Acta Materialia 139 (2017) 174–187

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Interfacial stresses within boundary between martensitic variants: Analytical and numerical finite strain solutions for three phase field models

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ARTICLE INFO

Article history:
Received 13 May 2017
Received in revised form
5 July 2017
Accepted 30 July 2017
Available online 2 August 2017

Keywords:
Phase field method
Martensitic phase transformation
Variant-variant boundary
Strain incompatibility
Interfacial stresses

ABSTRACT

The origin of a large elastic stress within an interface between martensitic variants (twins) within a finite strain phase field approach has been determined. Notably, for a sharp interface this stress is absent. Three different constitutive relations for the transformation stretch tensor versus order parameters have been considered: a linear combination of the Bain tensors (kinematic model-I, KM-I), an exponential-logarithmic combination (KM-II) of the Bain tensors, and a stretch tensor corresponding to simple shear (KM-III). An analytical finite-strain solution has been found for an infinite sample for tetragonal martensite under plane stress condition. In particular, explicit expression for the stresses have been obtained. The maximum interfacial stress for KM-II is more than twice that which corresponds to KM-I. Stresses are absent for KM-III, but it is unclear how to generalize this model for multivariant martensitic transformation. An approximate analytical solution for a finite sample has been found as well. It shows good correspondence with numerical results obtained using the finite element method. The obtain results are important for developing phase field approaches for multivariant martensitic transformations coupled to mechanics, especially at the nanoscale.

1. Introduction

Interfacial stresses. Interfacial stresses play an important role in the formation of the nanostructures, causing martensitic phase transformations (PTs) in the nanowires [1,2], and influencing the nucleation condition and evolution in the multivariant martensitic microstructures [3,4]. Interfacial stresses can also reduce the activation energy for intermediate melt nucleation within solid-solid interface by more than an order of magnitude [5]. Interfaces may have a complex internal structure, including the intermediate phases [6–9]. They may appear as an intermediate state during PTs, e.g., solid-solid PT via intermediate melting [10–15]. Interfacial stresses have been determined for external surfaces [1] and solid-melt interfaces [16–18] using atomistic simulations.

It is well-known [19] that each material surface is subjected to biaxial interface stresses. For phases that do not support deviatoric stresses at the equilibrium (liquids and gases), the interfacial force per unit length $\overline{\sigma}^S$ in both directions is equal to the surface energy γ. For interfaces in solids, or for solid-liquid and solid-gas interfaces, the magnitude of the surface stresses is determined by the Shuttleworth equation [20] $\overline{\sigma}^S = \gamma + \partial\gamma/\partial\varepsilon_i = \overline{\sigma}_{st} + \overline{\sigma}^S_e$, where ε_i is the mean interface strain. Thus, interfacial stress consists of two parts: the tensile structural stress, $\overline{\sigma}_{st}$, which is the same as for a liquid-gas interface, and another, $\overline{\sigma}^S_e$, which is caused by elastic deformation of an interface and which may be tensile or compressive.

Within the sharp interface approach, the constitutive equations and balance laws for elastic interfaces were derived in Refs. [20–27]. The challenges are (a) in finding the material parameters and (b) in the concern for whether the resultant interfacial stresses can be formalized through simple constitutive equations due to strongly heterogeneous interfacial fields like elastic moduli, transformation strains, and total strains across the interface.

Phase field approach. The phase field approach, which for the

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http://dx.doi.org/10.1016/j.actamat.2017.07.059
1359-6454/

conserved order parameters is also known as the Ginzburg-Landau approach, is broadly applied for studying the microstructure evolution during various first-order PTs. The most relevant to the current paper are works on modeling austenite - multivariant martensite and twinned microstructure evolution in crystalline solids [4,28–41]. We also mention works on transformations in liquids [42] and melting/solidification [43–45], in which interfacial stresses have been included. In the phase field models, the interface has a finite width, and its structure (i.e., distribution of all fields within an interface) is resolved. Interfacial stresses σ_{st} (here, force per unit area at each point within the interface) with the resultant force per unit length $\overline{\sigma}_{st}$ equal to the interface energy γ have been introduced in Refs. [42–44], but are not fully consistent; see the discussion in Ref. [46]. The problem of introducing of the interfacial stresses σ_{st} was solved for melting [47,48] and the solid-solid interface for small [3,46,49] and large [50,51] strains, including cases with anisotropic interface energy [51]. The interfacial stresses were also introduced and studied for a complex solid-melt-solid interface [5,52], which appears during solid-solid PT via the intermediate melt.

Elastic interfacial stresses σ_e^S (with resultant force per unit interface length $\overline{\sigma}_e^S$) appear automatically (i.e., without extra terms in the constitutive equations) as a result of solution of the coupled Ginzburg-Landau and elasticity equations, due to heterogeneity of the transformations strain and the elastic properties within interface. They were found numerically for a solid-melt interface [45,47,48], for the austenite-martensite [3] and martensite-martensite [4,33] interfaces, as well as for a complex solid-melt-solid interface [5,52,53]. In contrast, the theory in Ref. [54] introduces the explicit dependence of the gradient energy on the interfacial strain. This results in the additional interfacial stresses that depend on the gradient of the order parameter. In the sharp interface limit, this theory reduces to the theory in Ref. [23], in which interfacial energy depends on the interfacial strain. The theory in Ref. [54] does not include structural interfacial stresses σ_{st}. Since the boundary-value problem for stresses was not solved in Ref. [54], elastic stresses due to heterogeneity of material parameters within the interface were not discussed. At the same time, it is argued in Ref. [50] that it is not evident that such an additional dependence of the gradient energy on the interfacial strain is necessary, because stresses due to heterogeneous distribution of material parameters across an interface (neglected in Ref. [54]) may be large, exceeding what one wants to introduce. This was shown for the solid-melt interface in Refs. [47,48]. In this case, volumetric transformation strain (more precisely, the biaxial part of the transformation strain along the interface) determines the elastic interfacial stresses [47,48]. They appeared to be too large and unrealistic (they are significantly larger than stresses determined using molecular dynamic simulations in Refs. [16,17]). These stresses artificially suppress melting, and in order to restore consistency with experimental data on the size-dependence of the melting temperature for Al nanoparticles, various methods of their relaxation (in particular, introducing an additional equation for stress relaxation) have been proposed in Refs. [47,48]. This led to the conclusion that for melting it is not necessary to introduce additional elastic interface stresses. However, there have been only limited attempts to understand which parameters affect elastic interfacial stresses for a solid-solid interface and how they can be controlled; see, e.g., [4,55,56].

In the current paper, we have found a complete analytical solution for the simplest case of a solid-solid interface between two martensitic variants, or a twin interface. Since transformation strain for twinning is a simple shear, internal stresses do not appear within the sharp interface between martensitic variants or twins. It is intuitively expected that they should not appear within a phase field approach also. However, we will see that this is not the case.

Multivariant martensitic PTs. Microstructure evolution during martensitic PTs plays the central role in determining mechanical, electrical, and other properties in a broad range of materials, e.g. shape memory alloys, ferroelectric materials, and multiferroic materials. The microstructures in such materials usually consist of mixture of austenite, A, and N martensitic variants, M_i, where $i = 1, 2, \ldots, N$; see, e.g., [57,58]. Some of the martensitic variants can form twin boundaries that are coherent interfaces. Across a twin boundary, one variant can be obtained by simple shear deformation of the other. In experiments, one rarely sees interfaces between A and a single martensitic variant, since the stress-free lattices of A and M_i in most of the materials are not geometrically compatible (in the sense of Hadamard's compatibility) to form a coherent stress-free interface. The system prefers to form microstructures consisting of A separated from twinned martensite by a plane interface, which minimizes the elastic energy of the system [57,58].

Various continuum theories [57–63] have been used to study twinned microstructures within sharp interface approaches. On the other hand, various aspects of the phase field approach to martensitic PTs and twinning have been developed and used for simulations in various papers; see e.g., [4,28–41]. The main concept is related to the order parameters η that describe material instabilities during PTs from A to M_i in a continuous way.

The necessary conditions for the Landau (local) potential and transformation strain, which are functions of the order parameters, have been formulated and utilized in Refs. [30,33,64–66] for small strains and in Refs. [30,67] for large strains. They, in particular, introduce the conditions that the thermodynamically equilibrium values of the order parameters are fixed (i.e., 0 or 1) for A and M_i for any stress and temperature and that the crystal lattice instability conditions should be included in the theory. This results in a much more complex expression for the thermodynamic potential and transformation strain tensor as compared to those used in the other theories [34–39]. Large strain formulation for multivariant martensitic PTs were developed in Refs. [30–32,38,39,67]. Three different kinematic assumptions are currently used in various papers.

(a) *Kinematic model-I (KM-I)*: Symmetric right transformational stretch $\boldsymbol{U}_t$ is considered as a linear combination of the Bain stretch tensors $\boldsymbol{U}_{ti}$ of all the martensitic variants multiplied with a corresponding nonlinear interpolation function of the order parameters [30,67]. Such an expression satisfies all of the conditions formulated in Refs. [30,67]. However, as it was shown in Refs. [38,39], it does not conserve the determinant of the transformation stretch (i.e., volumetric transformation strain) within the transition region between the variants where $0 < \eta < 1$. In particular, this means that while all martensitic variants have the same specific volume, the transformation process $M_i \leftrightarrow M_j$ is not isochoric. This requirement is not a mandatory one, because, for dislocational slip, for example, there is a volume change along the shearing process between two stable atomic configurations [68]. In fact, defect cores in dislocations and twin boundaries may induce change in volume (see Chapter 7 and 8 of [69] and the references therein). However, the requirement for volume conservation sounds reasonable, at least, for the simplest model; it is good to have such a model. If volume change is observed during a transformation process between two martensitic variants, in principle, it could be included as a correction to the isochoric model.