Phase field approach to martensitic phase transformations with large strains and interface stresses

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1. Introduction

Phase field approach: The phase field or Ginzburg–Landau approach is broadly used for the simulation of various first-order phase transformations (PTs), including martensitic PTs (Jin et al., 2001a; Chen, 2002; Seol et al., 2003; Lookman et al., 2008;
Levitas and Lee, 2007; Levitas et al., 2004; Vedantam and Abeyaratne, 2005; Artemev et al., 2001; Finel et al., 2010, see also recent review Mamivand et al., 2013), reconstructive PTs (Toledano and Dmitriev, 1996; Denoual et al., 2010; Salje, 1991), twinning (Clayton and Knap, 2011a,b; Hildebrand and Miehe, 2012; Levitas et al., 2013), dislocations (Jin and Khachaturyan, 2001; Wang et al., 2003; Hu et al., 2004; Koslowski et al., 2002; Rodney et al., 2003; Wang and Li, 2010; Levitas and Javanbakht, 2012), PTs in liquids (Lowengrub and Truskinovsky, 1998), and melting (Wheeler and McFadden, 1997; Anderson et al., 2001; Slutsker et al., 2006). The main concept is related to the order parameters $\eta_i$ that describe material instabilities during PTs in a continuous way. Here we focus on the theories in which order parameters $\eta_i$ are related to the deformation of the crystal lattice from the high-temperature phase, austenite (A), into the lattice of martensitic variants $M_i$ (the low temperature phase), described by the transformation deformation gradient tensor $U_{ij}$. Shuffles—i.e., atomic displacements inside the crystal cell—are assumed to be excluded by energy minimization or neglected. Due to the symmetry of the crystal lattices of A and M, there is a finite number $n$ of crystallographically equivalent martensitic variants (Wayman, 1964; Bhattacharya, 2004). Since the theories by Jacobs et al. (2003), Lookman et al. (2008), Barsch and Krumhansl (1984) and Vedantam and Abeyaratne (2005), which relate the order parameters to the total strain have some problems discussed in Levitas and Preston (2002a,b) and Levitas et al. (2003), we will relate the order parameters to the transformation deformation gradient tensor $U_{ij}$ for each martensitic variant, similar to Jin et al. (2001a), Chen (2002), Artemev et al. (2001), Levitas and Preston (2002a,b), Levitas et al. (2003) and Levitas and Lee (2007). The Helmholtz free energy depends on the strain (or elastic strain) tensor, temperature, the set of the order parameters, and their gradient, which penalize the interface energy. Evolution of the order parameters and multi-connected multivariant martensitic microstructure is simulated by the solution of the Ginzburg–Landau equations, which represent linear relationships between $\eta_i$ and the generalized thermodynamic forces $X_i$ conjugate to them, and coupled to continuum mechanical equations. The main computational advantage of such an approach is that there is no need to explicitly track the interfaces; they appear and evolve automatically as a result of the solution to the Ginzburg–Landau equations. The solutions exhibit diffuse (i.e., finite-width) interfaces, within which order parameters continuously change between their values in contacting phases. The main property of the thermodynamic potential, which allows such a solution is that in some temperature and stress ranges it possesses minima in the space of the order parameters corresponding to austenite and each martensitic variant, separated by an energy barrier (Lookman et al., 2008; Barsch and Krumhansl, 1984; Vedantam and Abeyaratne, 2005; Jin et al., 2001a; Levitas and Lee, 2007; Chen, 2002). However, potentials developed in material science and physical literature (Lookman et al., 2008; Barsch and Krumhansl, 1984; Jin et al., 2001a; Chen, 2002; Finel et al., 2010) did not take proper care of the mechanics of martensitic PTs and did not have sufficient degrees of freedom to incorporate all material properties of $\alpha$ and $M_i$ (see Levitas and Preston, 2002a,b; Levitas et al., 2003). Also, PTs criteria should follow from the material instability conditions (Toledano and Dmitriev, 1996; Toledano and Toledano, 1998; Salje, 1991; Umantsev, 2012), which were never implemented in the physical and material partial literature for multivarient martensitic PTs. In Levitas and Preston (2002a,b) and Levitas et al. (2003), the requirements for the Gibbs potential were formulated and new potentials were found for small strains that are conceptually consistent with typical experimental stress–strain curves and instability conditions. Thus,

(a) The transformation strain tensor that followed from the potential was stress- and temperature-independent, like in crystallographic theories (Wayman, 1964; Bhattacharya, 2004). Stress hysteresis could be controlled and could be chosen, in particular, constant or weakly temperature-dependent.

(b) Desired PTs conditions for $A \rightarrow M_i$ and $M_i \rightarrow M_j$ transformations follow from the material instability conditions.

(c) All material properties of $A$ and martensitic variants $M_i$ were included in the thermodynamic potential.

(d) Transformation started at nonzero elastic moduli.

We do not know how to impose these conditions in the theory based on order parameters related to the total (rather than transformation) strain; that is why we consider transformation strain based order parameters only.

Theory in Levitas and Preston (2002a,b) and Levitas et al. (2003) was extended and applied to dynamic problems in Idesman et al. (2008) and Cho et al. (2012), to introducing athermal interface friction in Levitas and Lee (2007) and Levitas et al. (2010), to generalization for microscale in Levitas et al. (2004), Idesman et al. (2005) and Levitas and Ozsoy (2009a,b), and description of surface-induced phenomena for martensitic PTs in Levitas and Javanbakht (2010, 2011a,b). Similar advances have been applied to melting/solidification in Levitas and Samani (2011a,b, 2014), including nonisothermal melting with the two-temperature model during laser heating (Hwang and Levitas, 2013). While there are still various problems in the development of the phase field theory, we will focus on a combination of the two of them: geometrically nonlinear formulation and introducing interface stresses.

Large strain formulations: Various examples of finite transformation deformation gradient, both volumetric and deviatoric, are collected in Levitas (2013a). Thus, volumetric and normal components of transformation deformation gradient reach 1.5 or 0.5 for PTs in carbon and boron nitride (graphite-like to diamond-like phases) (Britun and Kurdyumov, 2000), silicon, germanium, Sn, and GaSb (Malyushitskaya, 1999). Finite rotations may occur under some conditions (loading) even at small strains and are important in crystallographic theory (Wayman, 1964; Bhattacharya, 2004). The transformation shear is 0.2 for PTs in steels and some shape-memory alloys and is 0.71 for twinning in bcc and fcc lattices. Large elastic strains can be caused by high pressure or general loading at the nanoscale, when their relaxation due to dislocations is suppressed. In several steps, the theory from Levitas and Preston (2002a,b) and Levitas et al. (2003) was generalized for
large-strain regimes in Levitas and Preston (2005) and Levitas et al. (2009), with the detailed derivation in Levitas (2013a) and numerical implementation in Levitas et al. (2009) and Levin et al. (2013). However, these papers did not include interface stresses, which will be discussed below. In particular, free energy depends on the gradient of the order parameters in the reference state.

Interface stresses: It is known (Gibbs, 1948) that each material surface or interface is subjected to biaxial interface stresses with the force per unit length $T$ (for isotropic interfaces, which we will focus in this paper at). For liquid–liquid and liquid–gas interfaces, the magnitude of the isotropic biaxial tensile stresses is equal to the surface energy $\gamma$ (Fig. 1), which causes a jump in normal stresses across an interface equal to $2\gamma\kappa$, where $\kappa$ is the mean interface curvature. Interfaces in solids, solid–liquid, and solid–gas generate additional surface stresses due to their elastic deformations, which may be both tensile or compressive. There is an extended literature devoted to the derivation of constitutive equations and balance laws for elastic interfaces (see, Cahn, 1979; Podstrigach and Povstenko, 1985; Gurtin and Struthers, 1990; Povstenko, 1991; Gurtin and Murdoch, 1975; Javili and Steinmann, 2010; Nix and Gao, 1998, and review articles by Duan et al., 2009; Fischer et al., 2008; Cammarata, 2009). One of the problems is that the material parameters for interfaces are unknown. Another problem is whether strongly heterogeneous across interface fields of properties, transformation and total strains, and stresses can be formalized through simple constitutive equations.

The problem of interface stresses was addressed in the phase field approach. However, even for liquid–liquid and liquid–vapor diffuse interfaces, for which problems with elastic stresses do not exist, the results are not completely consistent with a sharp-interface limit shown in Fig. 1. Namely, interface stress tensor contains an additional hydrostatic pressure (Wheeler and McFadden, 1997; Lowengrub and Truskinovsky, 1998; Anderson et al., 2001) or is not localized at the interface for nonequilibrium conditions (Wheeler and McFadden, 1997), see analysis in Levitas (2013b). The important point is that for liquid–liquid and liquid–vapor PTs, in contrast to solids, derivations are naturally presented in the actual (deformed) configuration and free energy depends on the gradient of the order parameter in the deformed state. That is why some contributions to the interface stresses appear automatically. For melting in Anderson et al. (2001), a solid is considered as a very viscous liquid and equations in the deformed configurations are considered as well. When the melting of an elastic solid was considered (Slutsker et al., 2006), additional surface stresses were not introduced. Surface stresses have been ignored until very recently in the phase field theories for multivariant martensitic and reconstructive PTs and twinning (Jin et al., 2001a; Chen, 2002; Lookman et al., 2008; Levitas and Lee, 2007; Levitas et al., 2004; Vedantam and Abeyaratne, 2005; Artemev et al., 2001; Finel et al., 2010; Denoual et al., 2010; Salje, 1991; Clayton and Knap, 2011a,b; Hildebrand and Miehe, 2012). However, the thickness of martensitic variants is on the order of magnitude of a few nanometers and they form sharp tips. Thus, for nanoscale simulations surface stresses should play an important role in nucleation and evolution of martensitic nanostructure. Even for plane interfaces, interface stresses change elastic stresses, which in turn affect PT thermodynamics, kinetics, and morphology (see phase field simulations in Levitas and Javanbakht, 2010, 2011a). Interface stresses at the plane external surface were the only reason for martensitic PT in nanowires in Diao et al. (2003).

The theory by Fried and Grach (1997) for PT in solids pays special attention to the interface stresses. While consideration is in the reference configuration and free energy depends on the gradient of the order parameter in the undeformed state, the gradient-dependent part of the energy also depends on the strain along the interface. Then differentiation of the gradient energy with respect to strain results in additional gradient-dependent interface stresses. In the sharp interface limit, this theory transforms to that in Gurtin and Struthers (1990), i.e., it has the same problem of determining the elasticity rule for interfaces. There were no efforts in Fried and Grach (1997) to obtain biaxial interface true stresses with a magnitude equal to the interface energy. One more point is that even without any extra gradient-related stresses, variation of the

![Fig. 1. Each isotropic material interface is subjected to biaxial stresses with the force per unit length $T$. For liquid–liquid and liquid–gas interfaces, the force $T$ is tensile and equal to the interface energy $\gamma$.](image-url)
transformation strain and elastic moduli across diffuse interface produces significant elastic interface stresses, even for a solid–melt interface (Slusker et al., 2006; Levitas and Samani, 2011a,b). In fact, they are much higher than those obtained in molecular dynamic simulations (Frolov and Mishin, 2010a,b). They suppress PT and, in order to describe experimental data on the size dependence of the melting temperature for Al nanoparticles, an additional equation for stress relaxation at the interface is included in Levitas and Samani (2011a,b). Consequently, for melting, there is no need to introduce additional elastic interface stresses. The need for adding extra elastic interface stresses for a solid–solid PT should be analyzed after the solution to the boundary-value problem and comparison with the experiment or atomistic simulations.

In a sharp interface approach, when the energy of the interface γ is considered with respect to the deformed area, for a small strain approximation various derivations lead to the magnitude of the surface stresses \( \sigma^S = \gamma + \partial \gamma/\partial \epsilon_i = \sigma_{\text{st}} + \sigma_{\text{el}}^S \), where \( \epsilon_i \) is the mean interface strain (the Shuttleworth equation, see review by Fischer et al., 2008). Thus, surface stress consists of two parts, one, \( \sigma_{\text{st}} \), is the same as for a liquid–liquid interface, and another, \( \sigma_{\text{el}}^S \), is due to elastic deformation of an interface. Subscript \( \text{st} \) means the structural part of the interface stresses. The main idea of our approach in Levitas and Javanbakht (2010) and Levitas (2013b,c) for martensitic PTs and in Levitas and Samani (2011a,b) for melting is that elastic contribution to the surface stresses comes directly from the solution of the Ginzburg–Landau and mechanics equations for a PT problem. Then, the main focus was to determine the structural contribution to the interface stresses \( \sigma_{\text{st}} \) (see Fig. 1 with \( T = \gamma \)), i.e., like for liquid–liquid or liquid–gas interfaces. It was found that in order to introduce interface stresses that represent biaxial tension with the magnitude equal to the interface energy, one needs to introduce some geometrically nonlinear features even in a geometrically linear theory. The problem was solved for a 2–3–4 degree polynomial for free energy in terms of an order parameter and the importance of interface stresses on microstructure formation was demonstrated (Levitas and Javanbakht, 2010, 2011a; Levitas, 2013a,b). The main limitation of this theory is that it is developed for small strain approximation.

Goals and outlook: Thus, the main goal of this paper is to develop general thermodynamic framework and specific models for the phase field approach to multivariant PTs with large strains and interface stresses. We generalize and elaborate our latest works on the large-strain phase field approach without interface stresses in Levitas (2013a) and the small-strain phase field approach with interface stresses in Levitas (2013b,c), and resolve some basic problems which were not discussed in Levitas (2013a,b).

We designate contractions of tensors \( A = [A_{ij}] \) and \( B = [B_{ij}] \) over one and two indices as \( A \cdot B = [A_{ij}B_{jk}] \) and \( A : B = A_{ij}B_{ij} \), respectively; \( A_{ij} \) and \( B_{ij} \) are the components of tensors in the Cartesian unit basis vectors \( e_i \). The subscripts \( s \) and \( t \) designate symmetric and skew-symmetric parts of a second-rank tensor; subscripts \( e, t, \) and \( \theta \) mean elastic, transformational, and thermal strains; subscript \( 0 \) means that the parameter is defined in the reference configuration \( \partial_0 \); superscript \( t \) means transposition of the tensor; \( \delta_{ij} \) is the Kronecker delta; \( V_0 \) and \( \nabla \) are the gradient operators in the undeformed and deformed states, respectively; \( I \) is the second-rank unit tensor, \( V_0^\prime = \nabla_0 \cdot \nabla_0 \) and \( \nabla^2 = \nabla \cdot \nabla \) are the Laplacians in the undeformed and deformed states, respectively; \( \approx \) means equal by definition, summation is assumed over the repeated indices, and \( \otimes \) designates a dyadic product. Cross product \( \times \) is defined for any tensor \( C = C^{ijkl}e_i \otimes e_j \otimes e_k \otimes e_l \) as \( R \cdot C = C^{ijkl}(R \cdot e_i) \otimes (R \cdot e_j) \otimes (R \cdot e_k) \otimes (R \cdot e_l) \) with some orthogonal rotation tensor \( R \).

The main goal of this paper is to develop a phase field theory, which for a solution corresponding to the nonequilibrium diffuse interface with isotropic interface energy, for neglected elastic and viscous interface stresses, produces structural true (Cauchy) stresses within the finite-width interface

\[
\sigma_{\text{st}} = \sigma_{\text{st}}(\eta, \nabla \eta)(I - k \otimes k); \quad k = \nabla \eta/|\nabla \eta|,
\]

(1)

corresponding to a biaxial tension and not producing any other stresses within or outside an interface. Here \( k \) is the unit normal to the diffuse interface in the current configuration, \( I - k \otimes k \) is the two-dimensional unit tensor within a diffuse interface, and \( \sigma_{\text{st}} \) is the magnitude of the biaxial interface stresses. Outside of an interface (in bulk), one has \( \eta = 0, \eta = 1 \), and \( \sigma_{\text{st}} = 0 \). In addition, the tangential force per unit interface length

\[
T = \int_{-\infty}^{\infty} \sigma_{\text{st}} \, d\zeta = \gamma,
\]

(2)

where \( \gamma \) is the energy of the nonequilibrium diffuse interface and \( \zeta \) is the coordinate along the \( k \).

In Section 2, the global first and second laws of thermodynamics are formulated and localized in the reference configuration. Additional thermodynamic forces conjugated to the order parameters \( \eta \) are introduced at the external surface, which will allow stricter treatment of gradient-type materials. In Section 3, the structure of the constitutive equations is derived utilizing multiplicative kinematic decomposition of the deformation gradient into elastic, thermal, and transformational parts. The linear relationship between \( \eta \) and the conjugated thermodynamic force resulted in the generalized Ginzburg–Landau equations for evolution of the order parameters. In Section 4, boundary conditions for the order parameters are formulated both in the reference and current configurations. They take into account change in the surface energy during PT, which leads to various surface-induced effects and nanostructures (Lipowsky, 1982; Pluijs et al., 1990; Levitas et al., 2006b; Levitas and Javanbakht, 2010; Levitas and Samani, 2011a,b). In Section 5, the structure of the Helmholtz free energy is suggested, which will lead to the desired expression for the interface stresses. Thus, the thermal part of the free energy is divided into two parts, one of which is multiplied by the Jacobian \( J \) of the deformation gradient and therefore produces contribution to the interface stresses. Gradient energy depends on the gradient of the order parameters in the current configuration and is also multiplied by \( J \). Elastic energy is defined per unit volume of the unloaded configuration, which is important for correct formulation of the elasticity rule. This also will result in the additional
contributions to the Ginzburg–Landau equations and the expression for entropy, which were previously neglected. Expressions for the first Piola–Kirchhoff stress and the Cauchy stress are derived, each of them consisting of elastic, viscous, and structural parts. As it will be shown, the structural part will reproduce the proper expression for the interface stresses. For the isotropic gradient energy, the Cauchy stress is proven to be symmetric. An isotropic expression for the gradient energy is specified and the corresponding expressions for stresses are found. In Section 6, explicit expressions for Ginzburg–Landau equations are derived in both reference and current configurations. Remarkably, only elastic stresses explicitly contribute to these equations, while interface and viscous stresses do not. In Section 7, equations for elastic stresses and Ginzburg–Landau equations are simplified for finite volumetric but small deviatoric elastic strains. In Section 8, consecutive simplifications for small deviatoric thermal and transformational strains, then small all volumetric strains and rotations are presented. Even for small strains, an additional term, related to the definition of the elastic energy in the unloaded configuration, remains in the Ginzburg–Landau equation; it was missing in previous works. In Section 9, equations for the entropy and temperature evolution have been derived. Specification of the Helmholtz energy for a single order parameter was performed in Section 10. The thermal part of free energy is decomposed in two parts, one of which, \( \psi^\theta \), should contribute to the interface stresses and another not. The criterion to chose this partitioning is that for the propagating interface, the interface stresses represent biaxial tension with the magnitude equal to the interface energy. In Section 11.1, this problem is solved for a static interface for a general form of the thermal free energy and it is shown that \( \psi^\theta \) represents a double-well potential. In Section 11.2, the solution is found for a nonequilibrium interface by utilizing an analytical solution for a specific 2 – 4 – 6 polynomial potential. Important equality of the gradient energy at each point of the moving interface is found, which, in fact, has defined \( \psi^\theta \) and interface stresses. In Section 12, interface energy is determined. While for static interface it is defined unambiguously, for propagating interface one needs to define in which part of the interface, the excess energy is calculated with respect to \( A \) and in which with respect to \( M \), i.e., to determine position of the Gibbsian dividing surface or sharp interface (Fig. 3). The choice is made from the condition of static equivalence equation (2), which provides a missing equation for the dividing surface. For the obtained position, the local and gradient contributions to the interface energy are equal for the nonequilibrium interface, like for an equilibrium interface. Since determination of the position of the dividing surface is a fundamental long standing problem, it is considered in more detail in Section 13 (some preliminary results are obtained in Levitas, 2014). One more static equivalence condition, namely that the moment of the interface stresses with respect to position of the sharp interface is zero, results in one more equation. It is demonstrated that for thermodynamic potential under study, both conditions lead to the same position of the dividing surface, i.e., the theory is self-consistent. Detailed analytical study of the energy, width,
entropy excess, and stresses for a nonequilibrium interface is presented in Section 14. Interface stresses for a critical martensitic nucleus are determined in Section 15. In addition to a biaxial tension, the critical nucleus is subjected to tensile interface pressure. In Sections 16 and 17, a complete system of equations is formulated for single and multiple martensitic variants, respectively. Equations are presented for both 2 – 3 – 4 and 2 – 4 – 6 polynomials. Section 18 contains concluding remarks.

2. Laws of thermodynamics

The motion of the elastic material with PTs will be described by a continuous vector function \( \mathbf{r} = \mathbf{r}(\mathbf{r}_0, t) \), where \( \mathbf{r}_0 \) and \( \mathbf{r} \) are the positions of points in the reference (undeformed) \( \Omega_0 \) and the actual (deformed) \( \Omega \) configurations, respectively; \( t \) is the time. The volume under study \( V_0 \) can be arbitrarily cut from an actual body, thus its surface \( S_0 \) is not an external surface and surface energy will not be included in the thermodynamics laws. Assume that material in the reference configuration is in the austenitic state. The deformation gradient is defined as \( F = \partial \mathbf{r} / \partial \mathbf{r}_0 = \nabla_0 \mathbf{r} = (\partial \mathbf{r}_i / \partial \mathbf{r}'_0) \mathbf{e}_i \otimes \mathbf{e}_j \), where \( r_i \) and \( r'_0 \) are the components of the vectors \( \mathbf{r} \) and \( \mathbf{r}_0 \) in the Cartesian unit basis vectors \( \mathbf{e}_i \). The first law of thermodynamics can be presented in the form of the global (i.e., for the entire body) energy balance equation

\[
\int_{S_0} (\mathbf{p} \cdot \mathbf{v} - \mathbf{h}_0 \cdot \mathbf{n}_0) \, dS_0 + \int_{V_0} \nabla_0^\mathbf{e} \mathbf{q}_0 \cdot \mathbf{n}_0 \, dS_0 + \int_{V_0} \rho_0 \mathbf{f} \cdot (\mathbf{v} + \mathbf{r}) \, dV_0 = \frac{d}{dt} \int_{V_0} \rho_0 (U + 0.5 \mathbf{v} \cdot \mathbf{v}) \, dV_0.
\]

(3)

Here \( \mathbf{v} = \dot{\mathbf{r}} \) is the material velocity, \( \mathbf{p} = \mathbf{P} \cdot \mathbf{n}_0 \) is the traction vector, \( \mathbf{P} \) is the first Piola–Kirchhoff stress tensor, \( \mathbf{h}_0 \) is the heat flux, \( \mathbf{n}_0 \) is the unit outer normal to \( S_0 \), \( U \) is the specific (per unit mass) internal energy, \( \rho_0 \) is the mass density in the reference configuration, \( \mathbf{f} \) is the body force and \( \mathbf{r} \) is the specific volumetric heat supply rate (e.g., due to electric heating), both per unit mass. As it will be seen below, we must include extra generalized surface forces \( \mathbf{Q}^0_\mathbf{e}_i \cdot \mathbf{n}_0 \) conjugated with \( \eta_i \) in order to balance terms due to dependence of the thermodynamic potential on \( \mathbf{v}_0 \eta_i \). Otherwise, Eq. (4) is not applicable for an arbitrary volume.

The second law of thermodynamics will be accepted in the form of the global entropy balance equation combined with the Clausius–Duhem inequality for the whole volume \( V_0 \):

\[
S_i = \frac{d}{dt} \int_{V_0} \rho_0 s \, dV_0 - \int_{V_0} \frac{\rho_0 r}{\theta} \, dV_0 + \int_{S_0} \frac{\mathbf{h}_0}{\theta} \cdot \mathbf{n}_0 \, dS_0 \geq 0,
\]

(4)

where \( s \) is the specific entropy, \( S_i \) is the total entropy production rate, and \( \theta \geq 0 \) is the temperature. Transforming surface integrals into integrals over the volume with the help of the Gauss theorem, we obtain after some transformations

\[
\int_{V_0} (\mathbf{P} \cdot \dot{\mathbf{F}} - \rho_0 \dot{\mathbf{U}} - \mathbf{v}_0 \cdot \mathbf{h}_0 + \rho_0 r + \mathbf{v}_0 \cdot (\mathbf{Q}_0^0 \eta_i)) \, dV_0 + \int_{V_0} \eta_i \mathbf{P} \cdot \mathbf{f} - \rho_0 \mathbf{v} \cdot dV_0 = 0.
\]

(5)

\[
S_i = \int_{V_0} (\rho_0 s - \rho_0 \frac{r}{\theta} + \mathbf{v}_0 \cdot \frac{\mathbf{h}_0}{\theta}) \, dV_0 \geq 0.
\]

(6)

For an observer that moves with the constant velocity \( \mathbf{v} - \mathbf{a} \) with respect to a fixed frame of reference, velocity \( \mathbf{v} \) in Eq. (5) should be substituted with \( \mathbf{v} - \mathbf{a} \). Since \( \mathbf{a} \) is an arbitrary vector and the energy balance should be independent of an observer, the term in parentheses in the second integral in Eq. (5) is identically zero: \( \mathbf{v}_0 \cdot \mathbf{P} + \rho_0 \mathbf{f} = \rho_0 \mathbf{v} \). Thus, adding generalized forces \( \mathbf{Q}_0^0 \eta_i \) does not affect the local momentum balance equation. Since equality (5) and inequality (6) are valid for an arbitrary volume, then they have to be valid for each material point:

\[
\mathbf{P} \cdot \dot{\mathbf{F}} - \rho_0 \dot{\mathbf{U}} - \mathbf{v}_0 \cdot \mathbf{h}_0 + \rho_0 r + \mathbf{v}_0 \cdot (\mathbf{Q}_0^0 \eta_i) = 0.
\]

(7)

\[
\rho_0 \dot{\mathbf{S}}_i = \rho_0 \dot{s} - \rho_0 \frac{r}{\theta} + \mathbf{v}_0 \cdot \frac{\mathbf{h}_0}{\theta} = \rho_0 \dot{s} - \rho_0 \frac{r}{\theta} + \frac{1}{\theta} \mathbf{v}_0 \cdot \mathbf{h}_0 - \frac{\mathbf{v}_0 \cdot \mathbf{h}_0}{\theta^2} \cdot \mathbf{h}_0 \geq 0,
\]

(8)

where \( \mathbf{S}_i \) is the local entropy production rate. Introducing the local dissipation rate

\[
\rho_0 \mathbf{D}_i = \rho_0 \theta \dot{\mathbf{S}}_i = \rho_0 \theta \dot{s} - \rho_0 \theta r + \mathbf{v}_0 \cdot \frac{1}{\theta} \mathbf{h}_0 - \mathbf{v}_0 \cdot \mathbf{h}_0 \geq 0
\]

(9)

and resolving Eq. (7) for the expression \( \mathbf{v}_0 \cdot \mathbf{h}_0 - \rho_0 r \), and substituting it in Eq. (9), one obtains the following dissipation inequality:

\[
\rho_0 \mathbf{D}_i = \mathbf{P} \cdot \dot{\mathbf{F}} - \rho_0 \dot{\mathbf{U}} + \rho_0 \theta \dot{s} + \mathbf{v}_0 \cdot (\mathbf{Q}_0^0 \eta_i) - \frac{\mathbf{v}_0 \cdot \mathbf{h}_0}{\theta} \cdot \mathbf{h}_0 \geq 0.
\]

(10)

It is more convenient to substitute \( U \) with the specific Helmholtz free energy per unit mass \( \psi = U - \dot{s} \theta \). Also, we assume that the heat conduction and other thermomechanical processes are mutually independent. Then the inequality (10) transforms to Fourier’s inequality \( -\mathbf{v}_0 \theta / \theta \cdot \mathbf{h}_0 \geq 0 \) and the mechanical dissipation inequality:

\[
\rho_0 \mathbf{D}_i = \rho_0 \mathbf{D} + \frac{1}{\theta} \mathbf{h}_0 \cdot \mathbf{v}_0 \theta = \mathbf{P} \cdot \dot{\mathbf{F}} - \rho_0 \psi - \rho_0 \theta \dot{s} + \mathbf{v}_0 \cdot (\mathbf{Q}_0^0 \eta_i) \geq 0.
\]

(11)
Let us introduce the Cauchy (true) stress tensor \( \sigma \) and deformation rate \( \mathbf{d}, \sigma = (\rho/\rho_0) \mathbf{P} : \mathbf{F}^t, \mathbf{d} = (\mathbf{F} : \mathbf{F}^{-1})_t \), where \( \rho \) is the mass density in the actual configuration. Then one can transform stress power to the actual configuration \( \mathbf{P} : \mathbf{F}^t = (\rho_0/\rho) \sigma : \mathbf{d} \), which will be utilized below.

### 3. Kinematics and constitutive equations

**Kinematics:** The multiplicative decomposition of the deformation gradient,

\[
\mathbf{F} = \mathbf{F}_e \cdot \mathbf{U}_\rho \cdot \mathbf{U}_t,
\]

into elastic, thermal, and transformational parts will be used (Levitas, 1998) (Fig. 2). Without loss of generality, \( \mathbf{U}_\rho(\theta, \eta_i) \) and \( \mathbf{U}_t(\eta_i) \) are considered to be symmetric (rotation-free) tensors and all rotations are included in \( \mathbf{F}_e \).

After a local release of stresses, elastic deformation disappears (i.e., \( \mathbf{F}_e = \mathbf{I} \)) and an unloaded configuration, characterized by \( \mathbf{U}_\rho \cdot \mathbf{U}_t \), is designated as \( \Omega_0 \). After returning temperature \( \theta \) to its reference values \( \theta_0 \), thermal strain disappears as well (i.e., \( \mathbf{U}_\rho = \mathbf{I} \)) and one obtains the transformed configuration \( \Omega_\theta \) characterized by transformation deformation gradient \( \mathbf{U}_t \). It is assumed that no reverse PT occurs during such an unloading and temperature change; otherwise, these procedures should be considered as the thought experiment under fixed phase state. After introducing Jacobians, which describe ratios of volumes \( V \) and mass densities \( \rho \) in the corresponding configurations,

\[
J = \frac{dV}{dV_0} = \frac{\rho_0}{\rho} = \det \mathbf{F}; \quad J_t = \frac{dV_t}{dV_0} = \frac{\rho_0}{\rho_t} = \det \mathbf{U}_t;
\]

\[
J_\rho = \frac{dV_\rho}{dV_0} = \frac{\rho_t}{\rho_0} = \det (\mathbf{U}_\rho \cdot \mathbf{U}_t) = J J_t.
\]

One obtains from Eq. (12):

\[
J = J_t J_e.
\]

We will also need the Jacobian for combined transformational and thermal strain

\[
J_{\rho \theta} = \frac{dV_{\rho \theta}}{dV_0} = \frac{\rho_0}{\rho_0} = \det (\mathbf{U}_\rho \cdot \mathbf{U}_t) = J J_t.
\]

**Constitutive equations:** Let \( \psi = \psi(\mathbf{F}, \mathbf{F}_e, \eta_i, \theta, \nabla_0 \eta_i) \). The order parameter \( \eta_i = 0 \) for austenite and 1 for the \( i \)th martensitic variant. Derivation will be more compact if we will change an argument of \( \psi \) from \( \mathbf{F}_e \) to \( \mathbf{F} \):

\[
\psi = \psi(\mathbf{F}, \mathbf{F}_e, \eta_i, \theta, \nabla_0 \eta_i) = \psi(\mathbf{F}, \mathbf{F}_e^{-1}(\eta_i) \cdot \mathbf{U}_0^{-1}(\theta_0, \eta_i, \theta, \nabla_0 \eta_i) = \psi(\mathbf{F}, \eta_i, \theta, \nabla_0 \eta_i).
\]

Let us evaluate the term

\[
\nabla_0 \cdot (\mathbf{Q}_{\theta i}^g)_{\eta_i} = (\nabla_0 \cdot \mathbf{Q}_{\theta i}^g)_{\eta_i} + \mathbf{Q}_{\theta i}^g \cdot \nabla_0 \eta_i = (\nabla_0 \cdot \mathbf{Q}_{\theta i}^g)_{\eta_i} + \mathbf{Q}_{\theta i}^g \cdot \nabla_0 \eta_i.
\]

Substituting \( \psi \) into Eq. (11) and taking into account Eq. (17), we obtain

\[
\rho_0 D = \left( \mathbf{P} - \rho_0 \frac{\partial \mathbf{F}}{\partial \mathbf{F}} \right) : \mathbf{F}^t - \rho_0 \left( s + \frac{\partial \mathbf{F}}{\partial \theta} \right) \theta - \left( \rho_0 \frac{\partial \mathbf{F}}{\partial \eta_i} - \nabla_0 : \mathbf{Q}_{\theta i}^g \right)_{\eta_i} + \left( \mathbf{Q}_{\theta i}^g - \rho_0 \frac{\partial \mathbf{F}}{\partial \mathbf{F}} : \nabla_0 \eta_i \right) \cdot \nabla_0 \eta_i \geq 0.
\]

Independence of the dissipation rate of \( \theta \) leads to the constitutive equation for entropy

\[
s = -\frac{\partial \mathbf{F}}{\partial \theta} \theta
\]

Assuming that the dissipation rate is independent of \( \nabla_0 \eta_i \), we obtain equations

\[
\mathbf{Q}_{\theta i}^g = \rho_0 \frac{\partial \mathbf{F}}{\partial \mathbf{F}} : \nabla_0 \eta_i
\]

which define the introduced generalized thermodynamic forces. The term in Eq. (18) conjugated to \( \mathbf{F}^t \) is the generalized dissipative or viscous stresses \( \mathbf{P}_v \); the terms conjugated to \( \eta_i \) are corresponding to dissipative forces \( X_i \). Then Eq. (18) simplifies to

\[
\rho_0 D = \mathbf{P}_v : \mathbf{F}^t + \rho_0 X_i \eta_i \geq 0.
\]

This leads to constitutive equations for the stress tensor and the evolution equation for \( \eta_i \)

\[
\mathbf{P} = \rho_0 \frac{\partial \mathbf{F}}{\partial \mathbf{F}} + \mathbf{P}_v; \quad \rho_0 X_i = -\rho_0 \frac{\partial \mathbf{F}}{\partial \eta_i} + \nabla_0 \cdot \left( \rho_0 \frac{\partial \mathbf{F}}{\partial \mathbf{F}} \right).
\]
provided that constitutive equations for $P_v$ and $X_i$ are given. Next, we assume that the generalized rates, i.e., deformation rate and $\eta_i$, are thermodynamically independent. Then two stricter inequalities are valid

$$ P_v \dot{\gamma} \geq 0; \quad X_i \dot{\eta}_i \geq 0. \quad (23) $$

To satisfy these inequalities, one has to assume that $P_v = P_v(\dot{\gamma})$ and $X_i = X_i(\dot{\eta}_i)$, otherwise, inequalities can be easily violated.

In particular, if one assumes linear relationships $\dot{\eta}_i = L_{ij}X_j$, where $L_{ij}$ are positive definite kinetic coefficients, for which $L_{ij} = L_{ij}$ according to the Onsager reciprocal relationships, then Eq. (22) transforms to the generalized Ginzburg–Landau equation

$$ \dot{\eta}_i = L_{ij} \left( \frac{\partial \gamma}{\partial \eta_i} + \frac{1}{\rho_0} \nabla_0 \cdot \left( \rho_0 \frac{\partial \gamma}{\partial \nabla_0 \eta_i} \right) \right). \quad (24) $$

If $\rho_0$ does not vary in space (initially homogeneous material), it disappears from Eq. (24).

Introducing dissipative (viscous) Cauchy stress tensor $\sigma_v = f^{-1}P_v \cdot \dot{\gamma}$, one obtains $P_v : \dot{\gamma} = \sigma_v(\dot{\gamma}) \geq 0; \quad \sigma_v = \sigma_v(\dot{\gamma})$.

4. Boundary conditions for order parameters

**Reference configuration:** Since we introduced generalized vector-forces $Q_{0i}^\eta$ at the external surface (see Eq. (20)), one can prescribe their normal component at the boundary (similar to the heat flux):

$$ n_0 \cdot Q_{0i}^\eta = n_0 \cdot \rho_0 \frac{\partial \gamma}{\partial \nabla_0 \eta_i} = H_{0i}, \quad (25) $$

where $H_{0i}$ are some given functions. Alternatively, one can prescribe periodic boundary conditions for $\eta_i$, which is always the case when spectral methods of solutions of the boundary value problems are used (Jin et al., 2001a; Chen, 2002; Lookman et al., 2008), or conditions $\eta_i = \text{const}$, (in particular, 0 or 1) are applied. Mixed boundary conditions are possible. Boundary conditions with the most important physically based option for functions $H_{0i}$ are (Lipowsky, 1982; Pluis et al., 1990; Levitas et al., 2006b; Levitas and Javanbakht, 2010; Levitas and Samani, 2011a,b)

$$ n_0 \cdot \rho_0 \frac{\partial \gamma}{\partial \nabla_0 \eta_i} = - \frac{\partial \gamma_{0i}(\eta)}{\partial \eta_i}, \quad (26) $$

where $\gamma_{0i}(\eta)$ is the surface energy per unit reference area. If surface energy is different for the parent and product phases, then it should depend on the order parameters. This leads to surface-induced pre-transformations and barrierless nucleation (Lipowsky, 1982; Pluis et al., 1990; Levitas et al., 2006b; Levitas and Javanbakht, 2010; Levitas and Samani, 2011a,b), which have been studied either without deformation or for small strains. In the earlier papers, mostly on surface melting, it was accepted $\gamma_{0i}(\eta) = B + C \eta^2$ with two constants (Lipowsky, 1982; Pluis et al., 1990). Alternatively, $\gamma_{0i}(\eta) = B + C \eta$ (Levitas et al., 2006b). It was justified in Levitas and Javanbakht (2010) and Levitas and Samani (2011a) for small strains that in order to avoid some artificial surface structures, one should accept $\gamma_{0i}(\eta) = \gamma_{0i}^A + (\gamma_{0i}^M - \gamma_{0i}^A)(a_i p^2 + (4 - 2a_i) p^3 + (a_i - 3) p^4)$, where $\gamma_{0i}^A$ and $\gamma_{0i}^M$ are the surface energies of A and M and $a_i$ is a parameter. Such a function $\gamma_{0i}(\eta)$ not only reduces to $\gamma_{0i}^A$ and $\gamma_{0i}^M$ for $\eta = 0$ and 1, respectively, but also possesses zero first derivatives at $\eta = 0$ and 1, providing smooth transition. Note that both $\gamma_{0i}^A$ and $\gamma_{0i}^M$ are determined per unit area of undeformed austenite, i.e., an experimentally measured value of the surface energy of a martensitic variant should be multiplied by the ratio of the area of martensitic elemental surface to the corresponding austenitic elemental surface. For the multivariant martensitic PT, one has (Levitas and Javanbakht, 2010)

$$ \gamma_{0i}(\eta) = \gamma_{0i}^A + (\gamma_{0i}^M - \gamma_{0i}^A)(a_i p^2 + (4 - 2a_i) p^3 + (a_i - 3) p^4); \quad p = \left( \sum_{i=1}^n \eta_i^2 \right)^{0.5}, \quad (27) $$

where $p$ is the “equivalent” order parameter. One can use the sixth-degree polynomial function $\gamma_{0i}(\eta)$ as well, see below. For equal surface energy of the phases, one has $H_{0i} = 0$.

Note that Eq. (26) could be obtained without introducing the thermodynamic forces $Q_{0i}^\eta$ at the surface $S_0$ in Eq. (4), but by including the rate of the surface energy $\gamma_{0i}(\eta)$ into the surface integral in Eq. (4). However, then global thermodynamics laws will be written not for an arbitrary body but for the actual body with the given surface and surface energy, which will require additional assumptions to localize them for a material point (Levitas, 2013a). This is the main reason to introduce the thermodynamic forces $Q_{0i}^\eta$ at the surface $S_0$ from the very beginning.

**Actual configuration:** In order to transform boundary conditions Eq. (26) to the actual configuration, let us formally introduce the thermodynamic forces $Q_i^\eta$ in the actual configuration by the equation

$$ Q_{0i}^\eta \cdot n_0 \, dS_0 = Q_i^\eta \cdot n \, dS_0, \quad (28) $$

where $n$ is the unit outer normal to the external surface $S$ the actual configuration. Utilizing Nanson’s relationship between oriented area in the deformed and undeformed states (Lurie, 1990; Malvern, 1977), $n_0 dS_0 = f^{-1}F \cdot n \, dS$, and substituting it in Eq. (28), one obtains

$$ Q_i^\eta = f^{-1}F \cdot Q_{0i}^\eta + \rho F \cdot \frac{\partial \gamma}{\partial \nabla_0 \eta_i} = f^{-1}F \cdot \frac{\partial \gamma}{\partial \nabla_0 \eta_i}, \quad (29) $$
where we used Eq. (216) for the last transformation. Combining Eqs. (26), (28), and (29), we obtain boundary conditions in the actual configuration
\[
\mathbf{n} \cdot \frac{\partial \sigma}{\partial \mathbf{n}} = - \frac{\partial \gamma_0^0}{\partial \eta_i} dS_0 = - \frac{\partial \gamma_s}{\partial \eta_i},
\]
where \(\gamma_s = \gamma_0^0 dS_0 / dS\) is the surface energy per unit deformed area. Thus, the structure of the boundary conditions in the reference and actual configurations is the same. When surface energy of the initial and final phases per unit area in the same configuration does not change during the PT, then
\[
\frac{\partial \gamma_0^0}{\partial \eta_i} = \frac{\partial \gamma_s}{\partial \eta_i} = 0 \Rightarrow \frac{\partial \sigma}{\partial \mathbf{n}} = 0,
\]
which offers a physical interpretation of the traditional boundary conditions.

It was stated in Levitas and Javanbakht (2011b) that there is an evident contradiction in the phase field approach: while the finite width of the phase interfaces and the surface transformed layer are resolved, the external surface is treated as the sharp surface with boundary conditions (i.e., like here). The finite-width external surface was introduced in Levitas and Javanbakht (2011b) with the help of an additional order parameter that describes a stationary solid–gas interface. This led to several interesting scale and mechanics effects and morphological transitions in surface-induced PTs. For melting of Al nanoparticles, a very rich temperature – width of a surface layer transformation diagram is found, which includes various barrierless and thermally activated transformations between solid, melt, and surface melt, complex hysteretic behavior, and bistable states (Levitas and Samani, 2014).

5. Structure of the Helmholtz free energy and expression for stresses

5.1. Structure of the Helmholtz free energy

Let us postulate the following structure of the free energy per unit mass:
\[
\psi(F, \eta_i, \theta, \nabla \eta_i) = \frac{1}{\rho_0} \psi^0 \left( F \cdot \nabla_i^{-1} (\eta_i) \cdot \nabla_i^{-1} \eta_i, \theta \right) + J \hat{\psi}^0(\eta_i, \theta_i) + J \hat{\psi}^0(\eta_i, \theta_i) + J \hat{\psi}^\gamma(\nabla \eta_i).
\]

Here \(\psi^0\) is the elastic energy, which depends on \(F, \eta_i, \theta\); \(\psi^\gamma\) is the gradient energy; \(\hat{\psi}^0\) and \(\hat{\psi}^\gamma\) are the parts of the thermal (chemical) energy; \(\hat{\psi}^\gamma\) is related to the thermal driving force for A–M PT (i.e., to the difference between the thermal parts of the free energies of \(M_i\) and \(A_i\), \(\Delta G^\gamma\)) and is equal to zero at phase equilibrium temperature \(\theta\), when \(\Delta G^\gamma(\theta) = 0\); \(\psi^\gamma\) is localized at the interfaces and is equal to zero in the bulk (i.e., when all order parameters are 0 or 1). We will demonstrate that consideration of the gradient \(\nabla \eta_i\) in the deformed configuration as an argument of \(\psi^\gamma\) and multiplication of \(\hat{\psi}^0\) and \(\psi^\gamma\) by the Jacobian \(J\) will lead (with the proper choice of \(\hat{\psi}^0\)) to the desired expression for interface stresses, at least for a single martensitic variant. Note that Jacobians and gradient with respect to deformed configurations in Eq. (32) should be kept even in small strain formulation (when they are traditionally neglected), otherwise, interface stresses will disappear (Levitas, 2013b). In the expression for the free energy per unit undeformed volume, \(\rho_0 \psi^0\) function \(\rho_0 \psi^0\) and constants in it are determined per unit undeformed volume as well. It follows from the expression \(\rho_0 \psi^0 \psi^0 dV_0 = \rho_0 \psi^0 \psi^0 dV\) that \(\rho_0 \psi^0\) and constants in it are determined per unit undeformed volume \(V\). The same is true for \(\rho_0 \psi^0\). Similar, equality \(\rho_0 (\partial \psi^\gamma / \partial \psi^\gamma) dV_0 = \psi^\gamma dV\) implies that the elastic energy is defined per unit volume in the unloaded configuration \(\Omega_0\), in which the elasticity rule is determined experimentally or in atomistic simulations (see Section 5.2). Note that the similar definition of the elastic energy was suggested for large anisotropic compositional expansion during lithiation–delithiation of silicon in Levitas and Attarzian (2013, 2014). It is assumed that free energy is invariant under superposed rigid-body motion in the actual configuration, i.e., it satisfies the principle of material objectivity.

Below we will use the relationship
\[
\nabla \eta_j = \nabla \eta_j; \quad \frac{\partial \eta_j}{\partial \eta_j} = \frac{\partial \eta_j}{\partial \eta_j}, \quad \frac{\partial \eta_j}{\partial \eta_j} = \frac{\partial \eta_j}{\partial \eta_j} = \frac{\partial \eta_j}{\partial \eta_j} F^{-1};
\]
\[
\frac{\partial \nabla \eta_j}{\partial \nabla \eta_j} = F^{-1}; \quad \frac{\partial (\partial \eta_j / \partial \eta_j)}{\partial (\partial \eta_j / \partial \eta_j)} = F^{-1}.
\]

Designating \(i = \nabla \eta_j\) and \(i = \nabla \eta_k\) for compactness, we rewrite Eq. (33)
\[
\zeta_j = \xi_j; \quad \xi_j = \xi_j; \quad \xi_j = \xi_j; \quad \frac{\partial \xi_j}{\partial \xi_j} = \xi_j; \quad \frac{\partial \xi_j}{\partial \xi_j} = \xi_j; \quad \frac{\partial \xi_j}{\partial \xi_j} = \xi_j.
\]

Let us express function \(\psi^\gamma\) in terms of \(\nabla \eta_j\) and \(F\), i.e., in the form used in general derivations:
\[
\psi^\gamma (\nabla \eta_k) = \psi^\gamma (\nabla \eta_k \cdot F^{-1}).
\]
5.2. Constitutive equations for stresses

Elastic stresses: Let \( \psi^e = \psi^e(F_e, \eta, \theta) \). We will use below the following kinematic equations

\[
F_e = R_e \cdot U_e = V_e \cdot R_e; \quad V_e = R_e \cdot U_e \cdot R_e^T; \quad E_e = 0.5(U_e \cdot U_e - I);
\]

\[
B_e = 0.5(V_e \cdot V_e - I) = R_e \cdot E_e \cdot R_e^T,
\]

where \( R_e \) is the proper orthogonal lattice rotation tensor, \( V_e \) and \( U_e \) are the symmetric left and right elastic stretch tensors, and \( E_e \) and \( B_e \) are the Lagrangian and Cauchy–Green strain tensors. Under superposition of the rigid–body rotation \( r^e = Q \cdot r \), we have \( F_e^* = Q \cdot F_e \). According to the principle of material objectivity, \( \psi^e(Q \cdot F_e, \eta, \theta) = \psi^e(F_e, \eta, \theta) \) for all \( Q \). Setting \( Q = R_e \), we obtain that function \( \psi^e(U_e, \eta, \theta) \) satisfies the principle of material objectivity. Usually, argument \( U_e \) is substituted with the equivalent one \( E_e \), i.e., \( \psi^e = \psi^e(E_e, \eta, \theta) \), where for simplicity we did not change designation for \( \psi^e \). By definition, for the elastic first Piola–Kirchhoff stress

\[
P_e = \rho_0 \left( \frac{\partial \psi^e}{\partial \mathbf{F}} \right) = \int_{\Omega_0} \frac{\partial \psi^e}{\partial \mathbf{F}} \mathbf{F}^* = \int_{\Omega_0} \frac{\partial \psi^e}{\partial \mathbf{F}} \cdot \mathbf{U}^{-1}_\eta (\theta, \eta) \cdot \mathbf{U}^{-1}_\eta (\theta, \eta) = \int_{\Omega_0} \frac{\partial \psi^e}{\partial \mathbf{F}} \mathbf{F}^e \cdot \mathbf{F}^e - 1,
\]

where multiplicative decomposition Eq. (12) was used. For true elastic stress

\[
\sigma_e = J_e^{-1} F_e \cdot (C(E_e) \cdot F^e); \quad P_e = J_e^{-1} F_e \cdot (C(E_e) \cdot F^e \cdot F^e - 1).
\]

Let us transform the equation for the Cauchy stress, using Eq. (36):

\[
\sigma_e = J_e^{-1} V_e \cdot (C(R_e) \cdot R_e) \cdot V_e = J_e^{-1} V_e \cdot (C(R_e) \cdot B_e) \cdot V_e,
\]

where \( C = \delta_{ij} e_i \otimes \delta_{ij} e_i \otimes \delta_{ij} e_i \otimes \delta_{ij} e_i \) and \( \delta_{ij} R_e \times C = \delta_{ij} R_e \times (R_e \cdot e_i) \otimes (R_e \cdot e_i) \otimes (R_e \cdot e_i) \) are the fourth-rank tensors of elastic moduli and rotated elastic moduli, and the validity of the transformations in Eq. (40) is easy to check in component form. Here Cartesian unit basis vectors \( e_i \) are related to the martensite crystal lattice in the unloaded configuration \( \Omega_0 \) and basis vectors \( R_e \cdot e_i \) are related to the stress-free martensite lattice rotated by tensor \( R_e \).

For small elastic strains but finite other strains and rotations, \( V_e \simeq I \), \( B_e \) transforms to small elastic strain \( e_e \) and the elasticity rule Eq. (40) transforms into Hooke’s law \( \sigma_e = C_k : e_e \).

Note that if elastic energy in Eq. (40) would be introduced with respect to reference configuration \( \Omega_0 \), i.e., \( \psi = (1/\rho_0) \psi^e + \cdots \), then Eq. (38) would change to \( \sigma_e = J_e^{-1} F_e \cdot \partial \psi^e / \partial E_e \cdot F^e, \) For the same quadratic form for \( \psi^e \) this equation simplifies to

\[
\sigma_e = (J_e^{-1})^{-1} V_e \cdot (C_k : B_e) \cdot V_e.
\]

For small elastic strains this equation simplifies to \( \sigma_e = (J_e^{-1})^{-1} C_k : e_e \). It is clear that if elastic constants \( C_k \) of martensite were determined with respect to the crystal lattice of martensite, the term \( (J_e^{-1})^{-1} \) should not be present in Hooke’s law for martensite. Since volumetric change during PT can be quite large (e.g., \( J_e^{-1} = 1.54 \) for P Ts from rhombohedral and hexagonal graphite to cubic or hexagonal diamond and similar P Ts in boron nitride, all at high pressure (Britton and Kurydyumov, 2000), error in the elasticity rule can be significant.

A similar transformation of the elasticity rule from the unloaded configuration \( \Omega_0 \) to the actual configuration \( \Omega \) can be performed in the general case. Let \( C_k = C_{kij} : e_i \otimes e_j : \cdots \) be the tensor parameters of different ranks characterizing nonlinear elastic anisotropy in the unloaded configuration \( \Omega_0 \). They are functions of temperature and \( \eta \) and at fixed \( \theta \) and \( \eta \), \( C_k \) are also fixed. Then for the rotated stress-free crystal lattice of martensite these tensors transform to \( C_k^e = C_{k}^{ijkl} : (R_e \cdot e_i) \otimes (R_e \cdot e_j) \otimes (R_e \cdot e_k) \otimes (R_e \cdot e_l) \) to \( C_k \). Then elastic energy can be presented in the actual configuration in the form \( \psi^e(B_e, C_k(\eta, \theta)) = \psi^e(E_e, C_k(\eta, \theta)) \).

Indeed, under rigid–body rotation \( r = Q \cdot r \), the left–hand side transforms to \( \psi^e(Q \cdot B_e, Q^T \cdot Q \cdot C_k(\eta, \theta)) \). Then setting \( Q = R_e \), we obtain \( \psi^e(R_e \cdot B_e, R_e \cdot C_k(\eta, \theta)) = \psi^e(E_e, C_k(\eta, \theta)) \), which proves equivalence of presentation. Thus, in the
constitutive equations in the actual configuration, all tensors describing material anisotropy should be explicitly shown.

Indeed, in contrast to the description in the reference configuration, these tensors are not constants because they rotate with the body and depend on rotations. In the unloaded configuration \( \Omega_{0} \), tensors \( C_k \) usually are not shown explicitly, because they are either constants or can be expressed in terms of their arguments \( \eta_i \) and \( \theta \). Then it follows from Eq. (38)

\[
\sigma = J^{-1} \mathbf{e} \cdot \frac{\partial \psi^e(E, C_k)}{\partial E} \cdot R^e \cdot \mathbf{e} = J^{-1} \mathbf{e} \cdot \frac{\partial \psi^e(B_e, C_{ik})}{\partial B_e} \cdot V_e,
\]

where equation \( R_e \cdot \frac{\partial \psi^e(E, C_k)}{\partial E} = \partial \psi^e(B_e, C_{ik}) / \partial B_e \) was used (see Levitas, 1996).

**Stresses due to gradient energy:** Since \( \psi^\gamma(\nabla \eta_i, F) \) depends on \( F \), it produces contribution \( P^\gamma \) to the first Piola–Kirchhoff stress according to Eq. (22)

\[
P^\gamma = \rho_0 \frac{\partial \psi^\gamma(\nabla \eta_i, F)}{\partial F}
\]

With the help of Eq. (22) from Appendix one obtains

\[
P^\gamma = - \rho_0 J \frac{\partial \psi^\gamma}{\partial \nabla \eta_i} \otimes F^{-1} - \rho_0 J \frac{\partial \psi^\gamma}{\partial \nabla \eta_i} \cdot F^{-1}
\]

and corresponding contribution to the Cauchy stress

\[
\sigma^\gamma = J^{-1} P^\gamma \cdot F^{-1} = - \rho_0 J \psi(\nabla \eta_i) \otimes \frac{\partial \psi^\gamma}{\partial \nabla \eta_i}
\]

Thus, we multiplied by the Jacobian those contributions to free energy, which we would like to contribute to the spherical part of the Cauchy stress. This is even more evident for small strain formulation, when \( J = 1 + \varepsilon_0 + I \cdot \varepsilon \), and \( dJ / d\varepsilon = I \), where \( \varepsilon \) and \( \varepsilon_0 \) are the small strain tensor and its volumetric part.

**Total stresses:** Combining all contributions, one obtains for the nominal stress

\[
P = P_e + P_{sl} + P_{\gamma};
\]

\[
P_e = J \frac{\partial \psi^e}{\partial F_e} \cdot U^{-1}_e(\theta, \eta_i) \cdot U^{-1}_i(\eta_i) = J \frac{\partial \psi^e}{\partial F_e} \cdot F^{-1};
\]

\[
P_{sl} = P_d^l + P_{\gamma} = \rho_0 J (\psi^\theta + \psi^\beta) F^{-1} - \rho_0 J \frac{\partial \psi^\gamma}{\partial \nabla \eta_i} \otimes \frac{\partial \psi^\gamma}{\partial \nabla \eta_i},
\]

and for true stress

\[
\sigma = \sigma_e + \sigma_{sl} + \sigma_{\gamma};
\]

\[
\sigma_e = J^{-1} F_e \cdot \frac{\partial \psi^e}{\partial E_e} \cdot F^{-1} = J^{-1} \mathbf{e} \cdot \frac{\partial \psi^e}{\partial B_e} \cdot V_e;
\]

\[
\sigma_{sl} = \sigma^l + \sigma^\gamma = \rho_0 (\psi^\theta + \psi^\beta) I - \rho_0 \psi(\nabla \eta_i) \otimes \frac{\partial \psi^\gamma}{\partial \nabla \eta_i}.
\]

Stresses \( P_{sl} \) and \( \sigma_{sl} \) are called structural stresses at the interface, because for single martensitic variant we will prove that \( \sigma_{sl} \) reduces to biaxial stress with the magnitude equal to the interface energy. For small strain and rotations, one has \( P_{sl} = \sigma_{sl} \) and the expression for \( \sigma_{sl} \) does not change. Thus, while we needed large strain formulation to introduce surface stresses, surface stress does not disappear or even changes at small strains. This underlines the importance of a fully large strain formulation even for a small strain case, if one wants to introduce interface stresses.

All contributions to the Cauchy stress represent symmetric tensors, but the term \( \sigma^\gamma \), which contains a skew-symmetric part

\[
\sigma_a = - \rho_0 \left( \nabla \eta_i \otimes \frac{\partial \psi^\gamma}{\partial \nabla \eta_i} \right)_a = \rho_0 \left( \frac{\partial \psi^\gamma}{\partial \nabla \eta_i} \otimes \nabla \eta_i \right)_a.
\]

Below we consider a particular case for which \( \sigma_a = 0 \) can be proven.

**Isotropic interface energy:** For the case with isotropic interface energy and stresses, \( \psi^\gamma \) is an isotropic function of \( \zeta_i = \nabla \eta_i \), i.e., it depends on invariants \( a_{jk} = \zeta_j \cdot \zeta_k = a_{ij} \) for all \( k \) and \( j \). \( \psi^\gamma = \psi^\gamma(a_{jk}) \). Let us prove that

\[
\left( \frac{\partial \psi^\gamma}{\partial \zeta_j} \otimes \zeta_i \right)_a = 0
\]

for this case. Indeed, the second-rank tensor

\[
\frac{\partial \psi^\gamma}{\partial \zeta_i} \otimes \zeta_j = \frac{\partial \psi^\gamma}{\partial a_{jk}} a_{ij} \otimes \zeta_i = \frac{\partial \psi^\gamma}{\partial a_{jk}} (\zeta_k \otimes \zeta_i + \zeta_j \otimes \zeta_i) = \frac{\partial \psi^\gamma}{\partial a_{jk}} (\zeta_k \otimes \zeta_j + \zeta_j \otimes \zeta_k)
\]
is symmetric because $a_k$ is symmetric. Consequently, for isotropic interface energy $\sigma_a = 0$ and the Cauchy stress is symmetric.

**Specification of the gradient energy:** Let us specify a gradient-related term for an isotropic interface energy as

$$\psi^V = \frac{1}{2\rho_0} \nabla \cdot \left( a \nabla \psi \right); \quad a_i = \nabla \nabla_i \nabla \psi; \quad \nabla = \cdots + J \psi^V = \cdots + \frac{1}{2\rho_0} \nabla \cdot \left( a \nabla \psi \right),$$

where dots designate terms independent of $\nabla \psi$. Then the term contributing to stresses

$$\rho_0 \frac{\partial \psi^V}{\partial \nabla_i} = \frac{\partial \psi^V}{\partial a_i} = \beta_0 \nabla_i; \quad \beta_0 := \frac{\partial \psi^V}{\partial a_i}.$$

If all martensitic variants are equivalent, then

$$\beta_{ik} = \beta > 0; \quad \beta_{ij} = b \beta \; \forall k \neq j.$$

where $\beta_{ik}$ characterizes the austenite–martensite interfaces and $\beta_{ij} \forall k \neq j$ characterize the $M_i$–$M_j$ interfaces (Levitas, 2013a). The same is valid for the kinetic coefficients $L_{ij}$, Eq. (48) for interface stresses transforms to

$$\sigma_{st} = \rho_0 (\psi^a + \psi^V) \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi = \rho_0 (\psi^a + \psi^V) \mathbf{I} - \beta \sum_{i=1}^n \left( \nabla \psi_i \otimes \nabla \psi_i + b \nabla \psi_i \otimes \sum_{j=1}^n \nabla \psi_j \right).$$

If $\psi^V$ is the isotropic second degree polynomial in $\nabla \psi$, then

$$\psi^V = \frac{\beta_0}{2\rho_0} \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi = \frac{\beta}{2\rho_0} \left( \sum_{i=1}^n \sum_{j=1}^n \nabla \psi_i \otimes \nabla \psi_j \right);$$

$$\nabla = \cdots + J \psi^V = \cdots + \frac{\beta_0}{2\rho_0} \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi = \cdots + \frac{\beta}{2\rho_0} \left( \sum_{i=1}^n \sum_{j=1}^n \nabla \psi_i \otimes \nabla \psi_j \right),$$

and

$$\sigma_{st} = \left( \rho_0 (\psi^a + \psi^V) \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi \right) = \left( \rho_0 (\psi^a + \psi^V) \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi \right) = \left( \rho_0 (\psi^a + \psi^V) \mathbf{I} - \beta_0 \nabla \psi \otimes \nabla \psi \right).$$

In the majority of previous numerical simulations $b = 0$ was used, see Jin et al. (2001a), Chen (2002), Artemev et al. (2001), Finel et al. (2010) and Levitas and Lee (2007), i.e., $\psi^V$ depends on the single material parameter $\beta$ only. It was stated in Levitas and Javanbakht (2011a,b) that with a single material parameter, it is impossible to fit the energy and the width of the martensitic variant $M_i$ – martensitic variant $M_j$ interface to experimental or atomistically determined values since $\beta$ is fixed by the values of energy and width of the austenite $A$ – martensitic variant $M_i$ interface. To overcome this, Eq. (56) was introduced and used in simulations in Levitas and Javanbakht (2010, 2011a).

**6. Ginzburg–Landau equations**

**6.1. Elaborating gradient energy term**

Let us transform Ginzburg–Landau equation (24) to the actual configuration. We will work with a single order parameter, but the same can be repeated for multiple order parameters by substituting $\eta$ with $\eta_i$. As it was proven in Appendix (Eq. (217)),

$$\nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) = \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) = \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) = \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right).$$

With the help of Eqs. (58) and (24) can be transformed to the actual configuration

$$\frac{D\eta(r, t)}{Dt} = \frac{\partial \eta(r, t)}{\partial t} + \nabla \cdot \nabla \eta = L_{ij} \left( \frac{\partial \psi}{\partial \eta_i} + \frac{1}{\rho} \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) \right).$$

We substituted material time derivative of $\eta$ in the reference configuration with the corresponding expression in the current configuration but did not change the first terms in Eq. (59), because it is the same in any configuration.

For the specific expression for $\psi^V$ given in Eqs. (52)–(54), Eq. (59) transforms to

$$\frac{D\eta(r, t)}{Dt} = L_{ij} \left( \frac{\partial \psi}{\partial \eta_i} + \frac{1}{\rho} \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) \right).$$
If $\beta_{ii}$ are independent of position vector, then
\[
\frac{D\eta_i(t)}{Dt} = L_{ji} \left( -\frac{\partial \sigma}{\partial \eta_i} + \frac{\beta_{ii}}{\rho} \nabla^2 \eta_i \right) = L_{ji} \left( -\frac{\partial \sigma}{\partial \eta_i} + \frac{\beta}{\rho} \left( \nabla^2 \eta_i + \sum_{k=1, k \neq i}^{n} \nabla^2 \eta_k \right) \right).
\] (61)

Eq. (61) in the actual configuration has traditional form. In $\Omega_0$ one has
\[
a_{ij} = (F^{-1} \cdot \nabla \theta_i \cdot (\nabla \theta_j \cdot F^{-1})) = (F^{-1} \cdot F^{-1} \cdot \nabla \theta_i \otimes \nabla \theta_j).
\] (62)

To transform the Ginzburg–Landau equation to the reference configuration, we utilize Eq. (223):
\[
\nabla \cdot (\beta_0 \nabla \eta_i) = (F^{-1} \cdot F^{-1} \cdot \nabla_0)(\rho_0 \nabla \eta_i).
\] (63)

Substituting this equation in Eq. (73), we obtain
\[
\dot{\eta}_i = L_{ji} \left( -\frac{\partial \sigma}{\partial \eta_i} + \frac{1}{\rho} F^{-1} \cdot F^{-1} \cdot \nabla_0(\rho_0 \nabla \eta_i) \right) = L_{ji} \left( -\frac{\partial \sigma}{\partial \eta_i} + \frac{\beta}{\rho} (F^{-1} \cdot F^{-1} \cdot \nabla_0 \nabla_0 \eta_i) \right),
\] (64)

where in the last equality we assumed that $\beta_{ii}$ is independent of material coordinate. One can see that while isotropic function $\psi(\nabla \eta_i)$ in the actual configuration $\Omega$ results in isotropic contribution to the Ginzburg–Landau equation and isotropic interface energy in $\Omega$, in the reference configuration strain-induced anisotropy in the gradient and interface energy appears.

6.2. Specification of the boundary conditions

Utilizing Eq. (53), we specify the boundary conditions Eq. (30) in the actual configuration
\[
\mathbf{n} \cdot \rho \frac{\partial \sigma}{\partial \nabla \eta_i} = -\frac{\partial f}{\partial \eta_i} = \beta_0 \mathbf{n} \cdot \nabla \eta_i.
\] (65)

Let us transform the first term in the boundary conditions (Eq. (26)) in the reference configuration, taking into account relationships (34) and (53):
\[
\mathbf{n}_0 \cdot \rho_0 \frac{\partial \sigma}{\partial \nabla_0 \eta_i} = \rho_0 \frac{\partial \sigma}{\partial \nabla_0 \eta_i} \cdot \frac{\partial \mathbf{x}_i}{\partial \eta_i} \cdot \mathbf{n}_0 = \rho_0 \frac{\partial \sigma}{\partial \nabla_0 \eta_i} \cdot F^{-1} \cdot \mathbf{F}^{-1} \cdot \mathbf{F}^{-1} \cdot \mathbf{n}_0 = \beta_0 \mathbf{n}_0 \cdot F^{-1} \cdot F^{-1} \cdot \mathbf{n}_0.
\] (66)

Then the boundary conditions (Eq. (26)) in the reference configuration are
\[
\beta_0 \mathbf{n}_0 \cdot F^{-1} \cdot F^{-1} \cdot \mathbf{n}_0 = -\frac{\partial f_0}{\partial \eta_i}.
\] (67)

It is easy to check that the boundary conditions (Eq. (26)) in the reference configuration and in the actual configuration (Eq. (65)) are equivalent and can be transformed to each other by transforming all involved parameters from one configuration to another.

6.3. Elaborating local energy term

Let us obtain a more detailed form of the local term in the Ginzburg–Landau equation (61). Utilizing decomposition Eq. (32), we evaluate at constant $\mathbf{F}$, $\theta$, and $\eta$:
\[
\frac{\partial \sigma}{\partial \eta_i} = \int_{\Omega} \frac{\partial \sigma}{\partial \eta_i} \mathbf{P} \frac{\partial \mathbf{F}}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \eta_i} 
\] (68)

Note that $\frac{\partial f}{\partial \eta_i} = \mathbf{F} \mathbf{F}^{-1} = 0$ because differentiation is performed at constant $\mathbf{F}$. This is one more advantage of using $\sigma$ as a function of the total strain, rather than elastic strain. Let us evaluate the first term in Eq. (68)
\[
\frac{\partial f}{\partial \eta_i} = \beta_0 \mathbf{n}_0 \cdot F^{-1} \cdot F^{-1} \cdot \mathbf{n}_0.
\] (69)

where the second term is related to change in elastic properties of phases. We obtain
\[
\frac{\partial u}{\partial \eta_i} F = \mathbf{P} \cdot \mathbf{U} \cdot \frac{\partial u}{\partial \eta_i} F = \mathbf{P} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F = \mathbf{P} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F + \mathbf{F} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F = \mathbf{P} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F + \mathbf{F} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F - \mathbf{P} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F = \mathbf{F} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F + \mathbf{F} \cdot \mathbf{U} \cdot \mathbf{U}^{-1} \frac{\partial u}{\partial \eta_i} F.
\] (70)

In the above derivations, we took into account expression (37) for the elastic nominal stresses $\mathbf{P} = \int_{\Omega} (\partial \sigma / \partial \mathbf{F}) \cdot \mathbf{F}$ and expression $\mathbf{F} = \mathbf{U} \cdot \mathbf{U}^{-1} \cdot \mathbf{F}$. We also used that the identity $\mathbf{U} \cdot \mathbf{U}^{-1} \mathbf{I} = \mathbf{I} \cdot \mathbf{U}^{-1} = -\mathbf{d} \cdot \mathbf{U}^{-1}$, which was utilized in excluding derivatives $\partial \mathbf{U}^{-1} / \partial \eta_i$ and $\partial \mathbf{U}^{-1} / \partial \eta_i$. 
It is remarkable that elastic stresses only directly contribute to the driving force in the Ginzburg–Landau equation. For small elastic deviatoric strain, Eqs. (72) and (73) reduce to

\[ \frac{\partial U_r}{\partial t} = \frac{1}{\rho_e} \left( \sigma_e \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 - \mathbf{U}_1 \right) \cdot \mathbf{e}_r - J_0 \frac{\partial \psi}{\partial \eta_t} \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 \mathbf{e}_r \]

Substituting all terms in \( \partial \psi / \partial \eta_t \) in the Ginzburg–Landau equation (61) in the reference configuration, one obtains

\[ \frac{\partial \psi}{\partial \eta_t} = \frac{1}{\rho_e} \left( \sigma_e \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 - \mathbf{U}_1 \right) \cdot \mathbf{e}_r - J_0 \frac{\partial \psi}{\partial \eta_t} \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 \mathbf{e}_r \]

Substituting the same expression for \( \partial \psi / \partial \eta_t \) in the Ginzburg–Landau equation (73) in the current configuration and utilizing \( \mathbf{p}_e = J \mathbf{e}_r \cdot \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 - \mathbf{U}_1 \), one obtains

\[ \frac{\partial U_r}{\partial t} = \frac{1}{\rho_e} \left( \sigma_e \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 - \mathbf{U}_1 \right) \cdot \mathbf{e}_r - J_0 \frac{\partial \psi}{\partial \eta_t} \mathbf{F}_e^{-1} \cdot \mathbf{U}_0 \mathbf{e}_r \]

It is remarkable that elastic stresses only directly contribute to the driving force in the Ginzburg–Landau equation. While interface and dissipative stresses do not appear in the Ginzburg–Landau equation, they change elastic stresses through the solution of the mechanical problem and contribute to the Ginzburg–Landau equation indirectly.

### 7. Simplified equations for finite volumetric but small deviatoric elastic strains

We will simplify Eq. (42)

\[ \sigma_e = \mathbf{J}_e^{-1} \mathbf{V}_e \cdot \frac{\partial \psi}{\partial \mathbf{B}_e} \cdot \mathbf{V}_e \]

Let \( \mathbf{V}_e = a_I + \mathbf{e}_e \), where all components of the deviatoric elastic strain \( \mathbf{e}_e \) are much smaller than unity, \( \mathbf{I} \cdot \mathbf{e}_e = 0 \). Then the elastic Jacobian \( \mathbf{J}_e \cong a_I^2 \) and \( \mathbf{B}_e = (a_I^2 - 1)/2 + a_I \mathbf{e}_e \). We define the volumetric elastic strain \( \epsilon_{ve} = \mathbf{J}_e - 1 = a_I^2 - 1 \). Then

\[ \alpha_e = (\epsilon_{ve} + 1)^{1/2} \text{ and } \mathbf{B}_e \cong \frac{(\epsilon_{ve} + 1)^{3/2}}{2} \mathbf{I} + (\epsilon_{ve} + 1)^{1/2} \mathbf{e}_e \]

Assuming that \( \psi_e \) depends on \( \mathbf{B}_e \) through \( \epsilon_{ve} \) and \( \mathbf{e}_e \), we obtain

\[ \sigma_e = \frac{1}{\alpha_e^2} (a_I \mathbf{I} + \mathbf{e}_e) \cdot \left( \frac{\partial \psi}{\partial \epsilon_{ve}} + \frac{\partial \psi}{\partial \mathbf{e}_e} \frac{\partial \mathbf{e}_e}{\partial \mathbf{B}_e} \right) \cdot (a_I \mathbf{I} + \mathbf{e}_e) \cong \frac{1}{\alpha_e^2} \left( \frac{\partial \psi}{\partial \epsilon_{ve}} + \frac{\partial \psi}{\partial \mathbf{e}_e} \frac{\partial \mathbf{e}_e}{\partial \mathbf{B}_e} \right) \]

Double contraction of Eq. (75) with \( \mathbf{I} \) leads to

\[ \epsilon_{ve} = \frac{2}{3} \left( R_{e1}^1 + R_{e2}^2 + R_{e3}^3 \right) + 1 \]

We calculate \( \partial \epsilon_{ve} / \partial \mathbf{B}_e = a_I \mathbf{I} \) and \( \partial \mathbf{e}_e / \partial \mathbf{B}_e = (1/a_I) \mathbf{I} \). Then

\[ \sigma_e = \frac{\partial \psi}{\partial \epsilon_{ve}} + \frac{1}{\alpha_e^2} \frac{\partial \psi}{\partial \mathbf{e}_e} \frac{\partial \mathbf{e}_e}{\partial \mathbf{B}_e} \mathbf{p}_e \mathbf{I} + \mathbf{S}_e \]

where \( \mathbf{p}_e = \frac{1}{3} \mathbf{e}_e \mathbf{I} \) is the mean elastic stress and \( \mathbf{S}_e \) is the deviatoric part of the true stress. Let

\[ \psi_e = 0.5 \left( \mathbf{K}_0 + \Delta K \sum \phi_k(\eta_l) \right) \epsilon_{ve}^2 + \left( \mu_0 + \Delta \mu \sum \phi_k(\eta_l) \right) \mathbf{e}_e \cdot \mathbf{e}_e \]

where \( \mathbf{K} \) and \( \mu \) are the bulk and shear moduli, subscript 0 is for austenite, \( \Delta K \) and \( \Delta \mu \) are the difference in elastic moduli between ith martensitic variant and austenite, and functions \( \phi_k \) and \( \phi_k \) are equal to zero for \( \eta_l = 0 \), equal to unity for \( \eta_l = 1 \) and have a zero derivative at these points (Levitas and Preston, 2002a,b; Levitas et al., 2003; Levitas, 2013a). Then

\[ \sigma_e = \left( \mathbf{K}_0 + \Delta K \sum \phi_k(\eta_l) \right) \epsilon_{ve} \mathbf{I} + \frac{2}{\alpha_e^2} \left( \mu_0 + \Delta \mu \sum \phi_k(\eta_l) \right) \mathbf{e}_e \]

\[ \mathbf{P}_e = \frac{1}{\alpha_e^2} \left( \mathbf{K}_0 + \Delta K \sum \phi_k(\eta_l) \right) \epsilon_{ve} \mathbf{I} + 2 \mathbf{J}_e \left( \mu_0 + \Delta \mu \sum \phi_k(\eta_l) \right) \mathbf{e}_e \cdot \mathbf{V}_i^{-1} \cdot \mathbf{V}_t^{-1} \cdot \mathbf{R}_e \]

For small elastic deviatoric strain, Eqs. (72) and (73) reduce to...
8. Further geometric simplifications

Next, let \( V_\theta = \alpha_0 \mathbf{I} + \mathbf{e}_\theta \) and \( U_\theta = a_\theta \mathbf{I} + \mathbf{e}_\theta \), where all components of the deviatoric parts of the left \( \mathbf{e}_\theta \) and right \( \mathbf{e}_\theta \) thermal stretches are much smaller than unity; \( \mathbf{I}; \mathbf{e}_\theta = \mathbf{0} \) are then Eqs. (81)–(83) simplify to

\[
P_\varepsilon = \frac{J}{\alpha_0 a_0} \left( K_0 + \Delta K \sum_i \phi_\varepsilon(\eta_i) \right) \varepsilon_{00} \mathbf{I} + \frac{2J^2}{\alpha_0} \left( \mu_0 + \Delta \mu \sum_i \phi_\varepsilon(\eta_i) \right) \mathbf{e}_\varepsilon \cdot \mathbf{R}_\varepsilon; \tag{84}\]

\[
\dot{\eta}_\varepsilon = \frac{L_{\varepsilon \varepsilon}}{\rho_0} \left( a_\varepsilon \mathbf{e}_\varepsilon \cdot \mathbf{U}_\varepsilon^{-1} + \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \mathbf{R}_\varepsilon \right) - \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\varepsilon - \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \mathbf{R}_\varepsilon^t - J_{1\varepsilon} \frac{\partial \mathbf{R}_\varepsilon}{\partial \eta_i}; \tag{85}\]

and

\[
\frac{D \eta_i}{D t} = \frac{L_{\varepsilon \varepsilon}}{\rho} \left( \sigma^\varepsilon \cdot \mathbf{R}_\varepsilon \cdot \mathbf{U}_\varepsilon^{-1} + \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \mathbf{R}_\varepsilon \right) - \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\varepsilon - \frac{\partial \mathbf{U}_\varepsilon(\theta, \eta_\varepsilon)}{\partial \eta_i} \cdot \mathbf{R}_\varepsilon^t - J_{1\varepsilon} \frac{\partial \mathbf{R}_\varepsilon}{\partial \eta_i}; \tag{86}\]

Similar, if also \( V_\iota = a_\iota \mathbf{I} + \mathbf{e}_\iota \) and \( U_\iota = a_\iota \mathbf{I} + \mathbf{e}_\iota \), where all components of the deviatoric parts of the left \( \mathbf{e}_\iota \) and right \( \mathbf{e}_\iota \) transformational stretches are much smaller than unity, and \( \mathbf{I}; \mathbf{e}_\iota = \mathbf{0} \) are then Eqs. (84)–(86) reduce to

\[
P_\varepsilon = J^{2/3} \left( K_0 + \Delta K \sum_i \phi_\varepsilon(\eta_i) \right) \varepsilon_{00} \mathbf{R}_\varepsilon + 2J^{2/3} \left( \mu_0 + \Delta \mu \sum_i \phi_\varepsilon(\eta_i) \right) \mathbf{e}_\varepsilon \cdot \mathbf{R}_\varepsilon; \tag{87}\]

\[
\dot{\eta}_\iota = \frac{L_{\iota \iota}}{\rho_0} \left( a_\iota \mathbf{e}_\iota \cdot \mathbf{U}_\iota^{-1} + \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota \right) - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\iota - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota^t - J_{1\iota} \frac{\partial \mathbf{R}_\iota}{\partial \eta_i}; \tag{88}\]

and

\[
\frac{D \eta_i}{D t} = \frac{L_{\iota \iota}}{\rho} \left( \sigma^\iota \cdot \mathbf{R}_\iota \cdot \mathbf{U}_\iota^{-1} + \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota \right) - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\iota - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota^t - J_{1\iota} \frac{\partial \mathbf{R}_\iota}{\partial \eta_i}; \tag{89}\]

Usually, thermal strains are small, and one can put \( a_\varepsilon \approx 1 \) and \( \det \mathbf{U}_\varepsilon \approx 1 \). At moderate pressure, elastic volumetric strain is also small, \( a_\iota \approx 1 \) and \( \det \mathbf{U}_\iota \approx 1 \). Then Eqs. (80) and (87)–(89) reduce to

\[
\sigma^\varepsilon = \left( K_0 + \Delta K \sum_i \phi_\varepsilon(\eta_i) \right) \varepsilon_{00} \mathbf{I} + 2 \left( \mu_0 + \Delta \mu \sum_i \phi_\varepsilon(\eta_i) \right) \mathbf{e}_\varepsilon \cdot \mathbf{R}_\varepsilon; \tag{90}\]

\[
\dot{\eta}_\iota = \frac{L_{\iota \iota}}{\rho_0} \left( a_\iota \mathbf{e}_\iota \cdot \mathbf{U}_\iota^{-1} + \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota \right) - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\iota - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota^t - 3 J_{1\iota} \frac{\partial \mathbf{R}_\iota}{\partial \eta_i}; \tag{91}\]

and

\[
\frac{D \eta_i}{D t} = \frac{L_{\iota \iota}}{\rho} \left( \sigma^\iota \cdot \mathbf{R}_\iota \cdot \mathbf{U}_\iota^{-1} + \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota \right) - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \dot{\mathbf{R}}_\iota - \frac{\partial \mathbf{U}_\iota(\theta, \eta_\iota)}{\partial \eta_i} \cdot \mathbf{R}_\iota^t - 3 \psi C \left( \frac{\partial \mathbf{R}_\iota}{\partial \eta_i} \right) . \tag{92}\]
If \( a_e \) is also small, additional simplifications are possible

\[
P_e = \left( K_0 + \Delta K \sum \phi_K(\eta_i) \right) e_{0e} R_e + 2 \left( \mu_0 + \Delta \mu \sum \phi_\mu(\eta_i) \right) e_e \cdot R_e - \sigma_e \cdot R_e;
\]  
(93)

\[
\eta_j = \frac{L_{ij}}{\rho_0} \left( P_e \cdot \frac{\partial U_0(\theta_0, \eta_j)}{\partial \eta_i} \right)_R + \frac{L_{ij}}{\rho_0} \left( \frac{\partial U_0(\theta_0, \eta_j)}{\partial \eta_i} \right)_R - \frac{\partial \psi^e \eta_j}{\partial \eta_i} R_e - 3\psi^e \eta_j \left( \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} + \frac{\partial \mu_\mu}{\partial \eta_i} \right) - J_1 \frac{\partial \theta^0}{\partial \eta_i} - \frac{\partial \phi^0}{\partial \eta_i} + \nabla_0 \cdot (\beta_\theta \nabla_0 \eta_j)
\]  
(94)

and

\[
\frac{D\eta_j(t, \tau)}{D\tau} = \frac{L_{ij}}{\rho_0} \left( \sigma_e \cdot R_e + \frac{\partial U_0(\theta_0, \eta_j)}{\partial \eta_i} \right)_R - \frac{\partial \psi^e \eta_j}{\partial \eta_i} R_e - 3\psi^e \eta_j \left( \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} + \frac{\partial \mu_\mu}{\partial \eta_i} \right) - \frac{\partial \theta^0}{\partial \eta_i} - \frac{\partial \phi^0}{\partial \eta_i} + \nabla_0 \cdot (\beta_\theta \nabla_0 \eta_j)
\]  
(95)

Finally, when rotations are small (\( R_e \approx I \)), displacements are small, and consequently the difference between deformed and undeformed configurations is negligible, we obtain \( P_e = \sigma_e \) and

\[
\eta_j = \frac{L_{ij}}{\rho_0} \left( \sigma_e \cdot R_e \cdot \frac{\partial U_0(\theta_0, \eta_j)}{\partial \eta_i} \right)_R + \frac{L_{ij}}{\rho_0} \left( \frac{\partial U_0(\theta_0, \eta_j)}{\partial \eta_i} \right)_R - \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| R_e - 3\psi^e \eta_j \left( \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} + \frac{\partial \mu_\mu}{\partial \eta_i} \right) - \frac{\partial \theta^0}{\partial \eta_i} - \frac{\partial \phi^0}{\partial \eta_i} + \nabla_0 \cdot (\beta_\theta \nabla_0 \eta_j) \right|
\]  
(96)

with small strains \( \varepsilon_1 = U_1 - I \) and \( \varepsilon_2 = U_2 - I \). In comparison with the equations obtained within a small strain formulation from the very beginning, we have an additional term \( 3\psi^e \eta_j \left( \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} + \frac{\partial \mu_\mu}{\partial \eta_i} \right) \), which appeared due to formulation of the elasticity rule in the unloaded rather than in the reference configuration. It means that when the transformation and thermal volumetric strains change during PT, elastic energy, like effective pressure, produces the corresponding power that contributes to the driving force for change in \( \eta \). It is comparable to the term \( \frac{\partial \psi^e \eta_j}{\partial \eta_i} \), related to the change in elastic moduli and cannot be ignored even for small strain formulation. Also, starting with large strain formulation, we introduced interface stresses and demonstrated that elastic stresses only affect the Ginzburg–Landau equation.

9. Equation for entropy and temperature evolution

Let us elaborate Eq. (19) for the entropy. Utilizing Eq. (32) for free energy, we obtain

\[
-s = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| + \frac{1}{\rho_0} \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} \frac{\partial \mu_\mu}{\partial \eta_i} + \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} \frac{\partial \mu_\mu}{\partial \eta_i} + \frac{\partial \mu_\theta \eta_j}{\partial \eta_i} \frac{\partial \mu_\mu}{\partial \eta_i}
\]  
(97)

We used that \( \partial F / \partial \eta_i = \partial \psi^e \eta_j / \partial \eta_i = 0 \), because \( F \) is fixed. Next,

\[
\frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i}
\]  
(98)

where the last term is related to temperature-dependent elastic properties of phases. Further,

\[
F = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i}
\]  
(99)

We took into account Eq. (37) for the elastic first Piola–Kirchhoff stress, \( P_e \), multiplicative decomposition Eq. (12), and relationship \( \frac{\partial \psi^e \eta_j}{\partial \eta_i} = -U_1 - \frac{\partial \psi^e \eta_j}{\partial \eta_i} \), which follows from \( \partial(u_0 \cdot U_0) / \partial \eta_i = 0 \). Using the relationship (38) between the elastic first Piola–Kirchhoff and Cauchy stresses and symmetry of the Cauchy stress, one can transform

\[
P_e \cdot U_1 \cdot U_0 - F_e = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i} = \frac{\partial \psi^e \eta_j}{\partial F_e} \frac{\partial F_e}{\partial \eta_i}
\]  
(100)

Substituting these results in Eq. (32) and utilizing Eq. (56) for the gradient energy, we obtain for the entropy

\[
\frac{1}{\rho_0} \frac{\partial U_0}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right|
\]  
(101)

\[
\frac{1}{\rho_0} \frac{\partial U_0}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right| = \frac{\partial \psi^e \eta_j}{\partial \eta_i} \left| F \right|
\]  
(102)

One can see that if parameters \( \beta_\theta \) are temperature dependent, the entropy depends on the gradient of the order parameters. Neither interface stresses nor viscou stresses directly contribute to the expression for entropy, just elastic stresses. This is similar to the situation with the Ginzburg–Landau equations. One can sequentially simplify Eqs. (101) and (102) for small deviatoric and volumetric parts of all strains like we did for the Ginzburg–Landau equations. For the geometrically linear
which is important for the determination of entropy, specific heat, and temperature evolution in
where all derivatives of \( \beta \).

Here, the terms\( \partial \) are excluded with the help of elasticity rule. Substituting this equation in
Eq. (104), defining the specific heat at constant elastic Piola–Kirchhoff stress, \( c_p = \partial s / \partial \theta \), and resolving for the temperature rate, one derives
\[ c_p \dot{\theta} = P_e: F_e + \left( X_i - \frac{\partial s}{\partial \eta_i} \right) \eta_i + r - \rho_0 \partial \theta / \partial \eta_i, \]

where all derivatives of \( s \) can be evaluated utilizing the expression (101). Substituting the Fourier law in the reference
configuration, \( \mathbf{h}_0 = -\Lambda_0 \cdot \nabla \theta / \partial \eta_i \), where \( \Lambda_0 \) is the thermal conductivity tensor in the reference configuration, into Eq. (105), one obtains the temperature evolution equation
\[ c_p \dot{\theta} = P_e: F_e + \left( X_i - \frac{\partial s}{\partial \eta_i} \right) \eta_i + r - \rho_0 \partial \theta / \partial \eta_i, \]

10. Specification of the Helmholtz energy for a single order parameter

All previous results for multiple order parameters can be simplified for a single order parameter just by omitting
subscripts for \( \eta_i, \rho_0 \) and \( L_i \). Here we present a specific \( 2 - 4 - 6 \) polynomial for the Helmholtz free energy with the general structure in Eq. (32):
\[ \psi(f, \eta, \theta, \nabla \eta) = \frac{J_{90}}{\rho_0} \psi^o(f, \eta, \theta, \nabla \eta) + \frac{J_{90}}{\rho_0} \psi^o + \frac{J_{90}}{\rho_0} \psi^\eta (\nabla \eta); \quad \psi^\eta = \frac{\beta}{2\rho_0} |\nabla \psi|^2. \]

When surface stress is neglected, i.e., \( j = 1 \), the thermal part of free energy should reduce to that in Levitas et al. (2003) and Levitas (2013a):
\[ \psi^o + \psi^\eta = f(\theta, \eta) = G^o(\theta) + \Delta G^o(\eta^2) + 0.5A(\eta^2)^2(1 - \eta^2). \]

Here, the terms \( \Delta G^o(\eta^2) + 0.5A(\eta^2)^2(1 - \eta^2)^2 \) are parts of the thermal (chemical) energy \( f(\theta, \eta) \) related to the thermal driving force for PT and double-well barrier, respectively. Function \( G^o(\theta) \) is the thermal part of the free energy of \( A \), which is important for the determination of entropy, specific heat, and temperature evolution in \( A \). However, for our purposes below, we can set \( G^o(\theta) = 0 \) without loss of generality, which is equivalent to operating with an excess energy \( f(\theta, \eta) - G^o(\eta) \). Plots of function \( f \) for different temperatures are shown in Fig. 5. Importance of the proper division of \( f(\theta, \eta) \) into two functions, \( \psi^o \) and \( \psi^\eta \), is related to the fact that \( \psi^o \) contributes to the interface stresses Eq. (48) but \( \psi^\eta \) does not. For a single order parameter and gradient energy in Eqs. (107) and (48) reduces to
\[ \alpha_{st} = \left( \rho_0 \psi^o + \frac{\beta}{2} |\nabla \eta|^2 \right) I - \beta \nabla \eta \otimes \nabla \eta = \rho_0 |\nabla \eta|^2 (I - \kappa \otimes \kappa) + \left( \rho_0 \psi^o - \frac{\beta}{2} |\nabla \eta|^2 \right) I, \quad \kappa = \frac{\nabla \eta}{|\nabla \eta|}. \]

To obtain desired biaxial surface tension, the last term must be equal to zero for the propagating interface, which will be resolved below. For this purpose, we will treat the simplest version of the Ginzburg–Landau equation (96) for neglected stresses and elastic strain and in a small strain approximation reads
\[ \dot{\eta} = \Gamma \left( -\rho_0 \frac{\partial f}{\partial \eta} + \beta \nabla^2 \eta \right), \]

where \( \Gamma = L / \rho_0 \) is the kinetic coefficient. Such a formulation, and even treatment of Ginzburg–Landau equation without
mechanics at all can be strictly justified in a such way. Since our goal is partitioning a function \( f(\theta, \eta) \) of temperature and \( \eta 
only into two parts, if we complete this for a stress–strain free case, including strains or stresses cannot change the result, because \( f(\theta, \eta) \) by definition is independent of strains and stresses.

Note that parameters \( \beta, \A, \text{and} L \) can be calibrated utilizing an analytical solution for interface (like solution presented below) and values of the interface energy, width, and mobility determined experimentally or by atomistic simulations (Levitas et al., 2003, 2010; Monk et al., 2010). The same can be done to multiple order parameters, by considering interfaces between different phases.
11. Explicit expression for free energy and interface stresses

11.1. Stationary interface and arbitrary thermal energy

Following, for example Levitas et al. (2003) and Umantsev (2012), let us simplify Ginzburg–Landau equation (110) for a stationary 1D formulation with a spatial coordinate \( x \)

\[
\frac{df}{d\eta} = \rho_0 \frac{d}{dx} \frac{d\eta}{dx}.
\]

(111)

Note that function \( f \) is arbitrary in this subsection, with \( f(\eta) = 0 \). Since \( \eta \) is function of \( x \), which can be inverted, all functions of \( x \) can be considered functions of \( \eta \) as well. Using designation \( \eta_x = d\eta/dx \), one can transform the right side:

\[
\frac{df}{d\eta} = \frac{d\eta_x}{dx} d\eta_x = \frac{d\eta}{dx} \frac{d\eta_x}{d\eta} \eta_x = 0.5 \frac{d(\eta_x)^2}{d\eta} = \rho_0 \frac{d\psi^V}{d\eta}.
\]

(112)

Substituting Eq. (112) into Eq. (111), we obtain

\[
\frac{df}{d\eta} = \frac{d\psi^V}{d\eta}.
\]

(113)

Eq. (113) can be integrated over \( \eta \):

\[
\rho_0 \psi^V = 0.5 \rho \left( \frac{d\eta}{dx} \right)^2 = \rho_0 (f(\theta, \eta) - f_0),
\]

(114)

where \( f_0 \) is the integration constant. Thus, for any stationary solution, the gradient energy is equal to the excess of the local energy at each point. Let us consider a stationary plane interface, when one has \( A \) as \( x \to -\infty \) and \( M \) as \( x \to \infty \). Then \( d\eta/dx = 0 \) for \( x \to \pm \infty \), and \( f(-\infty) = f(A) = f_0 \) (i.e., \( f_0 = 0 \)) and \( f(\infty) = f(M) = f_0 = 0 \). Since \( f(A) = f(M) = f(1) = \Delta G^\theta = 0 \), then \( A \) and \( M \) are in thermodynamic equilibrium, and \( \theta = \theta_c \) (which is consistent with \( \Delta G^\theta(\theta_c) = 0 \)). Thus, for stationary interface Eq. (114) simplifies to

\[
0.5 \rho \left( \frac{d\eta_m}{dx} \right)^2 = \rho_0 f(\theta_c, \eta).
\]

(115)

Here subscript \( m \) designates that solution \( \eta_m \) is for an interface. To obtain biaxial interface stresses in Eq. (109) for the stationary interface, one has to define for the general case (i.e. for arbitrary distribution of \( \eta \)):

\[
\psi^\theta = \psi^V - \frac{\beta}{2 \rho_0} (\nabla \eta_m)^2 = f(\theta_c, \eta).
\]

(116)

Then for an interface, the last term in Eq. (109) disappears and surface stress represents biaxial tension within interface. Also,

\[
\psi^\theta = f(\theta, \eta) - f(\theta_c, \eta).
\]

(117)

The magnitude of the biaxial interface tension in Eq. (109) is equal to \( 2 \rho_0 \psi^V = 2 \rho_0 f(\theta_c, \eta) = \rho_0 \psi^V + \rho_0 f(\theta_c, \eta) \), i.e., to the total equilibrium energy at each point. Integrating it over the \( x \), we obtain that the magnitude of the force per unit interface length is equal to the equilibrium interface energy \( \gamma_c \), as required.

This is a general result, which is independent of specific expression for \( f(\theta, \eta) \), provided that it allows a stationary interface solution. Generally, one can present

\[
f(\theta, \eta) = \Delta G^\theta(\theta) f_d(\theta, \eta) + A(\theta) f_b(\theta, \eta),
\]

(118)

where \( f_d \) and \( f_b \) are parts of \( f \) describing the driving force and double well barrier respectively. They satisfy the following relationships:

\[
f_d(\theta, 0) = f_b(\theta, 0) = f_b(\theta, 1) = 0; \quad f_d(\theta, 1) = 1; \quad \frac{df_d(\theta, 0)}{d\eta} = \frac{df_d(\theta, 1)}{d\eta} = \frac{df_b(\theta, 0)}{d\eta} = \frac{df_b(\theta, 1)}{d\eta} = 0,
\]

(119)

which follow from the properties of \( f(\theta, \eta) \) (Levitas and Preston, 2002a) and the meaning of a double well function. According to Eqs. (116) and (117)

\[
\psi^\theta = A(\theta_c) f_b(\theta, \eta); \quad \psi^\theta = \Delta G^\theta(\theta) f_d(\theta, \eta) + A(\theta_c) f_b(\theta, \eta) - A(\theta_c) f_b(\theta, \eta),
\]

(120)

Since \( f_d(\theta, \eta) \) is localized at the diffuse interface (i.e., equal to zero outside of an interface), the same is true for \( \psi^\theta \), as required.

While the advantage of the above equations is that they do not require the knowledge of a specific function \( f(\theta, 0) \), they are limited to the equilibrium interface only.
11.2. Propagating interface

The solution to the Ginzburg–Landau equation (110) for the specific function \( f \) in Eq. (108) for the nonequilibrium plane interface moving in an infinite parallelepiped in the x-direction is (Levitas et al., 2010; Levitas, 2014):

\[
\eta_{in} = (1 + e^{-\zeta})^{-0.5}
\]

with

\[
\zeta = k(x - ct); \quad k = 2\sqrt{\frac{\rho_0(A(\theta) - 4\Delta G^0(\theta))}{\beta}}; \quad c = \frac{8\pi\rho_0\Delta G^0(\theta)}{k}.
\]

(121)

where \( k \) is inversely proportional to the interface width (see below) and \( c \) is the interface velocity. The most important property of solution (Eq. (121)) for us is

\[
\frac{\partial \eta_{in}}{\partial \zeta} = 0.5\eta_{in}(1 - \eta_{in}^2).
\]

(122)

Using it and the definition of \( k \) in Eq. (121), we obtain a key relationship for points of a propagating interface:

\[
\psi^\eta = \frac{A}{2\rho_0} \psi_u = \frac{\partial}{\partial \zeta} = \frac{1}{2} \frac{\partial}{\partial \zeta} = \begin{pmatrix} 0.5(\theta - 4\Delta G^0(\theta)) \eta_{in}^2(1 - \eta_{in}^2)^2 \end{pmatrix}.
\]

(123)

For phase equilibrium \((\Delta G^0(\theta) = 0)\), this relationship reduces to Eq. (115), which gave us a hint on how to find Eq. (122). To obtain biaxial interface stress in Eq. (109) for the propagating interface, one has to define for the general case (i.e. for arbitrary distribution of \( \eta \) rather than for \( \eta_{in} \)):

\[
\psi^\eta = \psi_u = \frac{1}{2} \frac{\partial \psi_u}{\partial \zeta} = \theta(\theta - 4\Delta G^0(\theta)) \eta_{in}^2(1 - \eta_{in}^2)^2.
\]

(124)

where Eq. (123) was used. It is clear that \( \psi^\eta \) is localized at the diffuse interface, as required. Then,

\[
\psi^\eta = f(\theta, \eta) = \psi_u = \Delta G^0(\theta) \eta_{in}^2(2 - \eta^2).
\]

(125)

Substituting Eq. (124) in the general expression for the interface stress (109), we obtain for propagating interface

\[
\sigma_{zz} = \eta |\nabla| \psi_u^2(I - k \otimes k) \sigma_{zz} = 2\rho_0 \psi_u^2(I - k \otimes k) = \sigma_{zz} = \eta |\nabla| \psi_u^2(I - k \otimes k).
\]

(126)

Still, it is necessary to check whether the magnitude of the force per unit interface length due to \( \sigma_{zz} \) is equal to the interface energy \( \gamma \).

12. Nonequilibrium interface energy: general expression

By definition of the interface energy under nonequilibrium condition (see, e.g., Gibbs, 1948; Kaplan et al., 2013; Levitas and Samani, 2011a; Levitas, 2014), it is equal to the excess energy with respect to austenite in the austenitic region \( \xi \leq \xi_{ds} \) and with respect to martensite in the martensitic region \( \xi > \xi_{ds} \):

\[
\gamma = \int_{-\infty}^{\xi_{ds}} \rho_0(\psi_{\text{A}} - \psi_u) d\xi + \int_{\xi_{ds}}^{\infty} \rho_0(\psi_{\text{M}} - \psi_u) d\xi.
\]

(127)

where \( \xi_{ds} = \xi/k \) moves together with the interface with velocity \( c \), \( \xi_{ds} \) is the sharp interface or Gibbsian dividing surface position (Fig. 3). All results in Levitas, (2013a,b) for a 2–3–4 polynomial have been obtained under assumption that \( \eta(\xi_{ds}) = 0.5 \), because a 2–3–4 polynomial is completely symmetric with respect to the exchange of A and M. However, this assumption does not allow us to receive the desired result for the current model; that is why we will keep \( \gamma = \eta(\xi_{ds}) \) as an arbitrary parameter and decide its value later. Setting \( \psi_{\text{A}} = 0, \psi_{\text{M}} = \Delta G^0(\theta) \), we obtain

\[
\gamma = \frac{\rho_0}{k} \int_{-\infty}^{\xi_{ds}} \frac{d\xi}{\Delta G^0} \psi_u^2 + \frac{\rho_0}{2k} \int_{\xi_{ds}}^{\infty} \left( \theta - \Delta G^0 \right) \psi_u^2 + \frac{\rho_0}{2} \int_{\xi_{ds}}^{\infty} \frac{d\xi}{\Delta G^0} \psi_u^2 + \int_{\xi_{ds}}^{\infty} \eta(3 - 2\eta^2) d\xi + \int_{\xi_{ds}}^{\infty} \eta(3 - 2\eta^2 - 1) d\xi.
\]

(128)

Utilizing Eq. (122), we evaluate

\[
\int_{-\infty}^{\infty} \eta^2(1 - \eta^2)^2 d\xi = 2 \int_0^1 \eta(1 - \eta^2) d\eta = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\xi}{\Delta G^0} \psi_u^2 = \frac{1}{2} \int_0^1 \eta(1 - \eta^2) d\eta = \frac{1}{8}
\]

\[
\int_{\xi_{ds}}^{\infty} \eta^4(3 - 2\eta^2)d\eta + \int_{\xi_{ds}}^{\infty} (\eta^4(3 - 2\eta^2) - 1) d\xi = 2 \int_0^{\eta_{ds}} \eta^3(3 - 2\eta^2) d\eta + 2 \int_{\eta_{ds}}^1 \eta^4(3 - 2\eta^2 - 1) d\eta = \ln \left( \frac{\eta^2}{1 - \eta^2} \right) = -1 + Z(\eta); \quad \eta = 1 + \ln \left( \frac{\eta^2}{1 - \eta^2} \right).
\]

(129)
The necessity of introducing function $Z$ will be clear shortly. Let us first evaluate the gradient energy contribution to the total interface energy, using Eq. (121) for $k$:

$$\psi^\gamma = \int_{-\infty}^{\infty} \rho_0 \psi^\gamma \, dx = \frac{k \beta}{2} \int_{-\infty}^{\infty} \left( \frac{d\eta}{d^2} \right)^2 \, dx = \frac{k \beta}{16} \sqrt{\beta \rho_0 (A(\theta) - 4\Delta G^e(\theta))}$$

(131)

The local interface energy according to Eqs. (128)–(130) and (121) for $k$ is

$$\psi^l = \frac{A \rho_0}{4k} - \frac{\rho_0 \Delta G^e}{k} (1 - Z) = \frac{\rho_0 (A - 4\Delta G^e)}{4k} + \frac{Z \rho_0 \Delta G^e}{k} = \frac{\sqrt{\beta \rho_0 (A(\theta) - 4\Delta G^e(\theta))}}{2k} + \frac{Z \rho_0 \Delta G^e}{k}.$$  

(132)

If $Z = 0$, then the local and gradient contributions to the interface energy are equal for the nonequilibrium interface, which was the case for the model in Levitas (2013a,b) for $\eta = 0.5$. Here,

$$Z = \ln \left( \frac{\eta^2}{1 - \eta^2} \right) = 0 \Rightarrow \eta = \frac{1}{\sqrt{1 + e^2}} = 0.5186,$$

where $e = 2.71828$ is Euler’s number. Thus, the value of $\eta$ is very close to 0.5 and can be considered as a reasonable definition of the interface position. For such a definition, the total interface energy is

$$\gamma = \psi^l + \psi^\gamma = 2\psi^l = 2\psi^\gamma = \frac{k \beta}{8} = \frac{\rho_0 (A - 4\Delta G^e)}{2k} = \frac{\sqrt{\beta \rho_0 (A(\theta) - 4\Delta G^e(\theta))}}{4}$$

(134)

Finally, we can prove that the magnitude of the force $T$ per unit interface length is equal to the nonequilibrium interface energy $\gamma$:

$$T = \int_{-\infty}^{\infty} \sigma_{\eta \eta} \, dx = \int_{-\infty}^{\infty} \beta |\nabla \eta|^2 \, dx = 2 \int_{-\infty}^{\infty} \rho_0 \psi^\gamma \, dx = 2\psi^\gamma = 2\psi^l = \gamma,$$

(135)

where Eqs. (126), (131) and (134) have been used. This completes the proof that the expression (109) for the interface stress for nonequilibrium propagating interface transforms to the desired Eq. (1) for the sharp interface limit. Note that for $Z \neq 0$, the force per unit length cannot be made equal to the interface energy. Thus $Z=0$ follows from the fundamental principle of statics, namely equivalence of the resultant force $T$ applied to the diffuse interface and force $\gamma$ applied to the sharp interface. This point will be further discussed in Section 13.

Thus, by introducing the free energy dependent on the gradient of the order parameters in the deformed (rather than reference) state and multiplying the gradient energy and the function $\psi$ determined by Eq. (124) by the Jacobian $J$, we introduced in Eq. (109) an additional contribution to the Cauchy stress tensor, $\sigma_{\eta \eta}$. It is called the surface stress tensor or the structural interface stress tensor, which is located at the diffuse interface (0 $\leq \eta \leq 1$) and is zero in bulk. For a nonequilibrium plane interface, the expression for surface stress reduces to biaxial tension (Eq. (126)), like for a sharp-interface approach. The force per unit area can be made equal to the surface energy $\gamma$ by a reasonable choice of the sharp interface (dividing surface) position. In fact, this also resolves long-standing problem of the definition of position of the dividing surface.

For the equilibrium interface, the choice of $\eta$ is irrelevant and substituting $\Delta G^e = 0$ in Eqs. (123) and (134), we obtain

$$\psi^\gamma = \frac{\beta}{2\rho_0} |\nabla \eta|^2 = 0.5 A(\theta_e) \eta^2_n (1 - \eta^2_n)^2; \quad \psi_{eq} = 2\psi^\gamma = A(\theta_e) \eta^2_n (1 - \eta^2_n)^2.$$  

(136)

and

$$\gamma_{eq} = 2\psi^\gamma = 2\psi_{eq} = \frac{\sqrt{\beta \rho_0 A(\theta_e)}}{4},$$

(137)

which are the known relationships (see, e.g., Levitas et al., 2003).

13. Position of the Gibbsian dividing surface for a nonequilibrium interface

**Principle of static equivalence:** We found in Eq. (133) the position of the dividing surface from the condition that the magnitude of surface stresses is equal to the interface energy. However, finding the position of the dividing surface was an unsolved fundamental problem in the interface and surface science, because an excess of any properties at the interface depends on the choice of $\delta_0$. Because it was not defined in Gibbs (1948) and later works, alternative definitions of the excess properties, which do not involve the dividing surface, were suggested for different purposes (Gibbs, 1948; Cahn, 1979; Kaplan et al., 2013; Frolov and Mishin, 2012; Sutton and Balluffi, 1995; Schimmele et al., 2007; Cammarata, 2009; Fischer et al., 2008; Umantsev, 2012). For example, interface energy is defined as a reversible work to create the interface. This does not resolve the problem because ambiguity in some other definitions still exists, see Gibbs (1948), Cahn (1979), Kaplan et al. (2013), Frolov and Mishin (2012), Sutton and Balluffi (1995), Schimmele et al. (2007), Cammarata (2009) and Fischer et al. (2008). Also, there is no direct connection between the distribution of properties for a finite-width interface and the interface excess properties, which is required, in particular, in the phase field approach to introduce proper interface stresses. Below, we solve this long-standing fundamental problem by utilizing the principle of static equivalence of two systems of forces: finite-width interface with distributed tensile stresses is statically equivalent to the sharp interface.
(dividing surface) with a single force and a couple if they possess the same resultant force and the same moment about any chosen point (Beer et al., 2006). For a sharp interface, the moment about position of the dividing surface is zero, which produces the equation to determine the position of the dividing surface. This is a general approach, which is independent of the method that is used to determine distribution $\sigma_{st}(\zeta)$, e.g., phase field or molecular dynamics or experiments (see also Levitas, 2014).

Thus, distributed interface stresses $\sigma_{st}(\zeta)$ in Fig. 4 are equivalent to the resultant force per unit interface length and moment about any chosen point $0$

$$T := \int_{-\infty}^{\infty} \sigma_{st} \, d\zeta; \quad M_{ds} := \int_{-\infty}^{\infty} (\zeta - \zeta_0) \sigma_{st}(\zeta) \, d\zeta. \quad (138)$$

**Interfaces that do not support elastic stresses:** Since we consider part of the interface stresses that are typical for a liquid–liquid or liquid–gas interface, let us focus on such interfaces. Then for a sharp interface, $T = \gamma$, which, as we have seen above, already allows one to determine the dividing surface. Also, for a sharp interface, the moment with respect to the position of the dividing surface $\zeta_{ds}$, $M_{ds} = 0$, because neither interface nor liquid or gas phases support moments. Thus, we obtain two conditions to determine position of the dividing surface:

$$T := \int_{-\infty}^{\infty} \sigma_{st} \, d\zeta = \gamma; \quad (139)$$

$$M_{ds} := \int_{-\infty}^{\infty} (\zeta - \zeta_{ds}) \sigma_{st}(\zeta) \, d\zeta = 0. \quad (140)$$

It is remarkable that for more than a century, there was not any condition to determine the position of the dividing surface; in the paper, we derived even two conditions, which may be potentially inconsistent with each other. In geometric interpretation, Eq. (140) means that the dividing surface passes through the centroid of the area below the $\sigma_{st}(\zeta)$ curve (Beer et al., 2006). If function $\sigma_{st}(\zeta)$ is symmetric with respect to axes passing through some point, then the dividing surface passes through this point. This was the case for the $2 - 3 - 4$ potential in Levitas (2013b) and our assumption that the dividing surface corresponds to $\eta = 0.5$ was correct.

While Eq. (139) was always utilized in some form, we are not aware that it was applied to determine the position of the dividing surface for a nonequilibrium interface. To our knowledge, Eq. (140) was never applied before. For a sharp interface the couple was not introduced in most of the works (see Gibbs, 1948; Cahn, 1979; Kaplan et al., 2013; Frolov and Mishin, 2012; Sutton and Balluffi, 1995; Schimmele et al., 2007; Cammarata, 2009; Fischer et al., 2008), which means that it is zero. Surprisingly, this condition was not used to determine the position of the dividing surface. Thus, the missing principle to determine position of the Gibbs dividing surface is found utilizing undergraduate statics.

To apply this approach for our specific model and to check whether the two Eqs. (139) and (140) lead to noncontradictory results, we present interface profile Eq. (121) as

$$\eta_{in} = (1 + e^{-kx + \ln 3})^{-0.5}. \quad (141)$$

Since the interface profile is the same for any $t$, we fixed time in a way that provides $\eta_{in} = 0.5$ for $x = 0$. Then substituting Eq. (161) into Eqs. (124) for $\sigma_{st} = 2\rho_0 \psi^0$ and substituting $\sigma_{st}$ into Eq. (138) with $x_o = 0$, we obtain moment with respect to a point corresponding to $\eta_{in} = 0.5$:

$$M_0 = \int_{-\infty}^{\infty} x \sigma_{st} \, dx = \frac{\rho_0 (A - 4\Delta C_i^3)}{2k^2} (\ln 3 - 1) = \frac{T}{k} (\ln 3 - 1). \quad (142)$$
where \( T = \rho_d(A - 4\Delta G^0)/2k \) was determined by substituting the same equation in Eq. (138)\textsubscript{1}. This is the same expression for \( T \) as for \( \gamma \) in Eq. (134), but since we did not define \( x_{st} \), yet, we do not identify \( T \) with \( \gamma \). Moment about any point \( x=b \) is

\[
M_{b} = \int_{-\infty}^{\infty} (x-b)\sigma_{st} \, dx = M_0 - bT. \tag{143}
\]

Zero moment \( M_{b}=0 \) corresponds to \( b = (\ln 3 - 1)/k \). Substituting \( x \) with \( x-b \) in the interface profile equation (Eq. (161)), we find

\[
\eta_{in} = (1 + e^{-k(x-b)} + \ln 3) - 0.5 = (1 + e^{-kx+1}) - 0.5. \tag{144}
\]

Then the position of the dividing surface coincides with \( x=0 \) and

\[
\eta_{in}(0) = (1 + e)^{-0.5} = \eta = 0.5186. \tag{145}
\]

This is exactly the value that we found in Eq. (132) from the condition that \( T = \gamma \). Thus, for the model under study, both conditions of static equivalency, Eqs. (139) and (140), results in the same position of the dividing surface. This demonstrates self-consistency of the developed theory. Only for such a position of the sharp interface the gradient and local contributions to the interface energy are the same. Note that for curved interface, the found position of the dividing surface and expression for the interface energy are also consistent with the expression for the velocity of the curved sharp interface (Levitas, 2014).

**Interfaces that support elastic stresses:** We would like to stress that the principle of static equivalence is the fundamental principle of mechanics (and consequently, physics) and its application is not optional. It must not be violated, and it is very surprising that it was completely neglected in the interface and surface science. One of the probable reasons is that because specific stress distributions across the interface became available only recently, they were considered mostly for equilibrium interfaces in the phase field approach (Lowengrub and Truskinovsky, 1998; Wheeler and McFadden, 1997; Anderson et al., 2001; Levitas and Javanbakht, 2010, 2011a; Levitas and Samani, 2011a,b) or in the molecular dynamics study in Frolov and Mishin (2010a). In this case the position of the dividing surface is not important. Only in Levitas (2013a,b) condition (139) was applied for stress distribution across the moving interface. However, due to symmetry of potential and stress distribution, the guess \( \eta = 0.5 \) was made and it allowed us to satisfy condition (139). We are not aware that the moment of stress distribution was calculated previously.

Thus, with elastic stresses, or for any more general case, Eqs. (138) are valid as well. If interface stresses are anisotropic, i.e., depend on \( k \) and direction within an interface, Eqs. (138) are valid for any direction. However, with elastic interface stresses, \( T \neq \gamma \), so this condition should not be satisfied and cannot be used for the determination of the dividing surface. In most works on the sharp interface approach (Gibbs, 1948; Cahn, 1979; Kaplan et al., 2013; Frolov and Mishin, 2012; Sutton and Balluffi, 1995; Schimmele et al., 2007; Fischer et al., 2008; Frolov and Mishin, 2010a), the bending moments (stress couples) were not introduced. This can be interpreted as the condition \( M_{st} = 0 \) is imposed. This condition applied to the sum of all type of interface stresses can be used to determine the position of the dividing surface. This new dividing surface can be used to determine total interface energy, including elastic energy. However, while for an interface without elastic stresses one needs position of the dividing surface in the course of the development of the theory in order to introduce interface stresses that satisfy condition \( T = \gamma \), with elastic stresses it is mostly for post-processing. The position of the dividing surface obtained from the condition \( M_{st} = 0 \) varies when stress state varies and when elastic stresses tend to zero, it tends to one corresponding to \( \eta = 0.5186 \). Thus, for solid–solid, solid–liquid, and solid–gas interfaces, our above procedure to introduce interface stresses \( \sigma_{st} \) is applicable and should not be changed. As we discussed, elastic contribution to the interface stresses is determined by solution of the boundary-value problem and does not require further elaboration.

However, results of solution of the phase field equations can be utilized for the development of the constitutive equations for the sharp interface model. If the dividing surface determined from the condition \( M_{st} = 0 \) is located outside of an interface or significantly shifted from the point with \( \eta = 0.5 \) (see such examples for stresses at solid–melt interface in Frolov and Mishin (2010a)), this is the sign that one must introduce couples in the sharp interface theory. Formal theories for interfaces with couple stresses are developed in Podstrigach and Povstenko (1985) and Povstenko (1991). Couple stresses may be necessary for a large transformation strain that varies across an interface from zero in austenite to the finite value in the martensite, which causes bending of a finite-width interface. In addition, for an anisotropic interface and unequal normal stresses in two principle directions (see Frolov and Mishin, 2016a), the dividing surface determined from the condition \( M_{st} = 0 \) for one of the principle directions may not in general coincide with that for another direction. Thus, any of them can be chosen as the dividing surface, and a couple for another direction should be incorporated in the sharp-interface model. However, this topic is outside of the current paper.

**14. Energy, width, entropy excess, and stresses for a nonequilibrium interface: parametric study**

We will follow as close as possible the similar treatment for the \( 2-3-4 \) potential in Levitas (2013b) and will mention differences.

**Energy and entropy excess:** It is usually assumed for any polynomial (Levitas and Preston, 2002a; Levitas et al., 2003)

\[
A = A_0(\theta - \theta_c), \quad A_0 > 0; \quad \Delta G^0(\theta) = -\Delta S_0(\theta - \theta_c), \quad \Delta S_0 < 0. \tag{146}
\]
where \( \theta_c \) is the critical temperature at which stress-free \( \Lambda \) loses its thermodynamic stability and \( \Delta s_0 \) is the difference in entropy between martensite and austenite at \( \theta = \theta_c \). Below we will use dimensionless temperature, \( \bar{\theta} \), parameter \( \sigma \), their combination, \( \gamma \), and parameter \( \tilde{A} \) defined by equations

\[
\bar{\theta} = \frac{\theta - \theta_c}{\theta_e - \theta_c}; \quad \sigma = -\frac{4\Delta s_0}{A_0} > 2/3; \quad \gamma = \bar{\theta}(1-\sigma) + 1 \geq 0; \quad \tilde{A} = A_0(\theta_e - \theta_c).
\]

(147)

While \( \bar{\theta} \) and \( \gamma \) are the same as in Levitas (2013b), \( \sigma \) and \( \tilde{A} \) have different numerical factors. Dimensionless local thermal energy,

\[
\tilde{f} = \frac{2\rho_0 f(\theta, \eta)}{A} = 0.5\sigma \eta^4 (3 - 2\eta^2) + (1+\bar{\theta})\eta^2 (1-\eta^2)^2,
\]

(148)
is plotted in Fig. 5 for \( \sigma = 1 \) and several temperatures \( \bar{\theta} \).

The expression (134) for the interface energy takes the form

\[
\gamma = \frac{\tilde{A}Y}{2k} = \sqrt{\bar{\theta}(\theta)\rho_0 A_0(\theta - \theta_e)(1-\sigma) + (\theta_e - \theta_c)} \frac{1.5\sigma(\theta_e - \theta_c)}{1 - 1.5\sigma}.
\]

(149)

Then the obvious inequalities \( \theta_{\text{M}} > \theta_e > \theta_c \) imply \( \sigma > 2/3 \). The critical temperatures in dimensionless form are

\[
\bar{\theta}_c = -1; \quad \bar{\theta}_{\text{M}} = \frac{1}{1.5\sigma - 1}.
\]

(150)

The expression (134) for the interface energy takes the form

\[
\gamma = \frac{\tilde{A}Y}{2k} = \sqrt{\bar{\theta}(\theta)\rho_0 A_0(\theta - \theta_e)(1-\sigma) + (\theta_e - \theta_c)} \frac{1.5\sigma(\theta_e - \theta_c)}{1 - 1.5\sigma}.
\]

(151)
The solution for a propagating interface exists and \( \gamma \) is a real number when \( \bar{\theta}(1-\sigma) + 1 \geq 0 \), i.e.,

\[
\bar{\theta} \geq \frac{1}{\sigma - 1} \quad \text{for} \quad \sigma < 1; \quad \bar{\theta} \leq \frac{1}{\sigma - 1} \quad \text{for} \quad \sigma > 1,
\]

(152)

with no limitations for \( \sigma = 1 \). Excess of an interface entropy is calculated below for \( \beta = \text{const} \):

\[
s_i = \frac{\partial S}{\partial \theta} = \frac{\sqrt{\bar{\theta}(\theta)\rho_0 A_0}}{8\sqrt{\theta_e - \theta_c}} \frac{\sigma - 1}{\sqrt{\bar{\theta}(1-\sigma) + 1}}.
\]

(153)

The dimensionless interface energy and excess entropy are defined as

\[
\gamma_i = 4\gamma / \sqrt{\bar{\theta}(\theta)\tilde{A}} = \sqrt{\bar{\theta}(1-\sigma) + 1} = \sqrt{Y}.
\]

(154)

\[
S_i = \frac{8S}{\sqrt{\theta_e - \theta_c}} = \frac{8S}{\sqrt{\theta_e - \theta_c}} \frac{\sigma - 1}{\sqrt{\bar{\theta}(1-\sigma) + 1}}.
\]

(155)

For the particular case \( \sigma = 1 \), the temperature-dependence of the interface energy is determined by \( \beta(\theta) \). If \( \beta \) is temperature-independent, the interface energy is temperature-independent resulting in zero interfacial entropy excess. It follows from Eq. (149) that for \( \sigma = 1 \) one has \( \theta_e = (2\theta_e + \theta_c) / 3 \). For the \( 2 - 3 - 4 \) polynomial, the temperature independent interface energy (for \( \beta(\theta) = \text{const} \)) corresponded to \( \theta_e = 0.5(\theta_e + \bar{\theta}_c) \) (Levitas, 2013b). Note that analysis of the dependence of \( \gamma \) and \( s_i \) versus \( \bar{\theta} \)
for various values of $m$ and versus $n$ for various values of $C$ and the corresponding plots coincide with those for the $2-3-4$ potential in Levitas (2013b) and will not be presented here. We just mention that the solution for a propagating interface exists even for $\theta > \theta_c$ (i.e., for $C > 1/(2m - 1)$) and for $\theta < \theta_c$ (i.e., $C < -1$), i.e., outside the temperature range, for which both phases have local minima, provided that $\gamma \geq 0$. However, homogeneous nucleation competes in this case with the interface propagation, as it was obtained numerically in Hwang and Levitas (2013) and Levitas and Samani (2011a,b).

**Interface width:** According to the definition Eq. (121) or the relationship to the interface energy Eq. (134), parameter $k$ is defined as

$$k = \frac{8y}{9} = 2 \sqrt{\frac{\rho_0 A_0 ((\theta - \theta_c)(1 - m) + (\theta_c - \theta_c))}{\beta(\theta)}} = 2 \sqrt{\frac{\hat{A} (1 - m) + 1}{\beta(\theta)}} \tag{156}$$

Then the diffuse interface width at arbitrary and equilibrium temperature is defined as

$$\hat{\delta} = \frac{10}{k} = 5 \sqrt{\frac{\beta(\theta)}{\hat{A} (1 - m) + 1}} \cdot \delta(\theta_c) = 5 \sqrt{\frac{\hat{A}(\theta_c)}{\hat{A}}} \tag{157}$$

The factor of 10 is an approximate width of the diffuse interface $\eta_m(\zeta)$ in terms of $\zeta$ in Eq. (121). There are various alternative definitions of the interface width, which gives a factor different from 10 (Levitas et al., 2003, 2010; Anderson et al., 2001; Svoboda et al., 2012; Levitas and Samani, 2011a).

With the same definition, the expression for $\delta$ here differs by a numerical factor from the corresponding expression for the $2-3-4$ potential in Levitas (2013b). The dimensionless width $\tilde{\delta}$ of the interface normalized by $\delta_c$ is

$$\frac{\delta(\theta)}{\delta(\theta_c)} = \frac{k(\theta)}{k(\theta_c)} = \sqrt{\frac{\beta(\theta)}{\beta(\theta_c)(1 - m) + 1}} = \sqrt{\frac{\hat{A}(\theta)}{\hat{A}(\theta_c)}} \tag{158}$$

or, alternatively

$$\tilde{\delta} = \delta_c \sqrt{\frac{\beta(\theta)}{\beta(\theta_c)}} = 1/\sqrt{\gamma} = 1/\gamma \tag{159}$$

In dimensionless form, the interface width coincides with the corresponding expression for the $2-3-4$ polynomial and the corresponding plots can be found in Levitas (2013b). While $\delta \to \infty$ for $\gamma \to 0$ and $\gamma \to \infty$ for $\delta \to 0$, their product $\gamma\delta = 1$ is finite.

**Interface stress:** The magnitude of the biaxial interface stresses is

$$\sigma_{st} = 2\rho_0 \psi^\beta = \rho_0 A_0 ((\theta - \theta_c)(1 - m) + (\theta_c - \theta_c)) \eta_0^2 (1 - \eta_0^2)^2 = \hat{A} \eta_0^2 (1 - \eta_0^2)^2 \tag{160}$$

Since the interface profile is the same for any $t$, we can fix time arbitrarily. For the comparison with the stresses for the $2-3-4$ potential in Levitas (2013b), we will utilize Eq. (161) and present

$$e^{-\zeta} = e^{-\lambda x + \ln 3} = e^{-10y/\bar{\delta} + \ln 3} = e^{-10y/\bar{\delta} + \ln 3} = e^{-10y/\bar{\delta} + \ln 3} = 3e^{-10y/\bar{\delta}}; \quad y = \frac{X}{\sigma e} \tag{161}$$

where the dimensionless coordinate $y$ is introduced in which the interface width $\zeta = 1$ at $\theta = \theta_c$. Shift of the interface profile by $\ln 3$ provides that $\eta = 0.5$ for $x = 0$, which is the position of the dividing surface for the $2-3-4$ potential in Levitas (2013b). For such a choice, the distribution of the surface stress is

$$\sigma_{st} = \hat{A} \eta_0^2 \frac{9e^{-20y/\bar{\delta}}}{(1 + 3e^{-10y/\bar{\delta}})^2} = \frac{\hat{A} \beta(\theta)}{\beta(\theta_c)} \frac{9e^{-20y/\bar{\delta}}}{(1 + 3e^{-10y/\bar{\delta}})^2} \tag{162}$$

where Eqs. (121) and (158) have been used. Then one can introduce dimensionless surface stresses that can be presented solely in terms of the dimensionless interface width $\tilde{\delta}$:

$$\sigma_{st} = \frac{\sigma_{st}(\theta_c)}{\hat{A}(\theta_c)} \frac{1}{\delta_c^2} \frac{9e^{-20y/\bar{\delta}}}{(1 + 3e^{-10y/\bar{\delta}})^2} \tag{163}$$

A plot of $\sigma_{st}(y)$ for several dimensionless interface widths $\tilde{\delta}$ is presented in Fig. 6a. The maximum dimensionless surface stresses is $4/27^2 \gamma$ at $y = \ln(3/2)/10$, which corresponds to $\eta = 1/\sqrt{3} = 0.577$. For comparison, for the $2-3-4$ potential, the maximum dimensionless surface stresses are $3/16^2 \gamma$ at $y = 0$, corresponding to $\eta = 0.5$ (Levitas, 2013b). Note that we increased the value for stresses for the $2-3-4$ potential from Levitas (2013b) by a factor of 3, in order to compare for the same total force per unit interface length, i.e., $\gamma$.

In Fig. 6b, plots of the interface profile $\eta(y)/7$ and $\sigma_{st}(y)$ for $\tilde{\delta} = 1$ are superposed for both $2-4-6$ and $2-3-4$ potentials. This allows us to analyze how stresses are distributed with respect to the interface and to compare results for two potentials. While for the $2-3-4$ potential the order parameter and stresses are symmetric with respect to $y = 0$, asymmetry in $\eta(y)$ for the $2-4-6$ potential causes asymmetry in interface stresses. This leads to a shift of the dividing surface from $\tau = 0.5$ ($y = 0$) to $\tau = 0.5186$ ($y = 0.1755$). Stress distribution for the $2-4-6$ potential is less localized and has smaller magnitude than for the $2-3-4$ potential (for the same $\gamma$). The relative configuration of $\eta(y)/(75)^2$ and $\sigma_{st}(y)$ is like in Fig. 6b for any $\gamma$.

If one substitutes the interface profile $\eta = (1 + e^{-10y/\bar{\delta} + 1})^{0.5}$ into Eq. (148) for $\bar{f}$, one can plot the distribution of the local energy across an interface (Fig. 7a). According to Eq. (124), the dimensionless gradient energy for propagating interface can
be presented in the form
\[
\psi = 2\rho_0 \psi \sim A \left( \frac{\theta}{C_0} + \frac{1}{C_0/C_1} \right) \eta^2 (1-\eta^2). \tag{164}
\]

A plot of the distribution of the total energy across an interface is shown in Fig. 7b for $\varpi = 1$. Since for $\varpi = 1$ the gradient energy is temperature independent, it adds the same contribution to all curves in Fig. 7a. The distribution of the gradient energy coincides with the distribution of the local energy in Fig. 7a for the equilibrium temperature $\theta = 0$ (dashed line). Since for $\varpi = 1$ the interface energy $\gamma$ is also temperature independent, the total dimensionless excess energy for all curves in Fig. 7b is the same and is equal to the area below the dashed curve for $\theta = 0$.

We would like to mention that for a finite sample with a stress-free surface, since the total traction is zero, the corresponding component of the elastic stresses at the intersection of the interface and external surface is equal to the negative component of the surface stress (Levitas and Javanbakht, 2010, 2011a).

15. Interface stresses for critical martensitic nucleus

Let us consider a critical martensitic nucleus within an austenitic matrix, which exists for $\theta \leq \theta_c$, with the boundary conditions $\eta_c(\pm \infty) = 0$ (Levitas et al., 2003). Since $d\eta_c/dx(\pm \infty) = 0$ and $f(\theta, 0) = 0$, substituting the boundary condition in Eq. (114) results in $f_0 = 0$. Then from Eq. (114), one obtains for each nucleus point
\[
\psi = f(\theta, \eta_c). \quad \psi(\theta, \eta_c) = \psi^\sim + f(\theta, \eta_c) = 2\psi^\sim = 2f(\theta, \eta_c). \tag{165}
\]
Substituting Eq. (165) into the general expression for the interface stress Eq. (109), one derives
\[
\sigma_{st} = \rho_0 \psi(\theta, \eta_c)(I - k \otimes k) - \rho_0 \psi^0 (\theta, \eta_c) I
\]
(166)
or in a more explicit form for the dimensionless magnitude of the biaxial tension and the tensile mean stress (negative pressure)
\[
\bar{\sigma}_{st} = \sigma_{st}/\bar{A} = 0.5 \bar{m} \bar{\eta}_c(3 - 2 \bar{\eta}_c^2) + (\bar{\eta} + 1) \bar{\eta}_c^2(1 - \bar{\eta}_c^2)^2 > 0;
\]
(167)
\[
p = - 4 \rho_0 \psi^0 /\bar{A} = - \bar{m} \bar{\eta}_c^2(2 - \bar{\eta}_c^2) > 0.
\]
(168)

Consequently, for a critical martensitic nucleus, the magnitude of the tensile biaxial interface tension is equal at each point to the local total free energy per unit volume \(\rho_0 \psi(\theta, \eta_c)\); i.e., it is positive (tensile). Thus, the total interface force is also equal to the total free energy of a critical nucleus. In addition, the tensile mean stress (negative pressure) \(\rho_0 \psi^0 > 0\) is applied to each point of a nucleus. The solution to Eq. (165) is (Levitas et al., 2003):
\[
\eta_c = 2 \left[4 - p + \sqrt{p^2 - 8p/3 \cosh(20 \sqrt{\bar{\theta} + 1} X)} \right]^{-1/2}; \quad P = \frac{3 \bar{m} \bar{\eta}_c}{\bar{\eta} + 1}, \quad l = 10 \sqrt{\frac{\bar{\rho}}{\bar{A}}}
\]
(169)
where \(l\) is a typical temperature-independent width of the critical nucleus. In fact, the actual width of the critical nucleus strongly depends on temperature and diverges at \(\theta_c\) (Levitas et al., 2003). Note that in the corresponding equation (146) in Levitas (2013b) \(l\) should be equal to \(l = 10 \sqrt{2 \bar{\rho} / \bar{A}}\) rather than \(l = 40 \sqrt{\beta / \bar{A}}\). Profiles of the critical nucleus \(\eta_c(z)\) (\(z = x/l\)) and the plots of \(\bar{\sigma}_{st}(z)\) and \(p(z)\) are shown in Fig. 8 for \(\sigma = 1\) and 3 and four temperatures. Since \(\sigma_{st} = 2 \rho_0 \psi^0\), it is evident that the surface stress is localized at the incomplete interfaces and is negligible at the center of a nucleus. The area below the \(\bar{\sigma}_{st}(z)\) curve is proportional to the total force per unit interface length and, consequently, to the energy of the critical nucleus. At the same time, mean stress is concentrated in the central region of the nucleus. Similar to the \(2 - 3 - 4\) potential, the effect of \(\sigma\) on the profile of the critical nucleus and interface stresses is much weaker than the effect of temperature. The magnitude of the mean stress is a nonmonotonous function of both \(\sigma\) and \(\bar{\eta}\). For small overcooling \(\bar{\theta} = -0.005\), the distribution \(\eta_c(z)\) is very close to two equilibrium austenite–martensite interfaces at \(\bar{\eta} = 0\) with almost complete austenite between them. Consequently, the mean stress is negligible and interface stress is close to that for a complete austenite–martensite interface and homogeneous austenite.

Note that since the critical nucleus in the phase field approach does not possess a complete structure of martensite but represents an intermediate heterogeneous state \(0 < \eta < 1\) without complete A–M interfaces, results are much different (and more precise) from those for critical nucleus within the sharp-interface approach. In particular, far from equilibrium, both interface energy and biaxial tension are essentially smaller than in the sharp-interface approach and additional mean stress appears.

![Fig. 8](image-url) Profile of the critical martensitic nucleus \(\eta_c(z)\), and distribution of the dimensionless biaxial surface stress \(\bar{\sigma}_{st}\) and mean stress \(p\) for four temperatures shown near curves: 1st row for \(\sigma = 1\) and 2nd row for \(\sigma = 3\).
16. Complete system of equations

Below we collect the final complete system of equations for a single order parameter and isothermal processes.

1. Kinematics

1.1 Decomposition of the deformation gradient $F$

$$F = \nabla_0 r = F_e \cdot U_0 \cdot U_t.$$  

1.2 Jacobians

$$J = \frac{\rho_0}{\rho} \det F; \quad J_e = \frac{\rho_0}{\rho_t} \det F; \quad J_0 = \frac{\rho_0}{\rho_\theta} \det U_0; \quad J_0 = \frac{\rho_0}{\rho_e} \det F_e;$$

$$J = J_0^t J_e; \quad J_0 = \det(U_0 \cdot U_t) = J_0^t J_e.$$  

1.3 Transformation $U_t$ and thermal $U_\theta$ deformation gradients

$U_t(\eta) = I + \epsilon_1 = I + \epsilon_{\Delta M} \delta a_1, \eta$;

$U_\theta(\theta, \eta) = I + \epsilon_\theta = I + \epsilon_{\theta M} \delta a_\theta, \eta$;

$\eta_0(a, \eta) = a \eta_0 / 2 + (3 - a) \eta^4 + (a - 4) \eta^6 / 2; \quad 0 < a < 6$;

$\eta_4(a, \eta) = a \eta_4 (1 - \eta)^2 + (4 \eta^2 - 3 \eta^4); \quad 0 < a < 6.$

2. Helmholtz free energy per unit mass and its contributions

$$\psi(F, \eta, \theta, \nabla \eta) = \frac{1}{\rho_0} \psi_e(F_e, \eta, \theta) + \frac{1}{\rho_0} \psi_0(\epsilon, \theta) + \frac{1}{\rho_0} \psi_\eta(\nabla \eta);$$

$$\psi_4 = \left( A(\theta) - 3 A \right) \psi_0^4 (1 - \eta)^2; \quad \psi_6 = \Delta G_4 (\theta) \eta^4 (3 - 2 \eta);$$

$$\psi_6 = 0.5 \left( A(\theta) - 4 A \right) \psi_0^6 (1 - \eta)^2; \quad \psi_8 = \Delta G_6 (\theta) \eta^6 (2 - \eta^2);$$

$$\psi_e = \frac{1}{2} \varepsilon_e \cdot C(\eta); \quad \varepsilon_e = \frac{1}{2} B_e \cdot C_e \cdot B_e; \quad C(\eta) = C_A + (C_M - C_A) \psi(\eta_0, \eta);$$

$$C_e = R_e \times C; \quad \psi_e = \beta \frac{1}{2 \rho_0} \nabla \eta^2.$$  

3. First Piola–Kirchhoff and Cauchy stress tensors

$$P = P_e + P_{sl} + P_d; \quad \sigma = \sigma_e + \sigma_{sl} + \sigma_d;$$

$$P_e = J_0 F_e \cdot \frac{\partial \psi_e}{\partial \varepsilon_e} - F_e \cdot F_e = J_0^{-1} F_e \cdot (C_e \cdot C_e);$$

$$\sigma_e = J_0^{-1} \varepsilon_e \cdot \frac{\partial \psi_e}{\partial \varepsilon_e} + \frac{1}{2} \sigma_{sl} \cdot \varepsilon_e;$$

$$\sigma_{sl} = \rho_0 (\psi_0 + \psi^\eta) I - \rho_0 \nabla \eta \otimes \frac{\partial \psi^\eta}{\partial \nabla \eta} = \rho_0 (\psi_0 + \psi^\eta) I - \beta \nabla \eta \otimes \nabla \eta;$$

$$P_{sl} = \rho_0 J \left( (\psi_0 + \psi^\eta) I - \beta \nabla \eta \otimes \nabla \eta \right) \cdot F_e^{-1} = \rho_0 J \cdot (\psi_0 + \psi^\eta) I - \beta \nabla \eta \otimes \nabla \eta \cdot F_e^{-1};$$

$$\sigma_v = \sigma_v(d); \quad P_v = J_0 \sigma_v(d) \cdot F_e^{-1}.$$  

4. Ginzburg–Landau equations

4.1 Compact form

$$\frac{\partial \eta(r, t)}{\partial t} = \nabla \eta \cdot \mathbf{V} + \tau \cdot \nabla \eta = \tau \left( \frac{\partial \eta}{\partial t} + \frac{1}{\rho_0} \nabla \cdot \left( \frac{\partial \eta}{\partial \nabla \eta} \right) \right);$$

$$\eta(0, t) = \tau \left( \frac{\partial \eta}{\partial t} + \frac{1}{\rho_0} \nabla \cdot \left( \frac{\partial \eta}{\partial \nabla \eta} \right) \right).$$
4.2 Detailed form

\[
\frac{Dη(r, t)}{Dt} = \rho \left( \sigma_e : F_e^{-1} \cdot U_0^{-1} \cdot \frac{∂U_0(θ, η)}{∂η} \cdot F_e + \sigma_e : F_e^{-1} \cdot U_0^{-1} \cdot \frac{∂U_1(ν)}{∂η} \cdot U_0 \cdot F_e \right) - \rho \frac{∂φ^ε}{∂η} \bigg|_{|ε|} - ∂F_e \bigg|_{|ε|} + ψ^ε \left( U_0^{-1} : \frac{∂U_0}{∂η} + U_0^{-1} : \frac{∂U_0}{∂η} \right) - \rho \frac{∂φ^ε}{∂η} - \rho \frac{∂φ^ε}{∂η} + j(\mathbf{F}^{-1} \cdot \mathbf{F}^{-1}) \cdot \nabla_0 (β φ^ε). \right]
\]

(181)

5. Momentum balance equation

\[
\nabla \cdot \sigma + j \mathbf{f} = \rho \frac{D\mathbf{v}}{Dt}; \quad \nabla_0 \cdot \mathbf{P} + ρ_0 \mathbf{f} = ρ_0 \mathbf{v}.
\]

(183)

6. Boundary conditions for the order parameter

\[
\mathbf{n} \cdot \frac{∂φ}{∂η} = - \frac{∂γ_0(ν)}{∂η} = \mathbf{β} \mathbf{n} \cdot \nabla_0 \mathbf{n} = \mathbf{n} \cdot \frac{∂φ}{∂η} = - \frac{∂γ_0(ν)}{∂η} = J_0 \nabla_0 φ \cdot \mathbf{F}^{-1} \cdot \mathbf{F}^{-1} \cdot \mathbf{n}.
\]

(184)

\[
γ_0(ν) = γ_0 + (γ_0 - γ_0) \nu(φ(a, ν)); \quad γ_0(ν) = γ_0 + (γ_0 - γ_0) \nu(φ(a, ν)).
\]

(185)

In addition to the equations derived in this paper, we utilized some equations from our previous papers. Thus, Eqs. (173) for transformation and thermal deformation gradient are taken from Levitas and Preston (2002b), Levitas et al. (2003), Levitas (2013a). Subscripts 4 and 6 designate the 2 – 3 – 4 and 2 – 4 – 6 polynomials. Monotonous functions φ(a, ν) with different parameters a smoothly connect properties of A and M and possess the following properties:

\[
φ(a, 0) = 0; \quad φ(a, 1) = 1; \quad \frac{∂φ(a, 0)}{∂η} = \frac{∂φ(a, 0)}{∂η} = 0.
\]

(186)

The last condition is necessary to have austenite and martensite as solutions of thermodynamic equilibrium conditions X = 0 for any temperature and stresses. Elastic energy (195) and elasticity rule (201) can be easily generalized for arbitrary nonlinear elastic rule (Levitas, 2013a). Equations for φ^ε and ψ^ε for the 2 – 3 – 4 potential have been derived in Levitas (2013b).

17. Generalization for multivariant transformations

Below we collect the final complete system of equations for multivariant PTs and isothermal processes.

1. Kinematics

1.1 Decomposition of the deformation gradient F

\[
\mathbf{F} = \nabla \mathbf{r} = \mathbf{F}_e \cdot \mathbf{U}_0 \cdot \mathbf{U}_1.
\]

(187)

1.2 Jacobians

\[
J = \frac{ρ_0}{ρ} = \det \mathbf{F}; \quad J_1 = \frac{ρ_0}{ρ_1} = \det \mathbf{U}_1; \quad J_0 = \frac{ρ_0}{ρ_0} = \det \mathbf{U}_0; \quad J = J_0 J_1 J_e = \det(\mathbf{U}_0 \cdot \mathbf{U}_1) = J J_0.
\]

(188)

(189)

1.3 Transformation \mathbf{U}_1 and thermal \mathbf{U}_0 deformation gradients

1.3.1 Fifth-degree polynomial

\[
\mathbf{U}_5 = I + ε_1 = I + \sum_{i=1}^{n} \epsilon_i \varphi_5(ε_i, η_k) - \sum_{i=1}^{n} \sum_{j=i}^{n} \eta_k \eta_j (\eta_i L_i^{(1)} + \eta_j L_j^{(1)}).
\]

\[
L_i^{(2)} = (a_1 - 3)ε_i + 3ε_i; \quad \varphi_4(ε_i, η_k) = a_1 (1 - η_k)^2 + (4η_k^2 - 3η_k^4); \quad 0 < a < 6.
\]

(190)
\[ \mathbf{U}_{\text{el}} = \mathbf{I} + \epsilon \alpha + \sum_{k=1}^{n} (\epsilon \alpha - \epsilon \alpha) \varphi \psi_{\alpha} (\alpha, \eta_k) - \sum_{i=1}^{n-1} \sum_{j=1}^{n} \eta_i^2 \eta_j^2 (\eta_i \mathbf{L}_i \eta_j + \eta_j \mathbf{L}_j \eta_i). \]

\[ \mathbf{L}_{\text{el}} = (a_0 - 3)(\epsilon \alpha - \epsilon \alpha) + 3(\epsilon \alpha - \epsilon \alpha). \]  

(191)

1.3.2 Sixth-degree polynomial

\[ \mathbf{U}_{\text{el}} = \mathbf{I} + \epsilon \alpha = \mathbf{I} + \sum_{k=1}^{n} (\epsilon \alpha \varphi \psi_{\alpha} (\alpha, \eta_k) - \sum_{i=1}^{n-1} \sum_{j=1}^{n} (\mathbf{Z}_i^1 \eta_i^2 \eta_j^2 + \mathbf{Z}_j^1 \eta_i^2 \eta_j^2); \quad 0 < a < 6; \]

\[ \mathbf{Z}_i^1 = 0.5[(d^2 - 3) \epsilon \alpha + 3 \epsilon \alpha]; \quad \varphi \psi_{\alpha} (\alpha, \eta_k) = \alpha \eta_k^2 / 2 + (3 - a) \eta_k^4 + (a - 4) \eta_k^6 / 2. \]

(192)

\[ \mathbf{U}_{\text{el}} = \mathbf{I} + \epsilon \alpha + \sum_{k=1}^{n} (\epsilon \alpha - \epsilon \alpha) \varphi \psi_{\alpha} (\alpha, \eta_k) - \sum_{i=1}^{n-1} \sum_{j=1}^{n} (\mathbf{Z}_i^1 \eta_i^2 \eta_j^2 + \mathbf{Z}_j^1 \eta_i^2 \eta_j^2); \quad 0 < a < 6; \]

\[ \mathbf{Z}_i^1 = 0.5[(d^2 - 3) \epsilon \alpha - \epsilon \alpha + 3(\epsilon \alpha - \epsilon \alpha)]. \]

(193)

2. Helmholtz free energy per unit mass and its contributions

\[ \psi (\mathbf{F}, \eta_i, \theta, \nabla \eta_i) = \frac{J_{\text{el}}}{\rho_0} \psi^0 (\mathbf{F}, \eta_i, \theta) + J\psi^\theta (\theta, \eta_i) + \psi^V (\nabla \eta_i). \]

(194)

\[ \psi^0 = \frac{1}{2} \epsilon \alpha \mathbf{C} (\eta_i) : \mathbf{E}_\eta; \quad \mathbf{E}_\eta = \frac{1}{2} \mathbf{C} (\eta_i) : \mathbf{B}_\iota; \quad \mathbf{C} (\eta_i) = \mathbf{C}_A + \sum_{i=1}^{n} (\mathbf{C}_\iota - \mathbf{C}_A) \varphi (\alpha, \eta_i); \]

(195)

\[ \psi^V = \frac{\beta_{\iota j}}{2 \rho_0} \nabla \eta_i : \nabla \eta_j = \frac{\beta}{2 \rho_0} \left( \sum_{i=1}^{n} |\nabla \eta_i|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \nabla \eta_i : \nabla \eta_j \right); \]

(196)

2.1 Thermal energy for the fifth-degree polynomial

\[ \psi_5^\theta = \sum_{k=1}^{n} (A(\theta) - 3 \Delta \psi \psi_{\theta} (\theta, \eta_k) (1 - \eta_k)^2 + \sum_{i=1}^{n-1} \sum_{j=1}^{n} F_{\theta i} (\theta, \eta_i, \eta_j); \quad \psi_4^\theta = \sum_{k=1}^{n} \Delta \psi \psi_{\theta} (\theta, \eta_k^2 (3 - 2 \eta_k)). \]

(197)

2.2 Thermal energy for the sixth-degree polynomial

\[ \psi_6^\theta = \sum_{k=1}^{n} 0.5 (A(\theta) - 4 \Delta \psi \psi_{\theta} (\theta, \eta_k^2 (1 - \eta_k^2)^2 + \sum_{i=1}^{n-1} \sum_{j=1}^{n} F_{\theta i} (\theta, \eta_i, \eta_j); \]

(198)

3. First Piola–Kirchhoff and Cauchy stress tensors

\[ \mathbf{P} = \mathbf{P}_e + \mathbf{P}_{\text{el}} + \mathbf{P}_{\text{d}}; \quad \sigma = \sigma_e + \sigma_{\text{el}} + \sigma_{\text{d}}; \]

(199)

\[ \mathbf{P}_e = J_{\text{el}} \mathbf{F}_e \cdot \frac{\partial \psi^\theta (\mathbf{E}_\iota, \eta_i)}{\partial \mathbf{E}_\iota} \cdot \mathbf{F}_e \cdot \mathbf{F}_e^{-1} = J_{\text{el}}^{-1} \mathbf{F}_e \cdot (\mathbf{C} : \mathbf{E}_\iota) \cdot \mathbf{F}_e \cdot \mathbf{F}_e^{-1}; \]

(200)

\[ \sigma_e = J_{\text{el}}^{-1} \mathbf{V}_e \cdot \frac{\partial \psi^\theta (\mathbf{C}, \mathbf{E}_\iota, \eta_i)}{\partial \mathbf{E}_\iota} ; \quad \mathbf{V}_e = J_{\text{el}}^{-1} \mathbf{V}_e \cdot (\mathbf{C} : \mathbf{B}_\iota) \cdot \mathbf{V}_e; \quad \mathbf{C}_\iota = \mathbf{R}_e \times \mathbf{C}; \]

(201)

\[ \sigma_{\text{el}} = \rho_0 (\psi^\theta + \psi^V) I - \rho_0 \nabla \eta_i \cdot \frac{\partial \psi^V}{\partial \nabla \eta_i} = \left( \mathbf{I} - \beta \nabla \eta_i \otimes \nabla \eta_i \right) \left( \rho_0 \psi^\theta + \beta \left( \sum_{i=1}^{n} |\nabla \eta_i|^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \nabla \eta_i \cdot \nabla \eta_j \right) \right) I - \beta \sum_{i=1}^{n} \left( \nabla \eta_i \otimes \nabla \eta_i + \nabla \eta_i \otimes \sum_{j=1}^{n} \nabla \eta_j \right) \right); \]

(202)
4. Ginzburg–Landau equations

4.1 Compact form

\[
\frac{D\eta_i(r, t)}{Dt} = \frac{\partial \eta_i(r, t)}{\partial t} + \nabla \cdot \nabla \eta_i = L \eta_i \left( -\frac{\partial \eta_i}{\partial \eta_j} + \frac{1}{\rho_0} \nabla \cdot \left( \rho_0 \frac{\partial \eta_i}{\partial \nabla \eta_j} \right) \right);
\]

\[
\frac{\partial \psi}{\partial t} + \nabla \cdot \nabla \psi = L \psi \left( -\frac{\partial \psi}{\partial \theta} + \frac{1}{\rho} \nabla \cdot \left( \rho \frac{\partial \psi}{\partial \nabla \eta} \right) \right);
\]

(203)

4.2 Detailed form

\[
\frac{D\eta_i(r, t)}{Dt} = \frac{L}{\rho} \left( \sigma_{ij} \epsilon_{ij} - \eta_i \eta_j \right) \cdot \nabla \eta_i + \frac{1}{\rho_0} \nabla \cdot \left( \rho_0 \frac{\partial \eta_i}{\partial \nabla \eta_j} \right);
\]

\[
-1 \frac{\partial \eta_j}{\partial t} \int_{\eta_i} \left( \epsilon_{ij} \frac{\partial \epsilon_{ij}}{\partial \eta_i} \cdot \epsilon_{ij} \frac{\partial \epsilon_{ij}}{\partial \eta_j} \right) - \frac{\partial \psi}{\partial \theta} \frac{\partial \psi}{\partial \nabla \eta_i} + \frac{\partial \psi}{\partial \eta_i} \frac{\partial \psi}{\partial \nabla \eta_j} \right);
\]

(204)

5. Momentum balance equation

\[
\nabla \cdot \sigma + \rho \dot{f} = \frac{\partial \psi}{\partial \nabla \eta_i} \cdot \nabla \cdot \dot{\psi} = \rho_0 \dot{\psi}.
\]

(206)

6. Boundary conditions for the order parameters

\[
\eta_0(p) = \gamma_0^0(r) + \gamma_0^0 \phi(a_0, p);
\]

\[
\gamma_1(p) = \gamma_1^0 + \gamma_1^0 \phi(a_1, p).
\]

(207)

(208)

Here, \( C_i \) are the elastic moduli tensor for the \( i \)th martensitic variant, \( \eta \) characterizes the energy barrier between martensitic variants, \( B, D, \) and \( H \) are constants that control the behavior of the potential away from energy minima. Note that for the 2–3–4 potential for a single martensitic variant, some functions for the multiple variants are fifth-degree polynomials, and they are designated with sub- or superscript 5. In addition to equations derived in this paper, we utilized some equations from our previous papers. Thus, Eqs. (190)–(193) for transformation and thermal deformation gradient are taken from Levitas and Preston (2002b), Levitas et al. (2003) and Levitas (2013a). Elastic energy (195) and the elasticity rule (201) can be easily generalized for arbitrary nonlinear elastic rule (Levitas, 2013a). Equations for \( \psi^0 + \psi^0 \) can also be found in Levitas and Preston (2002b), Levitas et al. (2003) and Levitas (2013a). In contrast to the strict partitioning for a single martensitic variant of the total thermal energy into two parts, \( \psi^0 \) and \( \psi^0 \), for the multiple martensitic variant it is not the case (Levitas, 2013b). Eqs. (197) and (198) for \( \psi^0 \) and \( \psi^0 \) provide correct expressions for the structural interface stresses for the \( A\text{–}M_i \) interface (i.e., biaxial tension with the magnitude equal to the interface energy). This is easy to check because for each martensitic variant \( M_i \), all \( \eta_k = 0 \) for \( k \neq i \) and general equations and solutions for the \( A\text{–}M_i \) interface reduce to those for a single variant. However, this cannot be proved for the \( M_i \text{–}M_j \) interface, because it is described by simultaneous variation of two order parameters and there is no analytical solution for such a case. The only additional condition that we satisfy is that interface stress is localized at the \( M_i \text{–}M_j \) interfaces. In Eqs. (197) and (198), all terms that localize at the diffuse interfaces are included in \( \psi^0 \) and the function \( \psi^0 \) depends on the thermal driving force for the \( A\text{–}M_i \) transformation. While presented equations look logical, formally, the terms \( \psi^0 \) can be divided between \( \psi^0 \) and \( \psi^0 \) in various ways, if the corresponding justifications will be found. For example, in Levitas and Javanbakht (2010, 2011a), where the assumptions in Eq. (146) and \( \sigma = 1 \) have been used for the fifth degree polynomial, the following partitioning was accepted:

\[
\psi^0 = \sum_{k=1}^{n} A_0 (\theta_c - \theta_c) \eta_k^2 (1 - \eta_k)^2 + \sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{F}_{ij} (\theta_c, \eta_i, \eta_j);
\]

\[
\psi^0 = \sum_{k=1}^{n} \frac{1}{3} A_0 (\theta_c - \theta_c) \eta_k^2 (3 - 2 \eta_k) + \sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{F}_{ij} (\theta_c, \eta_i, \eta_j) - \tilde{F}_{ij} (\theta_c, \eta_i, \eta_j).
\]

(209)
In this case, the temperature-independent portions of all terms, which localize at the diffuse interfaces are included in \( \tilde{\psi} \), while \( \psi^{\prime} \) includes all temperature-dependent terms. Eqs. (209) for \( \theta \neq \theta_c \) do not reduce to the correct Eqs. (124) and (125) for \( A-M \) interface, that is why we do not consider them as an option. However, for \( \theta = \theta_c \) they are correct, as well as all calculations in Levitas and Javanbakht (2010, 2011a).

Note that one of the goals of the paper by Levitas et al. (2013) was to introduce such order parameters, for which each martensite–martensite interface is described by a single order parameter. It was achieved by using hyperspherical order parameters, similar to those introduced in Levitas et al. (2003). While more detailed study and justification for this potential are required, interface stresses for martensite–martensite interfaces can be introduced in a way completely similar to the austenite–martensite interfaces. Generalization for three arbitrary phases is presented in Levitas and Momeni (2014) and Momeni and Levitas (2014).

18. Concluding remarks and future directions

In this paper, a general thermodynamically consistent, the large strain phase field approach to multivariant martensitic PTs is developed with emphasis on correct introducing interface stresses. Interface stresses consist of elastic, viscous, and structural contributions. Elastic and viscous contributions to the interface stresses appear automatically as a result of the solution of the coupled system of the phase field and mechanics equations. The necessity of more sophisticated constitutive developments for these stresses can be determined after comparing the solution for the total interface stresses with experiments or atomistic simulations. The main focus is on the structural part, which is similar to the interface stresses for the liquid–liquid and liquid–gas interfaces. Thermodynamic potential was formulated, for which the structural part of the Cauchy interface stresses reduces for the propagating interface to the biaxial tension with the force per unit length equal to the nonequilibrium interface energy. Important point is that a physical phenomenon like interface stresses is introduced with the help of geometric nonlinearity, i.e., large strain contributions, which retain even in the small strain approximation. Thus, the gradient energy should depend on the gradient of the order parameters in the deformed configuration, which results in compressive stresses normal to the interface. In addition, the gradient energy and some specific part of the thermal energy (function \( \tilde{\psi} \) determined by Eq. (124)) should be multiplied by the Jacobian \( J \) (which for small strains reduces to \( J = 1 + \varepsilon_0 \)), which produces the tensile mean stress, exactly compensating normal stresses and leading to biaxial tension. These results have been obtained by utilizing an analytical solution for the nonequilibrium propagating interface for a \( 2-4-6 \) polynomial free energy in terms of the order parameters.

To prove that the magnitude of the biaxial tension is equal to the interface energy \( \gamma \), one needs to define position of the Gibbsian dividing surface in order to calculate the nonequilibrium interface energy \( \gamma \). Generally, this was a fundamental and unsolved problem in the interface and surface science, which has not been treated before in the phase field approach. In the previous papers for the \( 2-3-4 \) potential by Levitas (2013a,b), due to symmetry of the potential and stress distribution, an easy guess \( \pi = 0.5 \) resolves the problem. This is not the case for the \( 2-4-6 \) polynomial, which is nonsymmetric and leads to asymmetric stress distribution. Surprisingly, even two conditions have been found for the dividing surface based on static equivalence of force and moment applied to the diffuse interface and equivalent sharp interface (dividing surface). The first one, in fact followed from the condition that the resultant force is equal to the interface energy \( \gamma \). The second one follows from the condition that the moment of diffuse interface stresses with respect to position of the equivalent sharp interface is zero. While we have two equations for one unknown, we found that both conditions give the same sharp interface position for the \( 2-4-6 \) potential. Thus, we suggested a new approach, namely, application of the principle of static equivalence, and resolved the long-standing problem on the determination of the position of the Gibbsian dividing surface, and found a self-consistent solution for the interface stresses and energy. Note that for curved interface, the found position of the dividing surface and expression for the interface energy are also consistent with the expression for the velocity of the curved sharp interface (Levitas, 2014). Analytical expressions for energy, width, entropy excess, and the distribution of the interface stresses at the nonequilibrium propagating interface are obtained and analyzed for the \( 2-4-6 \) potential. For the critical martensitic nucleus, tensile mean stress distribution is found in addition to the biaxial tension.

The explicit expression for the Ginzburg–Landau equations have been found for fully geometrically nonlinear formulation, which was simplified for various geometrical approximations of smallness of some strain components and rotations. An important point in the current approach is that the elastic energy is defined per unit volume of unloaded (intermediate) configuration, in which elastic properties are usually determined in experiment and atomistic simulations. Such a choice leads to the correct expression for the elasticity rule and additional contributions to the Ginzburg–Landau equations and expression for the entropy. They should be kept even at small strains, while they could not be obtained within geometrically linear approximation and were not included in the previous theories. These results and the necessity to introduce some geometrically nonlinear terms even at small strains in order to introduce proper interface stresses demonstrate the importance of starting with a fully geometrically nonlinear formulation even for the case when strains are small. Moreover, even if the solution of the mechanical problem is based on small strain formulation, it is desirable to use the Ginzburg–Landau equation for finite strains and rotations. The reason is that in numerical simulations and analytical solutions, the total local part of the driving force has a similar magnitude but the opposite sign to the nonlocal term with the Laplacian. Thus, even a small difference in any of the terms due to geometric simplifications can lead to a significant change in the total driving force, direction of the PT, and interface velocity. Accuracy can be increased if the output of the small strain solutions will be used to determine terms in the fully large strain versions of the Ginzburg–Landau
Eqs. (204) and (205). If a small strain solution was found without updating geometry by adding displacements, then the Ginzburg–Landau equation (205) in the reference configuration should be used. When geometry is updated, then Ginzburg–Landau equation (204) in the actual configuration has to be solved.

Thus, strictly speaking, based on results of the current work and previous simulations (Levitas and Javanbakht, 2010, 2011a; Diao et al., 2003), the phase field approach at the nanoscale should always include finite strain formulation with interface stresses, unless it is proven that they can be neglected for some specific problems. It was found that the elastic stresses only contribute to the Ginzburg–Landau equations and to entropy. While interface stresses and viscous stresses do not contribute to these equations explicitly, they change elastic stresses, which in turn affect the Ginzburg–Landau equations and entropy.

For multiple martensitic variants, an expression for the interface stresses cannot be strictly derived, and we limited ourself to the best guess. This is because the martensite–martensite interface is described by two order parameters and there is no analytical solution for it. However, this problem can be resolved with the help of hyperspherical order parameters introduced in Levitas et al. (2003, 2013), for which each martensite–martensite interface is described by a single order parameter. We will pursue this direction in future works, see, for example, Levitas and Momeni (2014) and Momeni and Levitas (2014). Also, since particular cases of the developed theory have already been used for the finite element solution of various problems on microstructure evolution (Levitas and Javanbakht, 2010; Levitas et al., 2009, 2013; Levitas and Javanbakht, 2011b; Levin et al., 2013), it will not be difficult to implement the complete theory as well. This may be important for the study of interface-induced phenomena and instabilities (Grinfeld, 1991).

Generalization for anisotropic interface will be performed in future work. The most popular way is to consider \( \beta = \beta(k) \) (Wheeler and McFadden, 1997; Eggleston et al., 2001). In this case, Eq. (50) is not valid, the interface stress tensor is not symmetric, and torque rotates interface towards a lower-energy configuration. Still, any non-rotating propagating interface corresponding to a specific \( k \) is described by the same analytic solution Eq. (121) with corresponding \( \beta = \beta(k) \). Thus, the same approach is applicable, which will lead to the same expressions for \( \bar{\psi}^\theta \) and \( \bar{\psi}^\varphi \) in Eq. (124), because local energy is independent of \( k \). An additional problem appears for large strain formulation, since gradient of the order parameter is defined in the current configuration and application of the principle of objectivity and practical description of anisotropy in the current configuration is nontrivial. The description of unequal principle interface stresses is another necessary extension. The derivation of the constitutive equation for the sharp interface, including couple stresses, can be performed as a coarse-graining of the numerical solution for diffuse interface.

There may be a concern about the applicability of the phase field method to the scale of several atomistic distances. However, it should be underscored that this approach to any phenomena always includes treatment at an atomistic scale because it resolves interfaces, which are several atomic layers thick. For martensitic phase transformations and twinning, the interface width is \( \sim 1 \) nm, which is included in phase field calibration (Levitas et al., 2003, 2010). For simulation of dislocations, their height is two interatomic distances and Burgers vector is one interatomic distance; both should be resolved with the phase field approach (Levitas and Javanbakht, 2012). The phase field crystal approach (Elder and Grant, 2002) utilizes differential equations to model the position of each atom. All these continuum approaches at the nanoscale have been calibrated and verified for different cases with atomistic approaches and experiments. Solid–liquid interface width is 0.7 nm for Ni (Monk et al., 2010), which was determined by molecular dynamics and introduced in phase field modeling. Calibrated to experiment width of the solid–gas interface for Al is 0.8–1.2 nm (Levitas and Samani, 2014). This model demonstrates good comparison with experiments on the size dependence of the melting temperature and on the width of surface molten layer versus temperature in the range of 0.3–1.2 nm for plane interface (Levitas and Samani, 2011a). In some cases (for melting temperature of nanoparticles and for temperature of bi-stable state, see Levitas and Samani, 2011a, 2014) the phase field approach gives an even better description than molecular dynamics. The reason is that the phase field approach is based on and calibrated by thermodynamic functions in bulk and interface, and kinetics of interface, and nanoscale features are included through interface width and energy of an interface, which is few interatomic distances thick. In contrast, it is more difficult to include similar desired information in the interatomic potential in molecular dynamics. There are numerous examples in which the continuum approach works unexpectedly good even beyond its supposed limit of small-scale applicability.

The developed large strain thermodynamic approach and expression for the interface stresses can be adjusted or extended to other temperature- and stress-induced PTs, including liquid–liquid PT (Lowengrub and Truskinovsky, 1998), reconstructive PTs (Denoual et al., 2010), melting/solidification (Wheeler and McFadden, 1997; Anderson et al., 2001; Levitas and Samani, 2011a,b; Slutsker et al., 2006), evaporation, sublimation, amorphization/crystallization, and others. An important part of this application is the presence or possibility to find an analytical solution for a propagating interface. Alternatively, we will try to find a way to formulate potentials and the expression for interface stresses for the case when analytical solutions cannot be found, using approximate methods. Similar approaches can be developed for various other phenomena that are described by the phase field approach. This includes various electromagnetic PTs (Slutsker et al., 2008), diffusive PTs and chemical reactions described by the Cahn–Hilliard theory (Cahn and Hilliard, 1958; Hong and Xiao Wang, 2013) (e.g., spinodal decomposition, segregation, separation, and precipitation), twinning (Levitas and Preston, 2002b; Levitas et al., 2003, 2013; Clayton and Knap, 2011a), evolution of multigrain structure (Kobayashi et al., 1998), dislocation evolution (Wang et al., 2001; Rodney et al., 2003; Levitas and Javanbakht, 2012), fracture in crystalline and amorphous solids and void nucleation (Jin et al., 2001b), cavitation in liquids (Levitas et al., 2011), and interaction of cracks and dislocations with PTs (Levitas et al., 1998; Levitas, 2000; Idesman et al., 2000; Levitas and Javanbakht, 2012, 2013, 2014; Boulbitch and Toledano, 1998; Boulbitch and Korzhenevskii, 2011).
Analytical distributions of the interface stress tensor can be found for the microstructures, for which analytical solutions were found: for a critical austenitic nucleus on martensite in an infinite sample (Levitas et al., 2003) for both 2–3–4 and 2–4–6 potentials; for equilibrium austenite–martensite and martensite–martensite interfaces and critical nuclei in a finite sample (Levitas et al., 2006a) for the 2–3–4 potential (including functionally-graded structures in a sample smaller than the interface width), and for multiple surface-induced pre-transformed nanostructures in semi-infinite sample for a two-parabola potential (Lipowsky, 1982; Pluis et al., 1990) and infinite sample for the 2–3–4 potential (Levitas et al., 2006b).

Similar solutions can be found for other potentials, see, for example, Umantsev (2012) and Steinbach (2009). A new expression for surface stresses and finite strains can be introduced in the phase field approach for an external surface (Levitas and Javanbakht, 2011b), for single and multiple martensitic variants, and for melting (Levitas and Samani, 2011a). This would allow for more precise study of surface-stress-induced PTs in nanowires (Diao et al., 2003) and the contribution of surface stresses to formation of nanometer size third phases at the interfaces between phases (Levitas, 2005; Luo and Chiang, 2008; Levitas et al., 2012; Levitas and Momeni, 2014; Momeni and Levitas, 2014) and within grain boundaries (Lobkovsky and Warren, 2002).

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Appendix A. Some derivations

1. Let us prove that for a tensor $A$ of an arbitrary rank one has

$$\mathbf{\nabla} \cdot (\rho \partial A) = \mathbf{\nabla} \cdot (\rho A) - \rho \partial \mathbf{\nabla} \cdot (\rho A).$$

Indeed,

$$\frac{\partial (\rho \partial A_{j;k})}{\partial r_k} = \frac{\partial (\rho A_{j;k})}{\partial r_k} + \rho A_{j;k} \frac{\partial \rho}{\partial r_k}.$$  

Then

$$\frac{\partial \rho}{\partial r_k} = \frac{\partial F_{mn}}{\partial r_k}, \quad \frac{\partial F_{mn}}{\partial r_k} = \frac{\partial m}{\partial r_k} \frac{\partial m}{\partial r_k} = \delta_{mk},$$

and, consequently, in Eq. (211)

$$\frac{\partial (\rho \partial A_{j;k})}{\partial r_k} = \rho \partial A_{j;k}.$$  

which proves Eq. (210).

2. We will prove that

$$\mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = \mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = \mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = f \mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right).$$

First, transform

$$\frac{\partial \sigma}{\partial \nabla^0 \eta} = F \cdot \frac{\partial \sigma}{\partial \nabla^0 \eta}.$$  

or in direct vector notations

$$\frac{\partial \sigma}{\partial \nabla^0 \eta} = F \cdot \frac{\partial \sigma}{\partial \nabla^0 \eta}.$$  

Substituting Eq. (215) in Eq. (214), we obtain

$$\mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = \frac{\partial \sigma}{\partial \eta} \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = \frac{\partial \sigma}{\partial \eta} \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right) = f \mathbf{\nabla} \cdot \left( \rho \frac{\partial \sigma}{\partial \nabla^0 \eta} \right).$$

Eq. (210) was utilized for the last transformation.

3. Let prove that

$$P^V = \rho_0 \frac{\partial V}{\partial F} \nabla \eta_k \otimes \frac{\partial V}{\partial \nabla \eta_k} = \rho_0 f \mathbf{\nabla} \cdot \frac{\partial V}{\partial \nabla \eta_k}.$$  

(218)
One has in the component form in the Cartesian system with basis vectors $\mathbf{e}_i$:

$$
\frac{\partial \psi \nabla (\zeta_k F^{-1})}{\partial \mathbf{f}_{ab}} = \frac{\partial \psi \nabla \eta_k}{\partial \mathbf{f}_{ab}} = \frac{\partial \psi \nabla \eta_k}{\partial \mathbf{f}_{ij}} \frac{\partial F^{-1}}{\partial \mathbf{f}_{ij}} = -\frac{\partial \psi \nabla \eta_k}{\partial \mathbf{f}_{ij}} \delta_{ij} F^{-1} = -\frac{\partial \psi \nabla \eta_k}{\partial \mathbf{f}_{ij}} \nabla \eta_k F^{-1},
$$

(219)

where the equalities

$$
\frac{\partial F^{-1}}{\partial \mathbf{f}_{ij}} = -F^{-1} F^{-1} F^{-1}; \quad \zeta_k^m = \zeta_k^m F^{-1}; \quad \frac{\partial \eta_k}{\partial \mathbf{f}_{ij}} = \frac{\partial \eta_k}{\partial \mathbf{f}_{ij}} \delta_{ij}
$$

(220)

have been eqd. Eq. (220) is the consequence of the chain $F^{-1} \cdot F - F^{-1} \cdot d F = 0$, and $d F^{-1} = -F^{-1} \cdot d F \cdot F^{-1}$.

Eq. (220) coincides with Eq. (34), and Eq. (220) is the consequence of Eq. (220). Then

$$
\frac{\partial \psi \nabla (\nabla \eta_k)}{\partial F} = -\frac{\partial \psi \nabla \eta_k}{\partial \nabla \eta_k} \nabla \eta_k F^{-1} \mathbf{e}_a \otimes \mathbf{e}_i = -\nabla \eta_k \otimes F^{-1} \cdot \frac{\partial \psi \nabla}{\partial \nabla \eta_k} \cdot F^{-1}.
$$

(221)

Substituting Eq. (221) into Eq. (218) we obtain for the gradient contribution to the first Piola–Kirchhoff stress

$$
\mathbf{P}^v = -\rho_0 \nabla \eta_k \otimes F^{-1} \frac{\partial \psi \nabla}{\partial \nabla \eta_k} \cdot F^{-1}.
$$

(222)

4. To transform the Ginzburg–Landau equation to the reference configuration, we evaluate:

$$
\nabla \cdot (\rho \beta \nabla \eta) = \frac{\partial}{\partial \tau_b} \left( \rho \beta \frac{\partial \eta}{\partial \tau_b} \right) = \rho \beta \frac{\partial \eta}{\partial \tau_b} \frac{\partial}{\partial \tau_b} \rho \beta \frac{\partial \eta}{\partial \tau_b} = \frac{\partial}{\partial \tau_b} \left( \rho \beta \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \right) = \frac{\partial \rho \beta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} + \rho \beta \frac{\partial}{\partial \tau_b} \left( \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \right) = \frac{\partial \rho \beta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} + \frac{\partial \rho \beta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} + \rho \beta \frac{\partial}{\partial \tau_b} \left( \frac{\partial \eta}{\partial \tau_b} \frac{\partial \eta}{\partial \tau_b} \right).
$$

(223)

References


