of Hadamard's compatibility. The system rather prefers to form microstructures consisting of mixture of austenite and twinned martensite, which are laminated microstructures with planar interfaces, and are minimizer of the total elastic energy of the system (Ball and James, 1987; Bhattacharya, 2004; Pitteri and Zanzotto, 2003). The interface between A and twinned martensite in such microstructures is diffused, i.e. has a finite width. The compatibility condition therein is satisfied in an average sense, and the local incompatibility is accommodated by elastic strains. However, away from the A − M interface the elastic stresses vanish. On the other hand, twin boundaries are compatible sharp interfaces, and hence the elastic stresses are vanishing, both within the variants and twin boundaries.

Multiphase phase field approach to martensitic PTs. Besides various continuum studies of multivariant martensitic PTs within a sharp interface approach (Ball and James, 1987; Levitas and Ozsoy, 2009a, 2009b; Petryk and Stupkiewicz, 2010a, 2010b; Roytburd, 1974; Roytburd and Slutsker, 2001), the phase field approaches (also known as the Ginzburg–Landau approaches) have been widely used for studying microstructure evolution during martensitic PTs (Artemev et al., 2001, 2005, 2000; Chen, 2002; Clayton and Knap, 2011a, 2011b; Hildebrand and Miehe, 2012; Idesman et al., 2008; Jin et al., 2001; Lei et al., 2010; Levin et al., 2013; Levitas and Javanbakht, 2011; Levitas and Lee, 2007; Levitas et al., 2009; Levitas and Preston, 2002a, 2002b; Levitas et al., 2003, 2013; Li et al., 2001; Seol et al., 2002, 2003; Tůma and Stupkiewicz, 2016; Tůma et al., 2016). The central idea in all the phase field approaches is to introduce the order parameters for describing the PTs in a continuous way. The free energy of the system and the transformation strains are functions of the order parameters. These functions include interpolation of all material properties between their values in each phase, the energy barrier between phases, and the terms related to the gradient of the order parameters penalizing interfaces between phases. The interfaces are therefore of finite width and their structures are also resolved.

The evolution of the order parameters is governed by a system of Ginzburg–Landau equations. Here we consider the transformation strain related order parameters, (see, e.g. Artemev et al. (2001); Levitas (2014); Levitas and Preston (2002b); Levitas et al. (2003)), in contrast to the total strain related order parameters in Barsch and Krumhansl (1984), Falk (1983), Jacobs (1992) The latter cannot be used to satisfy some important requirements formulated in Levitas (2013a), Levitas and Preston (2002a, 2002b), Levitas and Roy (2016).

A critical analysis of the multiphase phase field approaches (MPFA) to PTs is now presented, highlighting their main features and drawbacks (see also Levitas and Roy (2015, 2016); Tóth et al. (2015)).

MPFA-I: In this approach N volume fraction related order parameters η_i along with a single constraint $\sum_{i=1}^{N}\eta_i = 1$ are considered for a system with $N+1$ phases; see Refs. Ankit et al. (2013), Bollada et al. (2012), Garcke et al. (1999), Kim et al. (2006), Moelans et al. (2008, 2009), Nestler (2005), Steinbach and Pezzolla (1999), Steinbach et al. (1996), Tóth et al. (2011a, 2015, 2011b). The models have been mostly used for studying solid↔liquid transformations and grain growth without mechanics, as well as for PTs between solid phases with mechanics (Schneider et al., 2015; Steinbach and Apel, 2006). The constraint plane is schematically shown in $\eta_i - \eta_j - \eta_k$ space in Fig. 1(a), and all the liquid↔solid (or A ↔ M_i) transformation paths belong to this plane. This single constraint alone cannot ensure that each of the PTs can be described by a single order parameter, which is an important condition for calibrating the model parameters, and also to prevent the appearance of a third (if spurious) phase between two others (Levitas and Roy, 2015, 2016). A specialized model for a three phase system was derived by Folch and Plapp (2003, 2005) which successfully prevents the spurious phase, but yields a restriction on the kinetic coefficients. Also, it is not clear how to generalize the model for a system with more phases. Conversely, there can be instances where a third phase can actually nucleate between two others and plays an important role; see, e.g. solid-solid PT via intermediate (virtual) melt (Levitas et al., 2004a, 2012). Hence a robust model should have a provision to control the nucleation of a third phase between two others and also the quantity. The disadvantages of imposing the constraint using the Lagrangian multipliers (used in Folch and Plapp (2003, 2005)) are analyzed and overcome in Ref. Bollada et al. (2012). Further improvement of the model is presented in Tóth et al. (2015) where the drawbacks of the previous models are analyzed in detail. The last model was analyzed in Levitas and Roy (2016). Note that none of these models containing the constraint describe the instability criteria, which are very important in PTs.

In this context, we also mention that the volume fraction related order parameters have also been used to study martensitic PTs, e.g. in Refs. Idesman et al. (2005), Lei et al. (2010), Levitas et al. (2004b), Tůma and Stupkiewicz (2016), Tůma et al. (2016), where all the interpolation functions are linear and represent the simple mixture rule. Such models work well in microscale modelings, in which the interface width is either artificially increased from its actual size of one to a few nanometers by one to several orders of magnitude. At the nanoscale, when one mimics actual processes practically at the atomistic scale, the interpolation functions must be smooth. The first derivative of the interpolation functions must vanish within the bulk – a criterion imposed by the thermodynamic equilibrium condition (Levitas, 2013a; Levitas and Preston, 2002a, 2002b). We will focus here on the nanoscale models.

MPFA-II: The authors in Refs. Artemev et al. (2001, 2000), Jin et al. (2001), Li et al. (2001), Seol et al. (2002, 2003) considered N order parameters η_i for a system with N variants, where each η_i describes A ↔ M_i transformations ($\eta_i = 0$ in A and $\eta_i = 1$ in M_i). Additional conditions for such a choice have been imposed in Levitas (2013a), Levitas and Preston (2002a, 2002b) for small and large strains, which in particular include lattice instability conditions, and lead to more complex thermodynamic potentials and expressions for the transformation strains. These functions are designed in such a way that the instability criteria for A ↔ M_i and M_i ↔ M_j transformations yield the expected phase transformation conditions. Since A ↔ M_i PTs are described with the single order parameter η_i (Fig. 1(b)), the analytical solution for static and propagat-

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