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Interface stress for nonequilibrium microstructures in the phase field approach: Exact analytical results

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An exact expression for the temperature-dependent interface stress tensor (tension) and energy is derived within a phase field approach. The key problem, of which part of the thermal energy should contribute to the surface tension, is resolved with the help of an analytical solution for a nonequilibrium interface. Thus, for a propagating interface at any temperature, the interface stress tensor represents biaxial tension with magnitude equal to the temperature-dependent interface energy. Explicit expressions for the distributions of interface stresses are obtained for a nonequilibrium interface and a critical nucleus. The results obtained are applicable for various phase transformations (solid-solid, melting-solidification, sublimation, etc.) and structural changes (twinning, grain evolution), and can be generalized for anisotropic interface energy, for dislocations, fracture, and diffusive phase transformations described by Cahn-Hilliard theory.

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I. INTRODUCTION

The phase field approach is broadly used for modeling microstructure evolution during various phase transformations and structural changes (like grain growth and twinning) at the nanoscale.[1] Due to the nanometer size of the structural units, such as the nuclei of the product phases, nanotwin and martensitic plates, and especially their tips, interface tension is expected to play an important part in the microstructure evolution. It is known[2] that any interface is subjected to a biaxial tension with magnitude equal to the surface energy γ. However, there are only a few papers devoted to introducing surface tension in the phase field approach. Known expressions for liquid-liquid[3] and liquid-solid[4] diffuse interfaces contain additional hydrostatic pressure, i.e., they are contradictory. In Ref. 5, a very general treatment of the diffuse interface stresses is considered and for the phase equilibrium temperature $\theta = \theta_e$, a consistent expression for interface tension is obtained. However, for $\theta \neq \theta_e$, these stresses are not localized at the diffuse interface but also produce a contribution in one of the phases. Recently, a more precise expression for the surface tension was suggested[6,7] for solid-solid, solid-liquid, and liquid-liquid interfaces, which is always localized at the diffuse interface and reduces to the proper biaxial tension just for $\theta = \theta_e$, i.e., for a stationary interface. This expression contains extra hydrostatic pressure for nonequilibrium interfaces. Also, the magnitude of the surface tension was temperature independent in Refs. 6 and 7 and could not be equal to the temperature-dependent interface energy. One more complication in developing a theory for the interface tension is that the expression for the interface energy is known for an equilibrium interface only. In this paper, a strict approach for introducing the interface stress tensor in the phase field approach is developed, which resolves this long-standing problem. We derived an equation for the energy of a nonequilibrium interface vs temperature, $\gamma(\theta)$, utilizing an analytical solution for the propagating interface,[8] which allowed us to calibrate the magnitude of the surface tension. Then we derived a general expression for the interface stress tensor that reduces to biaxial tension with magnitude $\gamma(\theta)$ for any propagating interface. Since all results are based on an explicit analytical solution, they are exact. Analytical distributions of the interface stresses are obtained for a nonequilibrium interface and a critical nucleus. The current work marks a transition from the educated guesses[3–7] at formulations of the expression for the surface stresses to a strict and unambiguous procedure, for an arbitrary nonequilibrium case. Possible generalizations are outlined in the concluding remarks.

Below, a subscript s means symmetrization of the second-rank tensor; := is equal by definition; $\boldsymbol{I}$ is the unit tensor; $\boldsymbol{\nabla}$ and $\boldsymbol{\nabla}\cdot$ are the gradient and divergence operators in the deformed states; and $\otimes$ is a dyadic product.

II. GENERAL MODEL

Note that all equations of this section were first derived in the fully geometrically nonlinear formulation[6] and then linearized for small-strain regimes. We will keep only those geometrically nonlinear terms that are necessary for introducing the interface tension. For simplicity and to make the results obtained accessible to a broader audience, we will present here the small-strain version of the theory only. Thus, the equations for the stress tensor $\boldsymbol{\sigma}$ and the Ginzburg-Landau equations are

$$\boldsymbol{\sigma} = \rho_0 \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} - \rho \left(\frac{\partial \psi}{\partial \boldsymbol{\nabla} \eta} \otimes \boldsymbol{\nabla} \eta \right)_s, \tag{1}$$

$$\frac{1}{L}\frac{\partial \eta}{\partial t} = -\rho \frac{\partial \psi}{\partial \eta} + \boldsymbol{\nabla} \cdot \left(\rho \frac{\partial \psi}{\partial \boldsymbol{\nabla} \eta} \right). \tag{2}$$

Here η is the order parameter, L is the kinetic coefficient, $\boldsymbol{\varepsilon}$ is the strain tensor, and ρ and ρ_0 are the mass densities in the deformed and undeformed states. The Helmholtz free energy per unit mass $\psi(\boldsymbol{\varepsilon},\eta,\boldsymbol{\nabla}\eta,\theta)$ has local minima (extrema) at $\eta = 0$ for the high-symmetry phase H (e.g., melt or austenite), and $\eta = 1$ for the low-symmetry phase L (e.g., solid or martensite). To introduce surface tension, we accept the free energy in the following form:

$$\psi(\boldsymbol{\varepsilon},\eta,\theta,\boldsymbol{\nabla}\eta) = \psi^e + \frac{\rho_0}{\rho}\breve{\psi}^\theta + \tilde{\psi}^\theta + \frac{\rho_0}{\rho}\psi^\nabla, \tag{3}$$

$$\tilde{\psi}^\theta + \breve{\psi}^\theta = f(\theta,\eta) := \Delta G^\theta(\theta)\eta^3(4-3\eta) + A(\theta)\eta^2(1-\eta)^2, \tag{4}$$

$$\frac{\rho_0}{\rho} = 1 + \varepsilon_0, \quad \psi^\nabla = 0.5\frac{\beta}{\rho_0}|\nabla\eta|^2, \tag{5}$$

where ψ^e, f, and ψ^∇ are the elastic, thermal, and gradient contributions to the energy, ε_0 is the volumetric strain, ΔG^θ is the difference between the thermal parts of the energies of L and H $[\Delta G^\theta(\theta_e) = 0]$, and A and β are the double-well energy and gradient-energy coefficients. As will be demonstrated below, the division of the thermal energy f into two parts and multiplication of one of them and the gradient energy by ρ_0/ρ is required to reproduce the desired expression for the interface stresses. While usually in the small-strain approximation strains are neglected in comparison to unity, we keep ε_0 in Eq. (5) for ρ_0/ρ but neglect higher orders of ε_0 (and $\boldsymbol{\varepsilon}$, in general). Substituting Eq. (3) for ψ into Eq. (1), we obtain a decomposition of $\boldsymbol{\sigma}$ into elastic $\boldsymbol{\sigma}_e$ and surface tension $\boldsymbol{\sigma}_{st}$ tensors:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}_{st}, \quad \boldsymbol{\sigma}_e = \rho_0\frac{\partial\psi^e}{\partial\boldsymbol{\varepsilon}}, \quad \boldsymbol{n} := \frac{\nabla\eta}{|\nabla\eta|}, \tag{6}$$

$$\begin{aligned}\boldsymbol{\sigma}_{st} &= (\rho_0\breve{\psi}^\theta + 0.5\beta|\nabla\eta|^2)\boldsymbol{I} - \beta\nabla\eta\otimes\nabla\eta \\ &= \beta|\nabla\eta|^2(\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}) + (\rho_0\breve{\psi}^\theta - 0.5\beta|\nabla\eta|^2)\boldsymbol{I},\end{aligned} \tag{7}$$

where $\boldsymbol{n}$ can be interpreted as the unit normal to the diffuse interface [if the solution to the Ginzburg-Landau equation (2) represents an interface]. Thus, multiplication of $\breve{\psi}^\theta$ and ψ^∇ by $\frac{\rho_0}{\rho}$ (which depends linearly on the volumetric strain) and using the gradient in the deformed state in ψ^∇ results in Eq. (7) for the interface tension. The main problem is how to divide $f(\theta,\eta)$ into two functions $\tilde{\psi}^\theta$ and $\breve{\psi}^\theta$ to reproduce the desired expression for the interface tension for an arbitrary temperature. Equations (3) and (4) with a plausible (temperature-independent) guess for $\breve{\psi}^\theta$ were presented in Ref. 6. Here, we will derive an exact temperature-dependent expression for $\breve{\psi}^\theta$ by utilizing an analytical solution for a propagating interface. Since $\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}$ is the two-dimensional (2D) unit tensor at the interface, the first term in Eq. (7) represents the desired biaxial surface tension with equal stresses [provided that the magnitude of the stresses results in a force equal to $\gamma(\theta)$]. Thus, for a propagating interface, the last term should be equal to zero, which will be considered below.

III. NONEQUILIBRIUM INTERFACE

The solution of the Ginzburg-Landau equation (2) for a nonequilibrium plane interface moving in an infinite medium in x direction under stress-free conditions ($\psi^e = 0$) and $\rho_0 = \rho$ is[8]

$$\eta_{in} = \frac{1}{1+e^{-\zeta}}, \quad \zeta = k(x - ct), \tag{8}$$

$$k := \sqrt{\frac{2\rho_0[A(\theta) - 3\Delta G^\theta(\theta)]}{\beta}}, \quad c = \frac{6L\rho_0\Delta G^\theta(\theta)}{k}, \tag{9}$$

where c is the interface velocity. By the definition of the interface energy under a nonequilibrium condition (see, e.g., Ref. 7), it is equal to the excess energy with respect to H in the H region $x \leqslant x_i$ and with respect to L in the L region $x > x_i$:

$$\begin{aligned}\gamma &:= \int_{-\infty}^{x_i}\rho_0(\psi - \psi_H)dx + \int_{x_i}^{\infty}\rho_0(\psi - \psi_L)dx \\ &= \frac{\sqrt{2\beta\rho_0[A(\theta) - 3\Delta G^\theta(\theta)]}}{6} \\ &= 2\Psi^\nabla = \frac{\beta k}{6}, \quad \Psi^\nabla := \int_{-\infty}^{\infty}\rho_0\psi^\nabla dx\end{aligned} \tag{10}$$

(see the Appendix), where x_i is the interface position, at which we assume $\eta = 0.5$, and where Ψ^∇ is the gradient part of the total interface energy. An important result is that for a nonequilibrium interface the *total energy is twice the gradient energy*. This can be used as an initial guess for more sophisticated models, for which analytical solutions are not available. To obtain the biaxial interface tension in Eq. (7), one has to define with the help of Eq. (A2)

$$\begin{aligned}\breve{\psi}^\theta &:= [A(\theta) - 3\Delta\, G^\theta(\theta)]\eta^2(1-\eta)^2 \to \\ \tilde{\psi}^\theta &= f(\theta,\eta) - \breve{\psi}^\theta = \Delta G^\theta(\theta)\eta^2(3 - 2\eta).\end{aligned} \tag{11}$$

Substituting Eq. (11) in the expression for the surface tension (7), we obtain

$$\boldsymbol{\sigma}_{st} = \beta|\nabla\eta|^2(\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}) = 2\rho_0\breve{\psi}^\theta(\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{n}). \tag{12}$$

The magnitude of the force per unit interface length is equal to

$$\int_{-\infty}^{\infty}\beta|\nabla\eta_{in}|^2\,dx = 2\int_{-\infty}^{\infty}\rho_0\breve{\psi}dx = 2\Psi^\nabla = \gamma, \tag{13}$$

where Eqs. (A4) and (10) have been used. Thus, the magnitude of the force per unit interface length is equal to the nonequilibrium interface energy γ. This completes the proof that Eq. (7) for the surface tension transforms for the propagating interface to the desired expression.

Thus, by considering the gradient of the order parameter in the deformed state and multiplying the gradient energy and the function $\breve{\psi}$ determined by Eq. (11) by $\rho_0/\rho = 1 + \varepsilon_0$, we introduced in Eq. (7) an additional contribution to the stress tensor $\boldsymbol{\sigma}_{st}$, which is located at the diffuse interface ($\eta \neq 0$ and $\eta \neq 1$) and represents the surface tension (stress) tensor. For a propagating plane interface, the expression for surface tension reduces to the biaxial tension with the force per unit area equal to the surface energy γ, providing the correspondence with a sharp-interface approach. In the usual approximation[9]

$$\begin{aligned}A &= A_0(\theta - \theta_c), \quad A_0 > 0, \\ \Delta G^\theta(\theta) &= -\Delta s_0(\theta - \theta_e), \quad \Delta s_0 < 0,\end{aligned} \tag{14}$$

where θ_c is the critical temperature at which the stress-free H loses its thermodynamic stability and Δs_0 is the difference in entropy between L and H at $\theta = \theta_e$, one obtains for the interface energy and the magnitude of the biaxial surface stresses

$$\begin{aligned}\gamma &= \frac{\beta k}{6} = \frac{\sqrt{2\beta(\theta)\rho_0 A_0[(\theta - \theta_e)(1 - \varpi) + (\theta_e - \theta_c)]}}{6}, \\ \varpi &:= -\frac{3\Delta s_0}{A_0},\end{aligned} \tag{15}$$

$$\begin{aligned}\sigma_{st} &:= 2\rho_0\breve{\psi}^\theta = 2\rho_0 A_0[(\theta - \theta_e)(1 - \varpi) \\ &\quad + (\theta_e - \theta_c)]\eta_{in}^2(1 - \eta_{in})^2,\end{aligned} \tag{16}$$

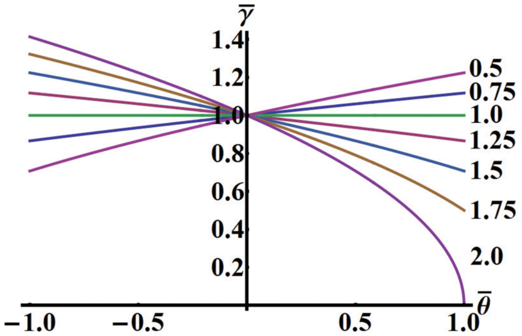

FIG. 1. (Color online) Dependence of the dimensionless nonequilibrium interface energy $\bar{\gamma}$ on the dimensionless temperature $\bar{\theta}$ for various values of ϖ shown near the curves.

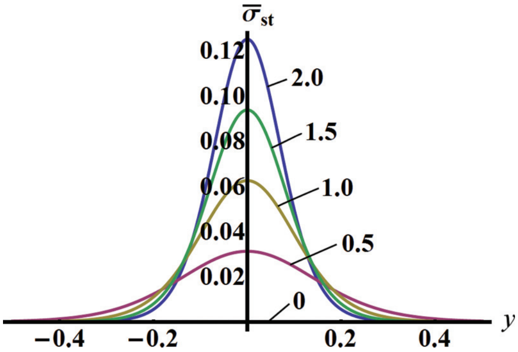

FIG. 2. (Color online) Distribution of the dimensionless magnitude of the biaxial surface tension $\bar{\sigma}_{st}(y)$ for a nonequilibrium interface for several parameters Π shown near the curves.

where the condition $\varpi \geqslant 0.5$ follows from Eq. (16) in Ref. 9. In the dimensionless form, the interface energy is

$$\bar{\gamma} := \frac{6\gamma}{\sqrt{2\beta(\theta)\rho_0 A_0(\theta_e-\theta_c)}} = \sqrt{\Upsilon}, \quad \bar{\theta} := \frac{\theta-\theta_e}{\theta_e-\theta_c},$$
$$\Upsilon := \bar{\theta}(1-\varpi)+1 \geqslant 0, \tag{17}$$

where $\bar{\theta}$ and Υ are the dimensionless temperature and a governing parameter that combines material properties and θ. Thus, for $\varpi = 1$, the temperature dependence of the interface energy is determined solely by $\beta(\theta)$. If β is independent of temperature, the same is true for the interface energy and it is the same as for θ_e. Note that $\varpi = 1$ corresponds to the case when θ_e is the average of the critical temperatures for the loss of stability of H and L.[9]

The relationship for the dimensionless interface energy $\bar{\gamma}$ vs $\bar{\theta}$ is presented in Fig. 1 for various values of ϖ. For $\theta = \theta_e$, $\bar{\gamma} = 1$ for any ϖ.

The deviation of $\bar{\gamma}$ from 1 increases with the magnitude of $\bar{\theta}$ and $1-\varpi$. Since for small $\bar{\theta}(1-\varpi)$ one has $\bar{\gamma}-1 \simeq 0.5\bar{\theta}(1-\varpi)$, the magnitude of the deviation of $\bar{\gamma}$ from 1 is an odd function of $\bar{\theta}$ and $1-\varpi$. For a larger magnitude of $\bar{\theta}(1-\varpi)$, the interface energy has a greater tendency to be reduced than to increase for $|\Upsilon| \leqslant 1$. For $\varpi < 1$ (or $\varpi > 1$), the interface energy grows (is reduced) with increasing temperature. Note that the solution for a propagating interface exists even for $\bar{\theta} > 1$ and $\bar{\theta} < -1$ (i.e., above and below the temperatures for which a minimum corresponding to one of the phases exists), provided that $\Upsilon \geqslant 0$.

Let us present for $t = 0$

$$e^{-\zeta} = e^{-10[k(\theta)/k(\theta_e)]y} = e^{-10\sqrt{\Upsilon[\beta(\theta_e)/\beta(\theta)]}y} = e^{-10\sqrt{\Pi}y}, \tag{18}$$

$$y := \frac{k(\theta_e)}{10}x, \quad \Pi := \Upsilon\frac{\beta(\theta_e)}{\beta(\theta)}, \tag{19}$$

where the factor of 10 is the approximate width of the diffuse interface $\eta_{in}(\zeta)$ in Eq. (8). The width δ of the diffuse interface $\eta_{in}(x)$ and its normalized value are

$$\delta := \frac{10}{k(\theta)}, \quad \bar{\delta} := \frac{\delta(\theta)}{\delta(\theta_e)} = \frac{k(\theta_e)}{k(\theta)} = \frac{1}{\sqrt{\Pi}}. \tag{20}$$

Then the dimensionless magnitude of the surface stresses is

$$\bar{\sigma}_{st} := \frac{\sigma_{st}\beta(\theta_e)}{2\rho_0 A_0(\theta_e-\theta_c)\beta(\theta)} = \Pi\eta_{in}^2(1-\eta_{in})^2$$
$$= \Pi\left(\frac{e^{-10\sqrt{\Pi}y}}{(1+e^{-10\sqrt{\Pi}y})^2}\right)^2. \tag{21}$$

The maximum of $\bar{\sigma}_{st}$ is $\Pi/16$. A plot of $\bar{\sigma}_{st}(y)$ for several parameters Π is presented in Fig. 2. It can be seen that the width of the interface is reduced with increasing Π.

IV. INTERFACE STRESSES FOR A CRITICAL L NUCLEUS

The stationary 1D Ginzburg-Landau equation (2) can be transformed to[10]

$$0.5\beta\left(\frac{d\eta}{dx}\right)^2 = \rho_0[f(\theta,\eta) - \text{const}]. \tag{22}$$

For a critical L nucleus $[\eta_c(\pm\infty) = 0,\ \theta \leqslant \theta_e]$ one has const $= 0$,

$$\psi^\nabla = f(\theta,\eta_c), \quad \psi(\theta,\eta_c) = 2\psi^\nabla = 2f(\theta,\eta_c) \tag{23}$$

and

$$\boldsymbol{\sigma}_{st} = \rho_0\psi(\theta,\eta_c)(\boldsymbol{I}-\boldsymbol{n}\otimes\boldsymbol{n}) - \rho_0\tilde{\psi}^\theta(\theta,\eta_c)\boldsymbol{I}. \tag{24}$$

Thus, for a stationary solution, the magnitude of the biaxial surface tension is pointwise equal to the local total energy $\rho_0\psi(\theta,\eta)$; consequently, the total force is equal to the total energy of the nucleus. However, an additional mean stress $-\rho_0\tilde{\psi}^\theta$ acts at each point of the nucleus. The solution to Eq. (23) is[10]

$$\eta_c = 6\left[6 - P + \sqrt{P^2-3P}\cosh\left(20\sqrt{\bar{\theta}+1}\frac{x}{l}\right)\right]^{-1}, \tag{25}$$

$$P := \frac{4\varpi\bar{\theta}}{\bar{\theta}+1}, \quad l := 20\sqrt{\frac{2\beta}{\rho_0 A_0(\theta_e-\theta_c)}}, \tag{26}$$

where l is a typical width of the critical nucleus. Plots of the critical nucleus η_c and the distributions of the dimensionless magnitude of the biaxial surface tension $\tilde{\sigma}_{st} := \frac{\psi(\theta,\eta_c)}{A_0(\theta_e-\theta_c)}$ and mean stress $p := -\frac{\tilde{\psi}^\theta(\theta,\eta_c)}{A_0(\theta_e-\theta_c)}$ in the nucleus are shown in Fig. 3 for $\varpi = 1$ and three temperatures. It is clear that the surface tension is concentrated at the incomplete interfaces and is zero

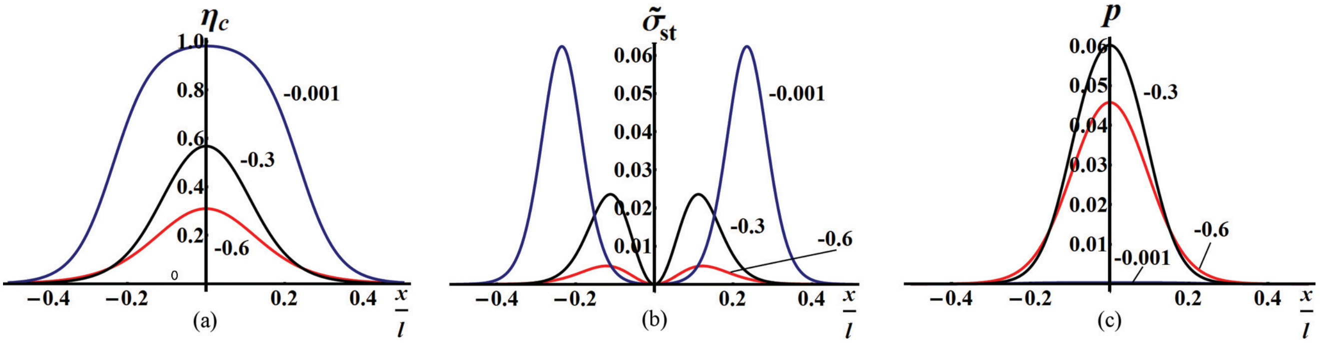

FIG. 3. (Color online) Plots of the critical nucleus profile $\eta_c(x/l)$ (a) and the distributions of the dimensionless magnitude of the biaxial surface tension $\tilde{\sigma}_{st} := \psi(\theta,\eta_c(x/l))/A_0(\theta_e - \theta_c)$ (b) and mean stress $p := \tilde{\psi}^{\theta}(\theta,\eta_c(x/l))/A_0(\theta_e - \theta_c)$ (c) for $\varpi = 1$ and three temperatures shown near the curves.

at the center of a nucleus, while the mean stress is concentrated in the center. For $\bar{\theta} = -0.001$, the nucleus profile is close to two equilibrium H-L interfaces at $\bar{\theta} = 0$ and that is why the mean stress is negligible, in agreement with our requirement.

V. CONCLUDING REMARKS

In summary, a thermodynamically consistent approach is developed and Eqs. (7) and (11) for interface stresses are derived for the phase field approach. Analytical expressions for the temperature-dependent energy of the propagating interface and the distributions of surface stresses for the propagating interface and critical L nucleus are determined. Since the problem is reduced to the determination of a single function $\tilde{\psi}^{\theta}(\theta,\eta)$ and is unambiguously solved, the results obtained can be considered as exact ones. This allows one to apply them to various microstructures different from propagating interfaces and obtain results which do not have counterparts in the sharp-interface approach. In particular, for the critical L nucleus, the biaxial surface tension is pointwise equal to the local total energy and an additional mean stress $-\rho_0\tilde{\psi}^{\theta}$ acts at each point of the nucleus. In addition, using analytical solutions for critical H nuclei,[10] functionally graded structures in a sample smaller than the interface width,[11] or surface-induced pretransformed structures,[12] one can find the analytical distribution of the $\boldsymbol{\sigma}_{st}$ tensor even for other cases when a complete interface does not exist and study its effect on the corresponding processes when mechanics is included. Surface stresses can be introduced in the phase field approach for an external surface.[13] A new expression for the interface stresses can be introduced instead of the previous results in all our numerical studies for martensitic phase transformations and melting, especially for nano-objects[7] and when stresses and stress relaxation at the interfaces are the main concern.[7,13] This will allow a more precise study of surface-stress-induced phase transformations in nanowires[14] and the contribution of surface stresses to the formation of nanometer-sized third phases at the interfaces between phases[15] and within grain boundaries.[16] Elastic interface stresses were not discussed in the current paper because they are determined in the same way as in Refs. 7 and 13, thus completing an advanced model for a coherent interface. This may lead to a more detailed phase field approach study of the surface phenomena which are currently treated using the sharp-interface approach,[17] including surface instabilities.[18] In most cases, the above processes occur far from the equilibrium temperature, which makes our temperature-dependent solution of special importance. After solution of the coupled phase field and mechanics boundary value problems,[7,13] the interface stresses can be compared to those obtained in atomistic simulations.[19] The developed approach can be applied for phase field approaches with different potentials (e.g., six-degree potentials, potentials in hyperspherical order parameters,[8,10] or two-parabola potentials).[12] The generalization for an anisotropic interface energy with $\beta = \beta(\boldsymbol{n})$ is straightforward[5] because it does not affect the division of f into two contributions in Eq. (11). The generalization for large strains can be done using approaches from Refs. 6 and 20. Similar developments can be applied for various phenomena described by the phase field approach, such as various phase transformations (martensitic,[1,6,20] reconstructive,[21] and electromagnetic phase transformations,[22] melting-freezing,[7,23] amorphization), diffusive phase transformations described by Cahn-Hilliard theory (e.g., spinodal decomposition, segregation, separation, and precipitation),[24] twinning,[20,25] grain evolution,[26] dislocations,[27] fracture,[28] and interaction of defects (cracks and dislocations) and phase transformations.[29] Finally, the expression obtained for the surface stresses can be included in commercial multyphysics codes, like COSMOL,[30] instead of the current simplified expressions.

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APPENDIX

One property of the solution Eq. (8) is

$$\frac{d\eta_{in}}{d\zeta} = \eta_{in}(1 - \eta_{in}). \qquad \text{(A1)}$$

Using this and the definition of k in Eq. (8), we obtain an important relationship for the points of a propagating interface:

$$\psi^{\nabla} = \frac{\beta}{2\rho_0}|\nabla\eta_{in}|^2 = \frac{\beta k^2}{2\rho_0}\left(\frac{d\eta_{in}}{d\zeta}\right)^2$$
$$= [A(\theta) - 3\Delta G^{\theta}(\theta)]\eta_{in}^2(1 - \eta_{in})^2. \qquad \text{(A2)}$$

We have in Eq. (10) $\psi_H = 0$, $\psi_L = \Delta G(\theta)$, and it follows from the condition $\eta = 0.5$ in Eq. (8) that $\zeta_i = 0$. Thus,

$$\begin{aligned}\gamma &:= \frac{\rho_0}{k}\int_{-\infty}^{0} \psi\, d\zeta + \frac{\rho_0}{k}\int_{0}^{\infty} [\psi - \Delta G(\theta)] d\zeta \\ &= \frac{\rho_0}{k}\int_{-\infty}^{\infty} A(\theta)\eta_{in}^2(1-\eta_{in})^2 d\zeta + \Psi^{\nabla} + \frac{\rho_0 \Delta G(\theta)}{k} \\ &\quad \times \left(\int_{-\infty}^{0} \eta_{in}^3(4-3\eta_{in}) d\zeta + \int_{0}^{\infty} [\eta_{in}^3(4-3\eta_{in}) - 1] d\zeta\right), \end{aligned} \tag{A3}$$

$$\Psi^{\nabla} := \int_{-\infty}^{\infty} \rho_0 \psi^{\nabla} dx = \frac{k\beta}{2}\int_{-\infty}^{\infty}\left(\frac{d\eta_{in}}{d\zeta}\right)^2 d\zeta. \tag{A4}$$

Evaluating the integrals with the help of Eqs. (A1) and (8) for k, one obtains the results in Eq. (10). For an equilibrium interface, substituting $\Delta G^{\theta} = 0$ in Eqs. (A2) and (10) results in the known relationships (see, e.g., Ref. 10)

$$\begin{aligned}\psi^{\nabla} &= A(\theta_e)\eta_{in}^2(1-\eta_{in})^2 \quad \text{and} \\ \gamma_e &= 2\Psi^{\nabla} = \sqrt{2\beta\rho_0 A(\theta_e)}/6. \end{aligned} \tag{A5}$$

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[1] Y. M. Jin, A. Artemev, and A. G. Khachaturyan, Acta Mater. **49**, 2309 (2001); L. Q. Chen, Annu. Rev. Mater. Res. **32**, 113 (2002); R. Ahluwalia, T. Lookman, and A. Saxena, Phys. Rev. Lett. **91**, 055501 (2003); V. I. Levitas, A. V. Idesman, and D. L. Preston, *ibid.* **93**, 105701 (2004); Y. Z. Wang and A. G. Khachaturyan, Mater. Sci. Eng., A **438**, 55 (2006); T. Lookman, A. Saxena, and R. C. Albers, Phys. Rev. Lett. **100**, 145504 (2008); W. F. Rao, M. Wuttig, and A. G. Khachaturyan, *ibid.* **106**, 105703 (2011).

[2] D. A. Porter and K. E. Easterling, *Phase Transformation in Metals and Alloys* (Van Nostrand–Reinhold, New York, 1992).

[3] J. Lowengrub and L. Truskinovsky, Proc. R. Soc. London, A **454**, 2617 (1998).

[4] D. M. Anderson, G. B. McFadden, and A. A. Wheeller, Physica D **151**, 305 (2001).

[5] A. A. Wheeller and McFadden, Proc. R. Soc. London, A **453**, 1611 (1997).

[6] V. I. Levitas and M. Javanbakht, Phys. Rev. Lett. **105**, 165701 (2010); Int. J. Mater. Res. **102**, 652 (2011).

[7] V. I. Levitas and K. Samani, Nat. Commun. **2**, 284 (2011); Phys. Rev. B **84**, 140103(R) (2011).

[8] V. I. Levitas, D.-W. Lee, and D. L. Preston, Int. J. Plast. **26**, 395 (2010).

[9] V. I. Levitas and D. L. Preston, Phys. Rev. B **66**, 134206 (2002).

[10] V. I. Levitas, D. L. Preston, and D.-W. Lee, Phys. Rev. B **68**, 134201 (2003).

[11] V. I. Levitas, D.-W. Lee, and D. L. Preston, Europhys. Lett. **75**, 84 (2006).

[12] R. Lipowsky, Phys. Rev. Lett. **49**, 1575 (1982); B. F. Henson and J. M. Robinson, *ibid.* **92**, 246107 (2004); V. I. Levitas, D.-W. Lee, and D. L. Preston, Europhys. Lett. **76**, 81 (2006).

[13] V. I. Levitas and M. Javanbakht, Phys. Rev. Lett. **107**, 175701 (2011).

[14] J. Diao, K. Gall, and M. L. Dunn, Nat. Mater. **2**, 656 (2003); H. S. Park, K. Gall, and J. A. Zimmerman, Phys. Rev. Lett. **95**, 255504 (2005).

[15] J. Luo and Y.-M. Chiang, Annu. Rev. Mater. Res. **38**, 227 (2008); A. M. Alsayed *et al.*, Science **309**, 1207 (2005); V. I. Levitas, B. F. Henson, L. B. Smilowitz, and B. W. Asay, Phys. Rev. Lett. **92**, 235702 (2004); J. Phys. Chem. B **110**, 10105 (2006); M. Baram, D. Chatain, and W. D. Kaplan, Science **332**, 206 (2011); V. I. Levitas, Phys. Rev. Lett. **95**, 075701 (2005).

[16] A. E. Lobkovsky and J. A. Warren, Physica D **164**, 202 (2002).

[17] F. D. Fischer *et al.*, Prog. Mater. Sci. **53**, 481 (2008); F. Delogu, J. Phys. Chem. B **110**, 12645 (2006).

[18] M. A. Grinfeld, *Thermodynamic Methods in the Theory of Heterogeneous Systems* (Longman, Sussex, 1991); Dokl. Akad. Nauk SSSR (Moscow) **251**, 824 (1980).

[19] T. Frolov and Y. Mishin, Phys. Rev. B **79**, 045430 (2009); Modell. Simul. Mater. Sci. Eng. **18**, 074003 (2010).

[20] V. I. Levitas, V. A. Levin, K. M. Zingerman, and E. I. Freiman, Phys. Rev. Lett. **103**, 025702 (2009).

[21] C. Denoual, A. M. Caucci, L. Soulard, and Y. P. Pellegrini, Phys. Rev. Lett. **105**, 035703 (2010).

[22] J. Slutsker, A. Artemev, and A. L. Roytburd, Phys. Rev. Lett. **100**, 087602 (2008); A. Artemev and A. L. Roytburd, Integr. Ferroelectr. **126**, 125 (2011).

[23] J. Slutsker, K. Thornton, A. L. Roytburd, J. A. Warren, and G. B. McFadden, Phys. Rev. B **74**, 014103 (2006).

[24] Y. Lu, C. Wang, Y. Gao, R. Shi, X. Liu, and Y. Wang, Phys. Rev. Lett. **109**, 086101 (2012); S. Inagaki and K. Yoshikawa, *ibid.* **105**, 118001 (2010); Q. Bronchart, Y. Le Bouar, and A. Finel, *ibid.* **100**, 015702 (2008).

[25] J. D. Clayton and J. Knap, Physica D **240**, 841 (2011).

[26] R. Kobayashi, J. A. Warren, and W. C. Carter, Physica D **140**, 141 (2000).

[27] D.-W. Lee, H. Kim, A. Strachan, and M. Koslowski, Phys. Rev. B **83**, 104101 (2011); Y. U. Wang, Y. M. Jin, A. M. Cuitino, and A. G. Khachaturyan, Acta Mater. **49**, 1847 (2001); V. I. Levitas and M. Javanbakht, Phys. Rev. B **86**, 140101(R) (2012).

[28] A. Karma and A. E. Lobkovsky, Phys. Rev. Lett. **92**, 245510 (2004); H. Henry and H. Levine, *ibid.* **93**, 105504 (2004).

[29] A. A. Boulbitch and P. Toledano, Phys. Rev. Lett. **81**, 838 (1998); A. Boulbitch and A. L. Korzhenevskii, *ibid.* **107**, 085505 (2011).

[30] Computer code COMSOL, COMSOL, Inc., website: www.comsol.com