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Thermodynamically consistent and scale-dependent phase field approach for crack propagation allowing for surface stresses

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Keywords
Phase field, crack propagation, surface tension, scale-dependent model

Disciplines
Aerospace Engineering | Heat Transfer, Combustion | Mechanical Engineering | Polymer and Organic Materials | Structures and Materials

Comments

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Thermodynamically Consistent and Scale-Dependent Phase Field Approach for Crack Propagation Allowing for Surface Stresses

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Abstract
A thermodynamically-consistent phase field approach for crack propagation which includes the following novel features is presented. (1) Scale dependency was included by relating the length scale to the number of cohesive interatomic planes at the crack tip. Because of this, the developed theory is applicable from the atomistic to the macroscopic scales. (2) The surface stresses (tension) are introduced by employing some geometrical nonlinearities even in small strain theory. They produce multiple contributions to the Ginzburg-Landau equation for crack propagation. (3) Crack propagation in the region with compressive closing stresses is eliminated by employing a stress-state-dependent kinetic coefficient in the Ginzburg-Landau equation. (4) The importance of analysis of the thermodynamic potential in terms of stress-strain curves is shown. The developed theory includes a broad spectrum of the shapes of stress-strain relationships. The finite element method is utilized to solve the complete system of crack phase field and mechanics equations. The effect of the above novel features is analyzed numerically for various model problems.

Keywords: Phase field; crack propagation; surface tension; scale-dependent model.

1. Introduction
There are two different approaches to any type of structural changes in materials, like phase transformations, twinning, dislocations, grain growth, and fracture. One of them is based on the “sharp defect” approach, like sharp phase, twin, and grain boundary interfaces and sharp crack

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surface. There is a jump of some parameters across interfaces or singularity (for linear fracture mechanics) of fields near crack tip. These theories are usually scale-free. Another one, a phase field approach, considers a finite-size (or diffuse) defects, for the same defects and problems. All jumps and singularities disappear. Each approach has its own advantages and disadvantages. The phase field approaches provide possibility to describe evolution of arbitrary complex evolving geometry, including multivariant martensitic variants (Artemev et al., 2001; Levitas and Javanbakht, 2010 and 2011), dendrites (Karma and Rappel, 1998), and branched cracks (Aranson et al., 2000; Henry and Levine, 2004), without giving any a priori information and any extra computational efforts to track interfaces or crack trajectories. Also, interaction with continuous heterogeneity and discrete heterogeneities (precipitates, different interfaces, and inclusions) does not require extra computational efforts as well.

**Phase field approach.** As one of the most powerful tools for modeling the complexity of microstructure evolution, the phase field approach has been widely used for the simulation of fracture (Aranson et al., 2000; Karma et al., 2001; Henry and Levine, 2004; Hakim and Karma, 2005; Spatschek et al., 2006; Hakim and Karma, 2009; Kühn and Müller, 2010; Miehe et al., 2010; Bourdin et al., 2011; Fleck et al., 2011; Borden et al., 2014; Ambati et al., 2015; Duda et al., 2015; Wu, 2017), damage (Mozaffari and Voyiadjis, 2015; Mozaffari and Voyiadjis, 2016; Wu, 2017), dislocations (Levitas and Javanbakht, 2015a), martensitic phase transformations (Levitas and Preston, 2002; Levitas 2013a, 2013b, 2014), and some of their interactions (Spatschek et al., 2007; Levitas and Javanbakht, 2015b; Ruffini and Finel, 2015; Schmitt et al., 2015; Zhao et al., 2016; Mozaffari and Voyiadjis, 2016).

The order parameter in phase field models is treated as a thermodynamic variable, which describes some type of material instability during microstructure evolution. Here, we introduce $\phi$ as the damage order parameter for fracture and include it as an internal variable in the free energy. This order parameter characterizes bond breaking in a solid and divides any sample into the following three parts: intact solid ($\phi=0$), completely broken bonds ($\phi=1$), and the crack surface with a narrow width in which the material is partially broken ($0<\phi<1$). The evolution of the damage order parameter occurs mainly in the crack tip zone. Thus, the damage growth is characterized by the evolution of the order parameter described by the Ginzburg-Landau equation. The Ginzburg-Landau equation coupled with mechanics, i.e. kinematics, constitutive law, and equilibrium equations, are used to obtain the evolution of the order parameter and stress-strain fields.

All phase field models for fracture can be divided into two categories: a) The models with a double-well potential, like for phase transformations (Levitas and Preston, 2002; Levitas, 2014), and b) the model with a single-well potential.

**Models with double-well potential.** The first phase field model for crack propagation based on the Ginzburg-Landau equation for phase transition was introduced in Aranson et al. (2000), where the order parameter was related to the relative concentration of point defects in an
amorphous material. The coupled elastodynamic equations with pure dissipative kinetics were used to determine the displacement field and the evolution of the order parameter for mode I crack growth. Also, the KKL (Karma-Kessler-Levine) phase field model for mode III of fracture (Karma et al., 2001) was similar to the conventional phase field modeling of dendritic solidification, i.e. to phase transformation. This model overcame some limitations in the previous model (Aranson et al., 2000), which could not fully relieve the bulk stress and thus had certain nonphysical features, such as a logarithmic dependence of the crack opening on the system size (Karma et al., 2001). The KKL model (Karma et al., 2001) was extended to modes I and II of crack growth under the plane strain conditions in Henry and Levine (2004), with the same double-well term. The KKL model was generalized in Hakim and Karma (2005), Hakim and Karma (2009) to predict quasi-static crack paths in anisotropic brittle materials. The KKL potential originally had the double-well term related to the energy barrier between the gas and the solid states responsible for the local fracture energy. The KKL model is revised in Hakim and Karma (2009), so the double-well term was replaced with the critical elastic energy, i.e. $\Psi^c$. The one-dimensional analytical solution for the KKL model is presented in Hakim and Karma (2009). We will show some drawbacks of the KKL model in Appendix C by analyzing the stress-strain curve for the homogenous state.

The phase field model can also be used as a mathematical regularization tool rather than a physical approach. In this work, the interface or the surface is smeared over a diffuse region for the sake of convenience of numerical solution. This application has been used to solve free-boundary problems of crack growth on the basis of the late stage of the Asaro-Tiller-Grinfeld instability (Spatschek et al., 2006; Spatschek et al., 2007). The phase field energy density in this group of models also contains the double-well term. The double-well term also appears in phase field modeling of damage (Mozaffari and Voyiadjis, 2015; Mozaffari and Voyiadjis, 2016).

The double-well term in phase field potentials originates from phase field modeling of first-order phase transformation as an energy barrier for phase transformation (Levitas and Preston, 2002; Levitas, 2014). The approaches with a double-well barrier consider fracture as a solid-gas transformation. Physically, however, fracture is a bond breaking rather than a solid-gas phase transformation. This misinterpretation causes crack widening and lateral growth during crack propagation, which has been discussed in Levitas et al. (2011), Bourdin et al. (2011). More details about the treatment of crack as phase transformation, by using double-well term, can be found in Farrahi et al. (2018).

Models with single-well potential. In contrast to phase field models with double-well potentials, there are some potentials with single-well energy, which are not related to phase transformation (Kuhn and Müller, 2010; Miehe et al., 2010; Bourdin et al., 2011; Borden et al., 2014; Ambati et al., 2015). Although there are similarities between these models and the previous type, there are several fundamental differences. Variational formulations for fracture and corresponding phase field modeling are presented in Francfort and Marigo (1998), Bourdin et al. (2000), Amor et al. (2009) to extend Griffith’s approach (Griffith, 1921). Potentials with single-well energy
eliminate some of the disadvantages of double-well potential, such as crack widening. In addition, it is possible to obtain a realistic stress-strain curve in this manner. However, they lack the flexibility needed to present the complex shape of the stress-strain curves obtained e.g. in atomistic simulations.

Besides the previous studies, which describe the nonlinear stress-strain curves in terms of weakening elastic moduli, there are some other models in which damage and stress-strain curve nonlinearities are described in term of eigen strain (Jin et al., 2001; Wang et al., 2002; Levitas et al., 2011). These models have some contradictions that will be discussed in Appendix D.

Surface tension. It is well known that each material interface or surface is subjected to biaxial stresses with the force per unit length, $T$ (Porter et al., 2009). For liquid-liquid and liquid-gas interfaces, which do not support elastic stresses and for which the surface stresses are independent of strain, the magnitude of the isotropic biaxial tensile stresses is equal to the surface energy $T=\gamma$. This causes a jump in normal stresses across an interface equal to $2\gamma\kappa$, where $\kappa$ is the mean interface curvature. The strain-dependent part, which is related to the surface elasticity and may be both tensile and compressive, appears for a solid surface or interface.

In the sharp surface approach, the surface stress tensor is related to the surface energy by $\sigma_s = \gamma I_s + \partial\gamma/\partial\varepsilon_s$, where $\varepsilon_s$ is the surface strain tensor and $I_s$ is the two-dimensional surface unit tensor (Cammarata and Sieradzki, 1994). This equation is usually used in literature to consider the effect of the surface stress on crack behavior (Chuang, 1987; Wang and Feng, 2007; Fu et al., 2008; Ou et al., 2008; Fu et al., 2010; Kim et al., 2011; Nan and Wang, 2012; Wang and Li, 2013; Li and Wang, 2015). The first part of the surface stress, $\gamma I_s$, is the residual surface stress, which is also called the structural part of the surface stress and is similar to that in liquids or gases. The second term, $\partial\gamma/\partial\varepsilon_s$, is the strain-dependent part of the surface stress. Based on the Gurtin-Murdoch surface elasticity model (Li and Wang, 2015), the linear constitutive law $\partial\gamma/\partial\varepsilon_s = C_s : \varepsilon$ is generally accepted in Wang and Feng (2007), Fu et al. (2008), Kim et al. (2009), Fu et al. (2010), Kim et al. (2010), Kim et al. (2011), Wang and Li (2013), Li and Wang (2015), where $C_s$ is the surface elastic moduli tensor; this suggests that the surface energy is a quadratic function of the surface strain. The elastic part of the surface stress can be neglected in the small strain framework (Ou et al., 2008; Wang and Li, 2013) because it is shown in atomistic simulations that the elastic constants in $C_s$ are of the same magnitude as $\gamma$ (Li and Wang, 2015). In addition, the material parameters for the surface are not known well. Another problem is uncertainty as to whether strong heterogeneity across the surface fields of properties, strains, and stresses can be formalized in terms of resultant stresses without moments.

The Griffith criterion for crack growth is based on the surface energy (Griffith, 1921) and neglects the surface stresses. However, large surface stresses act at sharp corners and a sharp crack tip. It was shown that the energy release rate can be negative in soft elastic materials with large surface stresses compared to elastic stresses, i.e. the surface tension can even cause crack healing (Liu et al., 2014). Due to the difficulties in surface stress measurements, there are few
quantitative predictions for the effect of surface stresses on crack growth. Surface stress was theoretically studied in Thomson et al. (1986) as line forces acting on the cleavage surface, whose influence on the stress intensity factor was investigated for the sharp crack tip. Wu (1999) analyzed an elliptic void with surface elasticity and concluded that the reduction of the applied stress intensity factor occurred due to surface stresses. Similar works for a crack tip have been done by using the surface elasticity theory for modes I (Wang and Feng, 2007; Fu et al., 2010; Wang and Li, 2013), II (Fu et al., 2008; Kim et al., 2011), III (Wang and Feng, 2007; Kim et al., 2009; Kim et al., 2010), and the mixed mode (Li and Wang, 2015). The crack tip curvature plays the main role in the strain-dependent part of the surface stress. The curvature radius not only affects the magnitude of stress, but also changes its deformation state from stretching to compression. Using data for the ionic crystals in Chuang (1987), it was shown that the stress-dependent part of the surface tension for SiO$_2$ glass is 3 times larger than the surface energy. Walton (2014) predicted that surface stresses would produce finite crack curvature and, consequently, finite crack-tip stresses and strains for plane strain deformations.

However, we are not aware of any works that include the surface stresses in the phase field approach to fracture. The problem of interface stresses was addressed in the phase field approach to phase transformations only. The most advanced theory is developed in Levitas and Javanbakht (2010), Levitas (2013b) for small strains and in Levitas (2014) and Levitas and Warren (2016) for large strains. The main point is that the elastic contribution to the surface stresses comes directly from the solution of the Ginzburg–Landau and elasticity equations, and the goal is to introduce the structural part of the surface stresses. To do this, the approach utilizes the gradient of the order parameters in the deformed configuration and the gradient and double-well energy defined per unit volume of the deformed configuration. This approach improves upon some earlier works (Wheeler and McFadden, 1997; Lowengrub and Truskinovsky, 1998; Anderson et al., 2001) in which the phase field is coupled to mechanics. The important point is that for liquid-liquid and liquid-vapor phase transformations, in contrast to solids, derivations are naturally presented in the deformed configuration and the free energy depends on the gradient of the order parameter in the deformed state. Because of this, some contributions to the interface stresses appear automatically. We will show in Appendix B that the approach to the surface stresses developed in the above works and based on energies per unit deformed volume is not applicable to the crack problem and that a new approach (see Sections 3.1 and 3.2) is required.

**Crack propagation under compressive stresses.** Traditional phase field models (Aranson et al., 2000; Karma et al., 2001; Hakim and Karma, 2009; Kuhn and Müller, 2010) do not distinguish between compressive and tensile loadings, which leads to unphysical crack propagation under compressive (closing) stresses. In Henry and Levine (2004), Miehe et al. (2010), Borden et al. (2014), Ambati et al. (2015), some parts of elastic energy, which are related to the compressive stresses/stRAINs by some definitions, are excluded from the driving force for crack propagation, which is energetically contradictory. Here, we present an alternative simple approach in which (a) the entire elastic energy reduction contributes to the driving force for crack propagation
(when crack can propagate), (b) but the kinetic coefficient is set to be zero if the stress normal to the crack surface is not tensile, which prevents crack propagation.

**Effect of spatial scales.** The question at which scale the crack propagation is considered within the phase field approach and how this is related to material properties is not properly treated in the literature. At the atomistic scale, the stress-strain curves and the corresponding elastic energy can be derived by using atomistic simulations and the maximum stresses are the theoretical strengths for tension, shear, etc. Critical stresses are much lower at macroscale. Here, we develop a phase field model which is applicable at an arbitrary scale. At macroscale, we implement a scale-dependent cohesive rule developed in Nguyen and Ortiz (2002) in the phase field approach. At nanoscale, we develop a two-parametric local elastic energy, which can be calibrated by atomistic simulations. We then apply scale-dependent interpolation between these two models, which is applicable for any intermediate scale.

The rest of the paper is organized as follows. The thermodynamics treatment for materials for which the Helmholtz energy depends on the order parameter and its gradient within small-strain formalism is presented in Section 2. Generalized force related to the gradient of the order parameter is included in the first law of thermodynamics. The elasticity rule, expression for the entropy, explicit expression for the driving forces for change in the order parameter, and Ginzburg-Landau equations are presented. In Section 3 we present the free energy, which includes the geometrically-nonlinear term producing surface stresses. The Ginzburg–Landau equation contains multiple terms due to surface stresses. The main requirements for thermodynamic potential terms, including the thermodynamic equilibrium conditions and instability conditions for homogeneous states, are formulated in Section 4. A general polynomial for a cohesive interpolation function that satisfies the formulated requirements is suggested. The equilibrium stress-strain curves for various values of the parameters in the interpolation function are presented in Section 5. A scale-dependent model, which interpolates between nanoscale and macroscale models, is suggested and analyzed in terms of stress-strain curves in Section 6. An analytical solution for the simplest version of the Ginzburg-Landau equation is presented and used for parameter calibration in Section 7. The total system of equations is summarized in Section 8. Numerical examples are presented in Section 9. Section 10 contains concluding remarks and future directions. Appendixes A-D contain some analysis of and comparisons with the previous (phase field) models for crack growth and surface stresses.

Outer and inner products between second-order tensors \( A = \{ A_i \} \) and \( B = \{ B_i \} \) are denoted by \( A \cdot B = \{ A_i B_j \} \) and \( A : B = \{ A_i B_j \} \), respectively; \( a \otimes b \) also represents a dyadic product of vectors \( a = \{ a_i \} \) and \( b = \{ b_i \} \); \( I \) and \( 0 \) are second-order unit and null tensors, respectively; \( A^T, A^{-1}, \nabla A, tr \) \( A \) and \( \dot{A} \) are the transpose, inverse, gradient (with respect to undeformed configuration), trace, and time derivative of \( A \), respectively; := stand for equality by definition.
2. General thermomechanical model

The general thermodynamic treatment will follow our works on phase field approach to phase transformations (Levitas, 2013a; Levitas, 2013b; Levitas, 2014).

Kinematics is described by the conventional relationship between the strain and the gradient of displacement in the small strain approximation

$$\varepsilon = \varepsilon_c = \frac{1}{2}[(\nabla u) + (\nabla u)^T].$$  

Still, some features of geometrically-nonlinear formulation will be utilized below (see Sections 3.1 and 3.2) to introduce surface stresses. The same was done in the phase field approach to phase transformations (Levitas, 2013b), but in very different way.

The laws of thermodynamics are written below for an arbitrary volume $V_0$ with an external surface $S_0$ that includes cracks. Cracks do not represent discontinuities in displacement, but rather narrow regions with a strong variation of the order parameter. The first law of thermodynamics is presented as:

$$\int_{S_0} (p \cdot \dot{u} - h \cdot n + G \phi \cdot n) dS_0 + \int_{V_0} (f \cdot \dot{u} + r) dV_0 = \frac{d}{dt} \int_{V_0} (U + \rho_0 \frac{u^2}{2}) dV_0.\) (2)

Here, $p$ is the traction vector acting on the boundary surface $S_0$; $u$ is the displacement vector; $h$ is the heat flux vector; $n$ is the unit outward normal to the boundary; $f$ is the body force per unit volume; $r$ is the specific volumetric heat supply rate; $U$ is the internal energy per unit undeformed volume; and $\rho_0$ is the initial density of the material. The vector $G$ (more precisely, its projection $G \cdot n$) represents the generalized surface force conjugate to $\phi$ at the surface. $G$ is introduced to balance the terms that appear due to the dependence of the free energy on the gradient of the order parameter. Without this term, Eq. (2) cannot be applied to an arbitrary volume and, consequently, cannot be localized. The second law of thermodynamics is a combination of the global entropy balance with the Clausius-Duhem inequality:

$$S_i := \frac{d}{dt} \int_{V_0} s dV_0 - \int_{V_0} r dV_0 + \int_{S_0} h \cdot n dS_0 \geq 0,\) (3)

where $S_i$ is the rate of total entropy production; $s$ is the entropy per unit volume, and $\theta$ is the temperature. Using the relationship between the Cauchy stress and the traction vector, conservation of mass, and Gauss’s divergence theorem, we transform the surface integral in Eq. (2) into a volumetric integral:

$$\int_{V_0} (\sigma : \varepsilon - \dot{U} - \nabla \cdot h + r + \nabla \cdot (G \phi)) dV_0 + \int_{V_0} (\nabla \cdot \sigma + f - \rho_0 a) \cdot \dot{u} dV_0 = 0,\) (4)

where $a$ is the acceleration vector. The objectivity property with respect to translational motion results in the equation of motion $\nabla \cdot \sigma + f - \rho_0 a$ without being affected by $G$. Thus, even with the extra surface force, the momentum balance remains the same.
Similarly, Eq. (3) reduces to

\[ S_i := \int_{V_i} (\dot{s} - \frac{r}{\theta} + \nabla \cdot \frac{h}{\theta}) dV_i \geq 0 . \]

(5)

Because we can make the volume infinitesimal, this results in the local form of the first and second laws of thermodynamics:

\[ \sigma : \dot{\varepsilon} - \dot{U} - \nabla \cdot \hat{h} + r + \nabla \cdot (G\dot{\phi}) = 0 ; \]

\[ D := \theta \dot{s} - r + \nabla \cdot \hat{h} - \frac{\nabla \theta}{\theta} \cdot \hat{h} \geq 0 , \]

where \( D \) is the dissipation rate. By combining Eqs. (6) and (7), we obtain

\[ D := \sigma : \dot{\varepsilon} - \dot{U} + \theta \dot{s} + \nabla \cdot (G\dot{\phi}) - \frac{\nabla \theta}{\theta} \cdot \hat{h} \geq 0 . \]

(8)

We assume that this inequality is separated into two stronger inequalities for mechanical and thermal dissipation rates:

\[ D_{\text{mech}} = \sigma : \dot{\varepsilon} - \dot{U} - \theta \dot{s} + \nabla \cdot (G\dot{\phi}) \geq 0 ; \]

\[ D_{\text{ther}} = -\frac{\nabla \theta}{\theta} \cdot \hat{h} \geq 0 . \]

(9)

(10)

It is more convenient to use the Helmholtz free energy per unit volume \( \psi = U - \theta s = \psi(\varepsilon, \theta, \phi, \nabla \phi) \) and transform

\[ D_{\text{mech}} = \sigma : \dot{\varepsilon} - \dot{\psi} - s \dot{\theta} + (\nabla \cdot G) \dot{\phi} + G \cdot \nabla \phi \geq 0 , \]

(11)

where we used

\[ \nabla \cdot (G\dot{\phi}) = (\nabla \cdot G) \dot{\phi} + G \cdot \nabla \phi. \]

(12)

Differentiating the free energy and using Eq. (12) results in:

\[ D_{\text{mech}} = (\sigma - \frac{\partial \psi}{\partial \varepsilon}) : \dot{\varepsilon} - (s + \frac{\partial \psi}{\partial \theta}) \dot{\theta} + (G - \frac{\partial \psi}{\partial \phi}) \cdot (\nabla \phi) + (G \cdot \nabla \phi - \frac{\partial \psi}{\partial \phi}) \dot{\phi} \geq 0 . \]

(13)

Assuming independency of the dissipation rate on \( \varepsilon, \theta \), and \( \nabla \phi \), we obtain the expression for stress and entropy

\[ \sigma = \frac{\partial \psi}{\partial \varepsilon} ; \]

\[ s = -\frac{\partial \psi}{\partial \theta} , \]

(14)

(15)

and the definition of the generalized force

\[ G = \frac{\partial \psi}{\partial \nabla \phi} . \]

(16)
Eq. (13) then simplifies to
\[ D_{\text{mech}} = \dot{\chi} \geq 0, \quad \dot{\chi} = \nabla \cdot \left( \frac{\partial \psi}{\partial \nabla \phi} \right) - \frac{\partial \psi}{\partial \phi}, \]  
(17)
where \( \dot{\chi} \) is the thermodynamic driving force conjugate to the rate of the order parameter, \( \dot{\phi} \).

Traditionally, assuming a linear relationship between the driving force and rate, we obtain the Ginzburg-Landau equation:
\[ \dot{\phi} = L \dot{\chi}, \]  
(18)
where \( L \) is the kinetic coefficient.

3. Phase field model

3.1. Expression for the energy

The free energy per unit undeformed volume is expressed as
\[ \psi = \psi^e(\phi, \varepsilon) + (1 + I_z : \varepsilon) \left( \psi^c(\phi) + \psi^s(\nabla \phi) \right), \]  
(19)
where \( \psi^e, \psi^c, \psi^s \) are the elastic, cohesion, and gradient contributions to the energy; \( I_z = I - m \otimes m = k \otimes k + t \otimes t \) is the two-dimensional unit tensor within constant \( \phi \) surfaces; \( m = \nabla \phi / |\nabla \phi| \) is a unit vector in the direction of \( \nabla \phi \), i.e. orthogonal to the constant \( \phi \) surfaces; \( k \) and \( t \) are the mutually-orthogonal unit vectors that are also orthogonal to \( m \) (see Fig. 1). Note that \( I_z = I_z : \varepsilon \) is the strain tensor of constant \( \phi \) surfaces and \( \varepsilon = I_z : \varepsilon = (k \otimes k + t \otimes t) : \varepsilon = (dS - dS_0) / dS_0 \) is the relative change in surface area from the initial \( dS_0 \) to the current \( dS \) value.

When a crack appears, constant \( \phi \) contours coincide with the crack surfaces. The multiplier \( 1 + I_z : \varepsilon \) is included to obtain biaxial surface stresses with the magnitude of the resultant force equal to the surface energy (see Eqs. (25)-(27) below). As we will see, the term \( \psi^c(\phi) + \psi^s(\nabla \phi) \) produces the surface energy \( \gamma \) per unit undeformed area and multiplication by \( dS / dS_0 \) produces the surface energy per unit deformed area. Thus, instead of \( \gamma dS_0 \), we introduce the term \( \gamma dS \), which produces surface tension in classical thermodynamics (see e.g. Porter et al. (2009)). Although we consider small strain theory and \( I_z : \varepsilon \) is negligible in comparison with unity in Eq. (19), these terms provide a finite contribution to the derivative of the energy with respect to strain, i.e. to stresses. Thus, even in the context of small strains, we retain some of the geometric nonlinearity that is required for reproducing surface stresses. Note that, for curved surfaces, the normal \( m = \nabla \phi / |\nabla \phi| \) varies in space.
Fig. 1. A crack with the finite width surfaces described by the level surfaces of the order parameter $\phi = \text{const}$ and designation of the mutually orthogonal unit vectors $m, k, t$ and distribution of the surface stresses $\sigma_{st}$. Vector $m$ is orthogonal to the level surfaces and vectors $k$ and $t$ are within level surfaces. Surface stresses have the same components along vectors $k$ and $t$, i.e., they are isotropic within level surfaces $\phi = \text{const}$.

**Gradient energy** is accepted in the traditional form for isotropic material:

$$\psi^v = \frac{\beta}{2} |\nabla \phi|^{2}; \quad \beta \geq 0. \quad (20)$$

**Elastic energy** per unit undeformed volume is accepted in the form

$$\psi'(\phi, \varepsilon) = I(\phi) \Psi' = I(\phi)\left(\frac{1}{2} \varepsilon : C_2 : \varepsilon + \frac{1}{3!} (\varepsilon : C_3 : \varepsilon) : \varepsilon + \frac{1}{4!} (\varepsilon : C_4 : \varepsilon) : \varepsilon + \ldots \right). \quad (21)$$

Here, $\Psi'$ is the elastic energy of damage-free material, $C_k$ is the $k$th-order elastic moduli tensors of the intact state, and the monotonously decreasing degradation function $I(\phi)$ will be defined below. When higher-order in strain terms are neglected, Eq. (21) reduces to its traditional form.

**Cohesion energy** $\psi^c(\phi)$, which is associated with the damage, is as usual accepted as

$$\psi^c(\phi) = A f(\phi), \quad (22)$$

where $A$ is the maximum cohesion energy for the completely-damaged state and $f(\phi)$ is the function that will be determined below.

3.2. Elastic and Surface Stresses

Combining Eqs. (14) and (19) results in the following expression for the stresses

$$\sigma = \frac{\partial \psi}{\partial \varepsilon} = \frac{\partial \psi^v}{\partial \varepsilon} + (\psi' + \psi^v)(I - m \otimes m). \quad (23)$$
We decompose the stress tensor into the elastic stress tensor $\sigma_e$, which is the same as the stress in bulk and in the previous phase field models for fracture, and the structural or surface stress part $\sigma_{ss}$, which has appeared in the damaged zone and crack surfaces due to the geometric nonlinearities introduced above:

$$\sigma = \sigma_e + \sigma_{ss},$$  \hspace{1cm} (24)

$$\sigma_e = \frac{\partial \psi^e}{\partial \varepsilon} = I(\phi) \left( C_2 : \varepsilon + \frac{1}{2} \varepsilon : C_3 : \varepsilon + \frac{1}{3!} \varepsilon : (C_4 : \varepsilon) + ... \right) = I(\phi) F(\varepsilon),$$ \hspace{1cm} (25)

$$\sigma_{ss} = \sigma_{ss} (I - m \otimes m) = \sigma_{ss} I_2 = \sigma_{ss} (k \otimes k + t \otimes t),$$ \hspace{1cm} (26)

where

$$\sigma_{ss} = \psi^e + \psi^s.$$

The surface tension can be expressed in the coordinate form:

$$\sigma_{ss} = \sigma_{ss} (I - m \otimes m) = -\left( \frac{(\psi^e + \psi^s)}{(\frac{\partial \phi}{\partial x})^2 + (\frac{\partial \phi}{\partial y})^2 + (\frac{\partial \phi}{\partial z})^2} \left[ \frac{\partial \phi}{\partial x} \frac{\partial \phi}{\partial y} + \frac{\partial \phi}{\partial y} \frac{\partial \phi}{\partial z} + \frac{\partial \phi}{\partial z} \frac{\partial \phi}{\partial x} \right] \right),$$ \hspace{1cm} (28)

where $x, y,$ and $z$ are the orthogonal Cartesian coordinates. The schematic of the surface stress distribution is shown in Fig. 1.

Let us consider an elastic-stress-free crack surface far away from the crack tip. The distribution of the order parameter can be considered to be one-dimensional, varying along the coordinate $\xi$ along the normal $m$. The resultant force for each crack surface $T$ and the energy of the crack surfaces is defined as an excess energy with respect to bulk material:

$$T = 0.5 \int_{-\infty}^{+\infty} \sigma_{ss} d\xi; \quad \psi^{surf} = 2\gamma = \int_{-\infty}^{+\infty} (\psi^e + \psi^s) d\xi = \int_{-\infty}^{+\infty} \sigma_{ss} d\xi = 2T,$$ \hspace{1cm} (29)

where we took into account that the crack possesses two material surfaces. Thus, according to Eqs. (27)-(29), the surface stresses represent biaxial tension along the surface with equal magnitude in all directions and with the resultant force equal to the surface energy. Thus, all desired conditions are fulfilled, which justifies introducing the term $\varepsilon_{ss} = I_2 : \varepsilon$ in Eq. (19).

Because the nonzero order parameter is localized in a thin surface layer (see Eq. (85) and Fig. 6), $\psi^e + \psi^s$ and the surface stresses are localized in this region as well and get zero away from the surfaces.

3.3. Ginzburg-Landau equation

After substituting the expressions for the energy (20)-(22) in Eq. (17), we obtain an explicit evolution equation for the order parameter:
\[
\frac{\dot{\phi}}{L} = -\frac{\partial \psi}{\partial \phi} + \nabla \cdot [(1 + I_2 : \varepsilon) \beta \nabla \phi - \beta \left(1 + \frac{\psi'}{\psi} \right) \nabla \phi \cdot \varepsilon \cdot I_2] = \\
-\frac{\partial \psi'}{\partial \phi} + \beta (1 + I_2 : \varepsilon) \nabla^2 \phi + \beta (I_2 : \nabla \varepsilon - 2m \cdot \nabla m) \cdot \nabla \phi - \\
\beta \left(1 + \frac{\psi'}{\psi} \right) (\nabla \nabla \phi : (I_2 : \varepsilon) + \nabla \phi \cdot (\nabla \varepsilon : I_2) - m \cdot \varepsilon \cdot (m \nabla^2 \phi + m \cdot (\nabla \nabla \phi)^T)) - \\
2(\psi') m \cdot (m \cdot \varepsilon \cdot I_2) + \frac{2 \beta \psi'}{\psi} m \cdot (\nabla \nabla \phi) \cdot (m \cdot \varepsilon \cdot I_2).
\] 

Eq. (30) describes crack nucleation and propagation. The current Ginzburg-Landau equation explicitly includes additional terms related to the surface stresses. This is in contrast to results for phase transformations (Levitas, 2014), in which interface stresses do not have a direct effect on the driving force for phase transformation. For phase transformations, interfacial stresses change elastic stresses through the equilibrium equation, thus implicitly affecting the driving force.

In a component form, Eq. (30) is presented as

\[
\frac{\dot{\phi}}{L} = -\frac{\partial \psi}{\partial \phi} + \beta (1 + I_{2,\beta}) \nabla^2 \phi + \beta (\epsilon_{i,j,k} I_{2,\mu} - \epsilon_{i,j,k} (m_{j,k,n} + m_{j,k,m})) \phi_{i,k} - \\
\beta \left(1 + \frac{\psi'}{\psi} \right) (\phi_{i,j,k} I_{2,\mu} + \phi_{j,i,k} I_{2,\mu} - \phi_{j,i,k} (m_{j,k,n} + m_{j,k,m})) - \\
\frac{(\psi') (\nabla \phi)^2 \phi_{i,k} - 2 \psi^2 \phi_{i,k} \nabla \phi \cdot (\phi_{i,j,k} I_{2,\mu})}{0.5 |\nabla \phi|^2}.
\] 

In small strain theory, when we neglect all terms proportional to strain \(\varepsilon\), Eq. (30) simplifies to:

\[
\frac{\dot{\phi}}{L} = -\frac{\partial \psi}{\partial \phi} + \beta \nabla^2 \phi + \beta (I_2 \cdot \nabla \varepsilon) \cdot \nabla \phi - \beta \left(1 + \frac{\psi'}{\psi} \right) (\nabla \phi \cdot (\nabla \varepsilon : I_2)) ,
\] 

or in component form

\[
\frac{\dot{\phi}}{L} = -\frac{\partial \psi}{\partial \phi} + \beta \nabla^2 \phi + \beta (\epsilon_{i,j,k} I_{2,\mu}) \phi_{i,k} - \beta \left(1 + \frac{\psi'}{\psi} \right) (\phi_{i,j,k} I_{2,\mu}) .
\] 

Neglecting \(\nabla \varepsilon\) as well leads to the conventional Ginzburg-Landau equation

\[
\frac{\dot{\phi}}{L} = -\frac{\partial \psi}{\partial \phi} + \beta \nabla^2 \phi .
\] 

Using Eq. (34) leads to the same effect of surface stresses on the Ginzburg-Landau equation as for phase transformations (Levitas, 2014), i.e. merely changing elastic stresses and, consequently, strains due to their contribution to the mechanical equilibrium equations.

### 3.3.1. Kinetic coefficient

It is known that crack cannot open under compressive stresses normal to the crack surface. This was first mimicked in Henry and Levine (2004), whose main difference from the previous
models (Aranson et al., 2000; Karma et al., 2001) was that it distinguished between the elastic energies for compression ($\varepsilon < 0$) and tension ($\varepsilon > 0$). Elastic energy for compression was artificially excluded from the coupling to the order parameter, i.e., it did not contribute to the driving force for the crack growth. In Miehe et al. (2010), the principle strain components are divided into positive (tensile) and negative (compressive) parts; the part of the stored energy that is expressed in terms of positive principle strains only is multiplied by the degradation function and contributes to the driving force for crack growth. In both approaches, if the release of compressive stresses acting along the crack surfaces occurs, it does not affect the driving force for crack propagation, which is counterintuitive. According to the expression for the $J$-integral, the total elastic energy reduction is the driving force for crack propagation. We present an alternative approach in which the entire elastic energy contributes to the driving force for crack growth, with an additional condition that the stress normal to the crack surface should be tensile. Thus, without changing the expression for elastic energy, we define the kinetic coefficient as

$$L = \begin{cases} 0 & m \cdot \sigma \cdot m \leq 0; \\ L_t & \text{otherwise.} \end{cases}$$

$L_t$ is the value of the kinetic coefficient when the crack is under tensile normal stresses. In this manner, under compression normal to the crack surface, the crack does not propagate. Instead of setting $L=0$ for $m \cdot \sigma \cdot m \leq 0$, one can equivalently set the driving force $\chi=0$ for $m \cdot \sigma \cdot m \leq 0$. While this changes the driving force for $m \cdot \sigma \cdot m \leq 0$, it does not change the driving force for $m \cdot \sigma \cdot m > 0$, when crack can propagate. Again, our approach is simple and consistent with the driving force for a sharp crack propagation based on the $J$-integral, i.e., on the total elastic energy reduction. This is in contrast to the previous approaches in Henry and Levine (2004), Miehe et al. (2010), Borden et al. (2014), and Ambati et al. (2015). Also, condition at which crack cannot propagate is more physical than in those papers.

3.3.2. Boundary conditions for the order parameter

Similar to the case with phase transformations, the following three boundary conditions are used:

$$n \cdot \frac{\partial \psi}{\partial \nabla \phi} = 0 \quad \text{or} \quad \phi = 1 \quad \text{or} \quad \phi = 0.$$  

(36)

The first condition physically means that the energy of the external surface does not change during the damage. The second and third conditions assume full damage or no damage on the external surface, respectively.

Boundary conditions are not needed at the crack surfaces because finite-width crack surfaces are described by the order parameter varying between 0 and 1. One can consider the condition $\phi = \text{const} < 1$ to be the definition of the “sharp” crack surface. The first boundary condition in Eq. (36) will then be met automatically. Because the crack surfaces do not differ from the external surfaces, the external surfaces can be described with the help of the order parameter $\phi$ in the same way.
4. Main requirements to the cohesion energy and degradation function

Similarly to the phase field theory for phase transformations (Levitas and Preston, 2002) and dislocations (Levitas and Javanbakht, 2015a), we will formulate the main requirements for the cohesion energy and degradation function, which prevent any contradiction in a model. According to the definition of the order parameter in Section 1, they should satisfy the following conditions:

1) In the intact state, the only existing energy is the elastic energy, i.e.
\[ f(0) = 0 \text{ and } I(0) = 1. \]  

2) Because \( A \) is the maximum cohesion energy for the fully damaged state, by definition,
\[ f(1) = 1. \]  

3) The elastic stresses and energy should be completely released in the fully damaged state, i.e.
\[ I(1) = 0. \]

The above requirements are mandatory and well known. All requirements below may be desirable for some conditions.

4) For the homogeneous state (i.e. \( \psi^\nabla = 0 \)), the stationary equilibrium solution for the Ginzburg-Landau equation \( \dot{\phi} = 0 \) is
\[ \frac{\partial \psi}{\partial \phi} = I'(\phi)\psi' + A(1 + I_2 : \varepsilon) f'(\phi) = 0. \]  

For homogeneously distributed order parameter, \( \nabla \phi = 0 \) and \( m = \nabla \phi / |\nabla \phi| \) is undefined. When we consider stress-strain curves for homogeneous states below, we assume that we know the decohesion plane and we define \( m \) just orthogonal to it.

Because \( \Psi' \) and \( A \) are independent nonzero function (excluding \( \varepsilon = \theta \)) and parameter, Eq. (40) results in the following damage equilibrium conditions

\[ I'(\phi) = 0 \quad \text{and} \quad f'(\phi) = 0 \quad \text{or} \quad \frac{\Psi'}{I + I_2 : \varepsilon} = -\frac{Af'(\phi)}{I'(\phi)}. \]  

Note that the denominator in Eq. (41) can be neglected for small strains. If we consider the case for which the order parameter \( \phi \leq 1 \) due to thermodynamic conditions rather than due to the non-thermodynamic constraint, then, according to Eq. (40), the requirement that the completely-damaged state must correspond to the thermodynamic equilibrium results in

\[ I'(1) = 0; \quad f'(1) = 0. \]  

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The condition $I'(1) = 0$ leads to a smooth transition to zero elastic driving force in the fully broken state. Similarly, the condition $f'(1) = 0$ results in a smooth transition to the constant cohesive energy in the completely-damaged state. We will not impose similar conditions for the undamaged state.

**Damage initiation.** The most important consequence of the equilibrium conditions is the third root in Eq. (41), which is an equilibrium relationship between strain and the order parameter. In combination with Eq. (25) for elastic stress, after excluding the order parameter, these equations represent the equilibrium stress-strain relationship. Along this curve, the criterion for damage initiation follows from the Eq. (41) for $\phi = 0$:

$$\Psi = \frac{Af'(0)}{1 + I'_z : \varepsilon - I'(0)}. \tag{43}$$

According to Eq. (41), because $I' \leq 0$, $f' \geq 0$. If polynomials $f'(\phi)$ and $I'(\phi)$ start with the same degree in $\phi$ for $\phi \rightarrow 0$, the right-hand side of Eq. (41) is finite and there is a critical strain energy at which damage starts. If damage starts immediately at $\varepsilon = 0$, then $f'(0)/I'(0) = 0$, i.e.

either $f'(0) = 0$ for finite $I'(0)$, or if $f'(0) = I'(0) = 0$, then $\lim_{\phi \rightarrow 0} f'(\phi)/I'(\phi) = 0$, i.e. $f(\phi)$ starts with a higher degree in $\phi$ than $I(\phi)$.

If the damage initiation corresponds to the material instability with respect to the variation of $\phi$ at fixed strain, the instability criterion is

$$\frac{\partial^2 \psi}{\partial \phi^2} = I''(0)\Psi' + A(1 + I'_z : \varepsilon) f''(0) \leq 0. \tag{44}$$

This condition is crucial for the determination of damage initiation, in particular when $f'(0)/I'(0)$ in Eq. (43) is undetermined.

We need to verify that the initial elastic moduli in the undamaged state coincide with the initial elastic moduli of the intact material, i.e. that infinitesimal damage causes an infinitesimal change in the initial elastic moduli. This requirement was formulated in Levitas et al. (2011) and was not fulfilled in Jin et al. (2001), Wang et al. (2002). Thus, because $F(0) = 0$ and $I(0) = 1$

$$\left. \frac{d\sigma}{d\phi} \right|_{\phi \to 0} = (I'(0) + I(0)) \frac{dF}{d\varepsilon} \frac{d\varepsilon}{d\phi} \left|_{\phi \to 0} = \frac{dF}{d\varepsilon} \frac{d\varepsilon}{d\phi} \right|_{\phi \to 0} \Rightarrow \frac{d\sigma}{d\varepsilon} \left|_{\phi \to 0} = \frac{dF}{d\varepsilon}, \tag{45} \right.$$ 

i.e. this condition is met. Note that this requirement is not imposed if damage starts at nonzero strains, as some realistic models have a significant jump in moduli; see Eq. (57) and (58).

**Damage completion.** Similar, for the complete damage

$$\Psi = \frac{Af'(1)}{1 + I'_z : \varepsilon - I'(1)}. \tag{46}$$
If both conditions in Eq. (42) are met, Eq. (46) is satisfied in one of these three options.

First, if \( \lim_{\varepsilon \to 0} \frac{f'(\phi)}{I'(\phi)} = 0 \), \( \Psi^e \) and, consequently, strain are zero at the end of the damage. This is an undesirable property because the damage is associated with residual strain.

Second, if \( \lim_{\varepsilon \to 0} \frac{f'(\phi)}{I'(\phi)} = \text{const} > 0 \), the complete damage is reached at the finite strain value.

Third, if \( \lim_{\varepsilon \to 0} \frac{f'(\phi)}{I'(\phi)} \to \infty \), the damage completes at infinite strains.

**Degradation function**: Discussion on several degradation functions can be found in Kuhn et al. (2015). \( I(\phi) = (1-\phi)^2 \) is the simplest degradation function used in the literature (Bourdin et al., 2000; Kuhn and Müller, 2010; Miehe et al., 2010). It has the properties \( I'(\phi) = -2(1-\phi), I(0) = 1, I(1) = 0, I'(0) = -2, \) and \( I'(1) = 0 \). We also consider \( I(\phi) = (1-\phi)^2 \) for the analysis in this part and will later define the degradation function for each scale separately.

**Interpolation function**: The unified PPR potential-based constitutive model for cohesive fracture is suggested in Park et al. (2009). Here, we present a phase field counterpart of the model (Park et al., 2009) in the form of

\[
f(\phi) = 1 - (1 + \frac{a}{b} \phi)^{b} (1-\phi)^{a}; \quad a>0, \quad b>0,
\]

which has such properties:

\[
f'(\phi) = a(1+\frac{a}{b}\phi)(1+\frac{a}{b}\phi)^{b-1}(1-\phi)^{a-1}; \quad f(0) = 0; \quad f(1) = 1;
\]

\[
f'(0) = 0; \quad f'(1) = 0 \quad \text{for} \quad a>1; \quad f'(1) = 1 \quad \text{for} \quad a=1, \quad \text{and} \quad f'(1) = \infty \quad \text{for} \quad a<1.
\]

The proposed \( f(\phi) \) and \( I(\phi) \) satisfy all mandatory conditions in Eqs. (37)-(39). Finally, we obtain the free energy:

\[
\Psi = (1-\phi)^2 \Psi^e(\mathbf{e}) + (1+I_2^e):\mathbf{e}\left[A[1-(1+\frac{a}{b}\phi)(1-\phi)^{a}]+\frac{\beta}{2}|
abla\phi|^2\right].
\]

Eq. (46) takes the form

\[
\frac{\Psi^e}{1+I_2^e} = \frac{1}{2} Aa(1+\frac{a}{b}\phi)(1+\frac{a}{b}\phi)^{b-1}(1-\phi)^{a-2}.
\]

In particular, for \( \phi=0 \) we have \( \Psi^e = 0 \), i.e. damage starts from the infinitesimal stresses. Also, in the fully damaged state, \( \phi=1 \) and

\[
\frac{\Psi^e}{1+I_2^e} = \frac{1}{2} Aa\phi^{a} 0^{a-2};
\]

which may result in one of these two types of curves:
a) For $0 < a < 2$: $\Psi^e \to \infty$ and damage completes at infinite strains like in Kuhn and Müller (2010), Miehe et al. (2010), Borden et al. (2014), Ambati et al. (2016).

b) For $a = 2$: $\Psi^e / (1 + I_2 : \varepsilon) = A(1 + 2/b)^b$ and damage completes at finite strains. In such a type of curve, a smaller $b$ results in a smaller final strain and, in the limit case, $\lim_{b \to 0} \Psi^e / (1 + I_2 : \varepsilon) = 0$.

The case $a > 2$ results in zero strain for the completely damaged state, which we exclude because the damage is associated with a residual strain.

5. Equilibrium stress-strain curves
Excluding the order parameter from Eq. (50), which is the relationship between the homogenous strain and the order parameter, and Eq. (25) leads to the equilibrium stress-strain relationship. For simplicity, we consider one-dimensional problem and use linear elastic behavior, i.e. $\Psi^e = 0.5E_2\varepsilon^2$, with no surface stresses. $E_2$ is defined as the Young’s modulus of linear elastic solid. Fig. shows $f(\phi)$ and uniaxial equilibrium tensile stress-strain curves for different values of $a$ and $b$. 

![Equilibrium stress-strain curves](image-url)
As we discussed above, the complete damage occurs at finite strain for $a=2$, while an infinite strain is required for the complete damage for $a<2$. When $b$ is reduced at $a=2$: 1) the strain for complete damage decreases; 2) the strain corresponding to the peak stress increases; 3) because the area under the curve should remain constant (see below), the value of elastic strain at which damage starts increases, as does the peak stress. When $a$ is increased for $b=const$, the peak stress and the corresponding strain grow.

**Calibration of $A$.** To calibrate the maximum cohesion energy, i.e. the parameter $A$, let us first evaluate the general three-dimensional homogenous expression for the work of the elastic stress tensor:

$$
\int_0^\varepsilon \sigma : d\varepsilon = \int_0^\varepsilon \frac{\partial \Psi}{\partial \varepsilon} : d\varepsilon = \int_0^\varepsilon d\Psi(\varepsilon, \phi) = \Psi(\varepsilon=1, \phi) - \Psi(\varepsilon=0, \phi) = A(1 + I_2 : \varepsilon) f(1) - A\Psi(0) = A_0 S_{\phi=1}
$$

where $\varepsilon$ is the strain at $\phi=1$. We used $d\Psi = (\partial \Psi / \partial \varepsilon) : d\varepsilon + (\partial \Psi / \partial \phi) d\phi$; $\partial \Psi / \partial \phi = 0$ due to the thermodynamic equilibrium condition, which determines the relationship between $\varepsilon$ and $\phi$: $I(0)=0$; $I(0)=1$; $\Psi(0)=0$; $f(0)=0$; and $f(1)=1$. Here, $S_0$ and $S_{\phi=1}$ are the surface of the crack in the undeformed state and deformed state at $\phi=1$. Eq. (52) is valid for any type of nonlinear hyperelastic material. For uniaxial tension, stress work is equal to the area under the stress-strain curve.

The elastic stress work within the undeformed volume $S_0 d$, where $d$ is the initial distance between two planes forming crack surfaces, i.e. the initial thickness of the cohesive layer, should be equal to the created surface energy. Thus, $(A S_{\phi=1} / S_0)(S_0 d) = 2\gamma S_{\phi=1}$, where $\gamma$ is the surface energy per unit current area, and we obtain

$$A = \frac{2\gamma}{d}.
$$

### 6. Scale-dependent phase field model: from nano to macro

Analyses concerning the suitable choice of the length scale in phase field models for fracture can be found in Amor et al. (2009), Bourdin et al. (2011). The length scale in the phase field approach is either a real material parameter of a gradient damage model, which must be selected according to experimental data (Amor et al., 2009; Kuhn et al., 2015; Mesgarnejad et al., 2015), or a mathematical parameter of the regularized model of brittle fracture (Amor et al., 2009). In the former case and at the atomic scale, when all interpolation functions can be obtained from atomistic simulations, the length scale is related to the distance between two atomic layers $d_0$. In
the latter case, when using the finite element method, the length scale \( d \) containing \( N = d/d_0 \) atomic planes in the cohesive layer should be connected to the element size.

There are two limit models. At macroscale, we will utilize the universal asymptotic form for the macroscopic cohesive law in the limit of \( N \), large but finite, developed in Nguyen and Ortiz (2002) and summarized in Appendix A. We will transform it into a corresponding phase field model. At the atomic scale, we will use a suitable phase field model that mimics atomistic behavior. We will then suggest an interpolation function for scale-dependent thermodynamic potential that matches both limit models. For any scale \( d \) much smaller than the sample size, the coincidence of the crack propagation criteria within a generic phase field and the sharp crack theories was justified in Hakim and Karma (2009). We demonstrated ability of our model to reproduce some known analytical solutions for sharp cracks as well.

6.1. Macroscale phase field model

The effective asymptotic macroscale thermodynamic potential for the cohesive energy is presented in Nguyen and Ortiz, 2002 and summarized in Appendix A. According to Eq. (41), a similar type of behavior within the phase field can be obtained by

\[
\begin{align*}
    f'(\phi) &= -I'(F) = I(\phi) = 1 - f(\phi) \text{ and} \\
    f'(0) &= -I'(0) = 0 \quad \text{and} \quad f'(1) = -I'(1) = 0 ,
\end{align*}
\]

where conditions for \( I(\phi) \) and \( f(\phi) \) at 0 and 1 were taken into account. The function \( f(\phi) \) has a minimum at 0 and a maximum at 1. If it has a saddle point at 1, we must impose the constraint \( 0 \leq f(\phi) \leq 1 \). Thus,

\[
\psi = (1 - f(\phi))\Psi' + (1 + I_2 : \varepsilon)(A f(\phi) + \psi^>) .
\]

Eq. (40) then has three solutions: \( \phi = 0 , \phi = 1 \), and

\[
\frac{\Psi'(\varepsilon)}{1 + I_2 : \varepsilon} = A ,
\]

which is independent of \( \phi \). For \( \Psi'(\varepsilon) < A (1 + I_2 : \varepsilon) \), the only stable equilibrium solution is the damage-free state \( (\phi = 0) \). When damage criterion (56) is met, the equilibrium value of \( \phi \) can be \( 0 \leq \phi \leq 1 \). For \( \Psi'(\varepsilon) > A (1 + I_2 : \varepsilon) \), the only stable equilibrium solution is \( \phi = 1 \). Thus, equilibrium damage starts, occurs, and ends at the satisfaction of the criterion in Eq. (56), which coincides with that in Hakim and Karma (2009) for the neglected denominator.

The corresponding elastic stress-strain curve is

\[
\begin{align*}
    \sigma_e &= C_2 : \varepsilon + \frac{1}{2} C_3 : \varepsilon + \frac{1}{3!} C_4 : \varepsilon + \ldots \quad \text{for} \quad \Psi'(<\varepsilon) < A (1 + I_2 : \varepsilon) ; \\
    \sigma_e &= 0 \quad \text{for} \quad \Psi'(\varepsilon) < A (1 + I_2 : \varepsilon) .
\end{align*}
\]
Fig. shows the bulk energy vs. the order parameter and the stress-strain curve for the macroscale model with linear elastic behavior for different values of $k := \Psi' / [A(1 + I_2 : \varepsilon)]$, which is similar to Hakim and Karma (2009). For $k=1$, undamaged, partially damaged, and completely damaged states are in indifferent thermodynamic equilibrium. Infinitesimal exceeding of $k$ over 1 leads to the disappearance of all local energy minima, except at $\phi=1$, and the complete transformation of the elastic energy into cohesion energy and dropping of stresses to 0.

Thus, condition (56) defines the damage surface in the six-dimensional strain space. The material behaves elastically within the damage surface. Outside of the damage surface, the material is completely damaged and the stresses are zero. We chose the interpolation function from Eq. (47) for $a=2$ and $b=1$, i.e.

$$f(\phi) = 1 - (1 + 2\phi)(1 - \phi)^2 = \phi^2(3 - 2\phi).$$

The degradation function is

$$I(\phi) = 1 - f(\phi) = (1 - \phi)^2(1 + 2\phi).$$

If the strains are small enough to allow neglecting of the higher-order terms in the elasticity rule, then the linear elastic behavior postulated in Nguyen and Ortiz (2002) is valid and we obtain

$$\sigma_{\text{max}} = 2\sqrt{\frac{E_d \gamma}{d}} \quad \text{and} \quad \varepsilon_{\text{c}} = 2\sqrt{\frac{\gamma}{E_c d}}.$$  

for maximum stress and strain, respectively. These are similar to Eq. Error! Reference source not found. and Error! Reference source not found.

6.2. Nanoscale phase field model
Here, we accept \( I(\phi) = (1 - \phi)^2 \). In general, complete bond breaking occurs at infinite displacement of the atomic planes (Anderson, 2017). Then, based on the analysis in Section 4 and Fig. , we should choose \( a < 2 \).

\( (a) \) In the simplest case, we may assume \( a = b = 1 \) and obtain the following interpolation function
\[
    f(\phi) = 1 - (1 + \phi)(1 - \phi) = \phi^2 ,
\]
and the corresponding stress-strain curve in Fig. . This function was used also in single-well potentials at the macroscale (Kuhn and Müller, 2010; Miehe et al., 2010; Bourdin et al., 2011). This potential is not appropriate at macroscale because it generates different stress-strain curves than in a macroscale model which satisfies asymptotic results in Nguyen and Ortiz (2002) (Fig.).

The thermodynamic equilibrium condition for homogeneous states has only one root:
\[
    \frac{\partial \psi}{\partial \phi} = -2(1 - \phi)\Psi' + 2A\left(1 + I_2 : \varepsilon\right)\phi = 0 \quad \rightarrow \phi = \frac{\Psi'}{\Psi' + A\left(1 + I_2 : \varepsilon\right)} .
\]
Because
\[
    \frac{\partial^2 \psi}{\partial \phi^2} = 2\Psi' + 2A\left(1 + I_2 : \varepsilon\right) > 0 \quad \text{for any } \Psi' ,
\]
the instability condition Eq. (44) is never satisfied. Therefore, the equilibrium solution in Eq. (63) corresponds to the minimum of the free energy and is followed by the system during damage growth, starting with the infinitesimal strains and ending at infinite strains.

\( (b) \) Interaction of atoms is almost negligible for large displacements. Therefore, alternatively, we impose complete damage at finite strain. We choose \( a = 2 \) and \( b = 1 \) and obtain:
\[
    f(\phi) = 1 - (1 + 2\phi)(1 - \phi)^2 = \phi^2 (3 - 2\phi) .
\]
This choice gives us the same interpolation function as at macroscale and will be used in our simulations. The analytical solution for maximum stress and strain for linear elasticity results in
\[
    \sigma_{\text{max}} = \frac{32}{25} \sqrt{\frac{3E_2\gamma}{5d_0}} = \frac{E_2\gamma}{d_0} \quad \text{and} \quad \varepsilon_{\text{p}} = \frac{2\sqrt{3\gamma}}{5E_2d_0} .
\]

The second expression for \( \sigma_{\text{max}} \) coincides with that in Anderson (2017), which was obtained by using a simple atomistic model. The thermodynamic equilibrium condition for homogeneous states has two roots
\[
    \frac{\partial \psi}{\partial \phi} = -2(1 - \phi)\Psi' + 6A\left(1 + I_2 : \varepsilon\right)\phi(1 - \phi) = 0 \quad \rightarrow \phi_1 = 1 ; \quad \phi_2 = \frac{\Psi'}{3A\left(1 + I_2 : \varepsilon\right)} .
\]
Damage starts at infinitesimal strains and is completed at \( \phi_2 = 1 \), i.e. at \( \Psi' = 3A\left(1 + I_2 : \varepsilon\right) \). We evaluate
\[
    \frac{\partial^2 \psi}{\partial \phi^2} = 2[\Psi' + 3A\left(1 + I_2 : \varepsilon\right)(1 - 2\phi)] ,
\]
and for \( \phi = \phi_2 \)
\[
\frac{\partial^2 \Psi}{\partial \phi^2} \bigg|_{\phi_2} = 2[3A(1 + I_z : \varepsilon) - \Psi'] > 0 \quad \text{for} \ \phi_2 < 1, \ \text{i.e.,} \ \Psi' < 3A(1 + I_z : \varepsilon) .
\] (69)

Thus, the instability condition Eq. (44) is never satisfied for the thermodynamic equilibrium value of the order parameter \( \phi_2 \) in Eq. (67).

6.3. Scale-dependent phase field model

Because the interpolation function in Eqs. (59) and (65) is the same for both nanoscale and macroscale theories, we assume that it does not change with the number of atomic layers \( N \). The degradation function for scale-dependent thermodynamic potential that matches both limit models is accepted as
\[
I(\phi, N) = (1 - \phi)^2 \left( 1 + 2\phi - 2\phi e^{(1 - N)c} \right).
\] (70)
The parameter \( c \) is chosen to specify the number of atomic planes that is sufficient to practically reach the limit transition to the macroscale model. In simulations, we use \( c=5 \), which corresponds to \( N \approx 20 \) to practically match the macroscale model.

It is evident that \( I(\phi, 1) = (1 - \phi)^3 \) and \( I(\phi, \infty) = (1 - \phi)^2 (1 + 2\phi) \), i.e. limit cases are met. Consequently, we obtain the following expression for the free energy:
\[
\Psi = (1 - \phi)^2 (1 + 2\phi(1 - e^{(1 - N)c}))\left( \frac{1}{2} \varepsilon : C_2 : \varepsilon + \frac{1}{3!}(\varepsilon : C_3 : \varepsilon) : \varepsilon + \ldots + (1 + I_x : \varepsilon)\left( \frac{2\gamma}{d} \phi^3 (3 - 2\phi) + \Psi' \right) \right). \] (71)

The thermodynamic equilibrium condition for homogeneous states has two roots
\[
\frac{\partial \Psi}{\partial \phi} = -2(1 - \phi)[1 - (1 - e^{(1 - N)c})(1 - 3\phi)]\Psi' + 6A(1 + I_z : \varepsilon)\phi(1 - \phi) = 0
\]
\[
\Rightarrow \phi_1 = 1; \quad \phi_2 = \frac{e^{(1 - N)c}\Psi'}{3[A(1 + I_z : \varepsilon) - (1 - e^{(1 - N)c})\Psi']}. \] (72)

Damage starts at infinitesimal strains for any finite \( N \) and is completed at \( \phi_2 = 1 \), i.e. when
\[
\Psi' = \frac{3A(1 + I_z : \varepsilon)}{3 - 2e^{(1 - N)c}} .
\]

Because
\[
\frac{\partial^2 \Psi}{\partial \phi^2} = 2[1 + (1 - e^{(1 - N)c})(-2 + 3\phi)]\Psi' + 6A(1 + I_z : \varepsilon)(1 - 2\phi) ,
\] (73)
and for \( \phi = \phi_2 \)
\[
\frac{\partial^2 \Psi}{\partial \phi^2} \bigg|_{\phi_2} = 2[3A(1 + I_z : \varepsilon) - (3 - 2e^{(1 - N)c})\Psi'] ,
\] (74)
which is always positive for $\phi_2 < 1 \rightarrow \Psi^c < \frac{3A(1 + I_2 : \epsilon)}{3 - 2e^{(1-N)c}}$. Thus, $\phi_2$ always corresponds to the stable minimum of free energy, which is energetically favorable for the system. For $N=1$ and for $N \rightarrow \infty$, these results reduce to the results obtained for the nanoscale and macroscale models, respectively.

Eq. (65) will be used in our simulations. If we choose Eq. (62) for $f(\phi)$ at nanoscale, we can then interpolate

$$f(\phi) = \phi^2 (3 - 2\phi - 2(1 - \phi)e^{(1-N)c})$$

(75)

This function also satisfies both limit cases.

6.4. Equilibrium stress-strain curve for the scale-dependent model

For the one-dimensional case and quadratic elastic energy, from Eq. (41) we obtain the relationship between the strain and the order parameter

$$\varepsilon^2 = -\frac{8\gamma f'}{E_d d^*} = -\frac{12\gamma}{E_d d^* N[(1-e^{(1-N)c})(1-3\phi) - 1]} \Rightarrow \varepsilon = \left(-\frac{12\gamma}{E_d d^* N[(1-e^{(1-N)c})(1-3\phi) - 1]} \phi \right)^{0.5}.$$  

(76)

For simplicity, we neglected the geometrically-nonlinear term $(1 + I_2 : \epsilon)$, which produces surface stresses. The one-dimensional elasticity rule gives

$$\sigma = \frac{\partial \psi}{\partial \varepsilon} = (1 - \phi)^2(1 + 2\phi - 2\phi e^{(1-N)c}) E_d \varepsilon.$$  

(77)

Similarly, for cubic elastic energy, i.e. $\Psi^c = \frac{1}{2} E_d \varepsilon^2 + \frac{1}{3!} E_d \varepsilon^3 = \frac{1}{2} E_d \varepsilon^2 + \frac{1}{3!} \omega E_d \varepsilon^3$, where we used $E_3 := \omega E_2$ with a parameter $\omega$ for convenience, we obtain for the strain-order parameter and stress-strain relationships, respectively:

$$\varepsilon^2 \left(1 - \frac{\omega}{3} \varepsilon \right) = -\frac{8\gamma f'}{E_d d^*} = -\frac{12\gamma}{E_d d^* N[(1-e^{(1-N)c})(1-3\phi) - 1]} \Rightarrow \varepsilon = \frac{2}{\omega} \cos(\theta / 3) + \frac{1}{\omega} \cos^{-1}\left[\frac{1}{\omega} - \frac{6\gamma f'}{NE_d d^* \omega^2} - \frac{2\pi}{3}\right];$$  

(78)

$$\sigma = \frac{\partial \psi}{\partial \varepsilon} = (1 - \phi)^2(1 + 2\phi - 2\phi e^{(1-N)c}) E_d \left(\varepsilon + \frac{\omega}{2} \varepsilon^2\right).$$  

(79)

Exclusion of $\phi$ from Eqs. (76) and (77) and Eqs. (78) and (79) leads to the desirable equilibrium stress-strain curves in Fig.
Fig. 4. Equilibrium stress-strain curve for various scale parameters $N$, $c=5$, and (a) quadratic elastic energy ($\omega=0$) or (b) cubic elastic energy ($\omega=0.33$). According to Eqs. (52) and (53), the area below the curve is proportional to $1/d$ or $1/N$.

For cubic elastic energy and $\omega=0.33$, the fitted expression for the peak stress is

$$\sigma_{\text{max}} = \sqrt{\frac{E d}{N}} \left( \frac{2.0}{\sqrt{N}} - 2.02 \frac{1}{(\sqrt{N})^2} + 0.81 \frac{1}{(\sqrt{N})^3} \right),$$

which approves $\sigma_{\text{max}} \propto \frac{1}{\sqrt{N}}$ for large $N$.

Fig. 5. Equilibrium stress-strain curve for various $\omega$ and $N=1$

For cubic elastic energy and for a large value of $\omega$, the stress reaches a maximum value even without damage. Because of this, we have not chosen values larger than 0.33. For higher-order elastic energy, there is no guarantee that there will be monotonous decaying elastic moduli. The effect of the 3rd-rank elastic coefficient is shown in Fig. 5. Note that the stress-strain curve can also be calibrated numerically for the general form of $f(\phi) = 1 - (1 + a\phi/b)^r (1-\phi)^s$. Thus, our model has provided some freedom to calibrate any constitutive law.
7. Parameters calibration

Let us elaborate upon the Ginzburg-Landau equation by substituting Eq. (71) into Eq. (34) for neglected surface stresses

\[
\dot{\phi} = L(-\frac{\partial \Psi}{\partial \phi} + \beta \nabla^2 \phi) = L \left[ 2(1-\phi)(1-(1-3\phi)(1-e^{i(1-\phi)}))\Psi - \frac{12\gamma}{d} \phi(1-\phi) + \beta \nabla^2 \phi \right].
\] (80)

For neglected elastic energy, the stationary Ginzburg-Landau equation in the one-dimensional case reduces to

\[
\frac{d\psi'}{d\phi} = \frac{d}{d\phi} \left( \frac{2\gamma}{d} f \right) = \beta \frac{d^2\phi}{dx^2},
\] (81)

where the coordinate \(x\) is along the direction normal to the crack surface \(m\). Utilizing

\[
\frac{d^2\phi}{dx^2} = \frac{d\phi'}{dx} = \frac{d\phi'}{d\phi} \frac{d\phi}{dx} = \frac{d\phi'}{d\phi} \frac{d\phi'}{2d\phi} = 1 \frac{d(\phi'^2)}{d\phi},
\] (82)

we transform Eq. (81) into the first-order differential equation

\[
\frac{d}{d\phi} \left( \frac{2\gamma}{d} f \right) = \beta \frac{d(\phi'^2)}{2d\phi}.
\] (83)

Eq. (83) has a sense of the energy integral for the equation of motion (81) if one uses an analogy with classical mechanics. Integration of Eq. (83) over \(\phi\) then leads to

\[
\frac{\beta}{2} \phi'^2 = \frac{2\gamma}{d} f.
\] (84)

\(\phi(\pm\infty) = \phi'(\pm\infty) = 0\) are used as boundary conditions for Eq. (83). Finally, the solution of Eq. (84) yields the explicit expression for the crack surface profile

\[
\phi = \frac{3}{2} (1 - \frac{-1 + \sqrt{1 + \frac{4}{3\beta d f \gamma}}}{1 + \frac{4}{3\beta d f \gamma}}). \] (85)

Fig. 6 represents a crack at the position \(x=0\) in an infinite bar based on Eq. (85).

Fig. 6. Finite-width profile of the crack surfaces. For \(x>0\) and \(x<0\) is two different crack surfaces are shown, and at \(x=0\) the separation plane is placed.
We can now repeat the procedure for the multidimensional case. Eqs. (81), (82), and (84) are generalized for the multidimensional case as

\[
\frac{d\psi}{d\phi} = \frac{d}{d\phi} \left( 2\gamma \frac{df}{d\phi} \right) = \beta \nabla^2 \phi, \tag{86}
\]

\[
\nabla^2 \phi = \nabla \nabla \phi = \frac{d\nabla \phi}{d\phi} \nabla \phi = \frac{1}{2} \frac{d(\nabla \phi)^2}{d\phi}, \tag{87}
\]

\[
\psi = Af. \tag{88}
\]

Eqs. (84) and (88) mean that the excess of the local energy is equal to the gradient energy. Due to the definition of surface energy, which is the excess of the strain-independent energy with respect to the energy of the intact phase, by allowing for Eq. (84) we evaluate the surface energy

\[
\psi_{\text{surf}} = 2\gamma = \int (Af + \psi) dx = 2A \int f dx = 4A \int f dx = 4A \int \frac{1}{0} f \frac{dx}{d\phi} d\phi = 2\sqrt{2}A\beta \int \sqrt{f} d\phi = 2\sqrt{2}A\beta Y, \tag{89}
\]

where \( Y = \frac{1}{0} \sqrt{f} d\phi \) is a number that can be evaluated, at least numerically, for any interpolation function \( f(\phi) \). It follows from Eq. (89), with allowing for Eq. (53):

\[
\beta = \frac{\gamma^2}{2AY^2} = \frac{\gamma d}{4Y^2}. \tag{90}
\]

For \( f(\phi) = \phi^2 (3-2\phi) \), we obtain \( Y = 0.639 \) and \( \beta = 0.612\gamma d \). For \( f(\phi) = \phi^2 \), we evaluate \( Y = 0.5, \beta = \gamma d \), and, in general, \( Y = Y(a,b) < 1 \). We should warn that the crack profile has two surfaces, which was taken into account here but was overlooked in the evaluation of material parameters in Kuhn and Müller (2010), Miehe et al. (2010), Kuhn et al. (2015).

The width \( \Delta \) of the crack surface is defined as a width of the region in which almost the entire perturbation occurs, e.g. such as

\[
\Delta = x_{\phi=0.01} - x_{\phi=1} = 1.46 \sqrt{\frac{\beta d}{\gamma} = 0.75 \frac{d}{Y}}. \tag{91}
\]

We took Eq. (89) into account. For \( f(\phi) = \phi^2 (3-2\phi) \), we have \( \Delta = 1.14d \), i.e. the surface width is approximately equal to the thickness of a cohesive layer.

8. Complete system of equations

The final system of equations is collected below.

1. Kinematics

\[
\mathbf{e} = \mathbf{e} = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right). \tag{92}
\]

2. Helmholtz free energy per unit undeformed volume
\[ \psi = \psi^e + (1 + \mathbf{I}_2 : \varepsilon) \left( \psi^e + \psi^\gamma \right); \]

2.1. Elastic energy

\[ \psi^e = (1 - \phi)^2 \left( 1 + 2\phi(1 - e^{(1-N)c}) \right) \Psi^e; \]
\[ \psi^e = \frac{1}{2} \varepsilon : C_2 : \varepsilon + \frac{1}{3!} \left( \varepsilon : C_3 : \varepsilon \right) + \frac{1}{4!} \varepsilon : (\varepsilon : C_4 : \varepsilon) + \ldots. \]  

2.2. Cohesion energy

\[ \psi^c = \frac{2\gamma}{d_0 N} \phi^2 (3 - 2\phi). \]

2.3. Gradient energy

\[ \psi^\gamma = 0.306 \gamma d_0 N \left| \nabla \phi \right|^2. \]

3. Stress tensor

\[ \sigma = \sigma^e + \sigma^c; \]
\[ \sigma^e = \frac{\partial \psi^e}{\partial \varepsilon} = (1 - \phi)^2 \left( 1 + 2\phi(1 - e^{(1-N)c}) \right) \left( C_2 : \varepsilon + \frac{1}{2} \varepsilon : C_3 : \varepsilon + \frac{1}{3!} \varepsilon : (\varepsilon : C_4 : \varepsilon) + \ldots \right); \]
\[ \sigma^c = (\psi^e + \psi^\gamma)(I - \mathbf{m} \otimes \mathbf{m}); \quad \mathbf{m} = \nabla \phi / |\nabla \phi|. \]

4. Ginzburg-Landau equation

For neglected surface stresses

\[ \dot{\phi} = L \left( \frac{\partial \psi}{\partial \phi} + \beta \nabla^2 \phi \right) = \\
L \left( 2(1 - \phi)(1 - (1 - 3\phi)(1 - e^{(1-N)c})) \Psi^e + \frac{\gamma}{d_0 N} \left( -12\phi(1 - \phi) + 0.612 (d_0 N)^2 \nabla^2 \phi \right) \right). \]  

With surface stresses

\[ \dot{\phi} = L \left[ 2(1 - \phi)(1 - (1 - 3\phi)(1 - e^{(1-N)c})) \Psi^e + 0.612 d_0 N \gamma \nabla^2 \phi + 0.612 d_0 N \gamma (I_2 : \nabla \varepsilon) \cdot \nabla \phi - 0.612 d_0 N \gamma (1 + \frac{3.27\phi^2 (3 - 2\phi)}{(d_0 N \nabla \phi)^2}) \nabla \phi \cdot (\nabla \varepsilon : I_2) \right]. \]

5. Momentum balance equation

\[ \nabla \cdot \sigma + f = \rho_a a. \]

6. Boundary condition for \( \phi \)

\[ n \cdot \frac{\partial \psi}{\partial \nabla \phi} = 0 \text{ or } \phi = 1 \text{ or } \phi = 0. \]

9. Numerical examples
In this Section, five example problems corresponding to the known methods of testing fracture of materials, including propagation of a curvilinear crack, are solved and analyzed to demonstrate the main features of the model. In particular, we would like to study the behavior of a sample of fixed size when \( N \) varies; damage of geometrically similar samples, whose sizes increase proportionally to \( N \); lack of damage in a zone with compressive stresses; and the evolution of surface stresses and their effect on crack propagation. We reproduced known solutions for the cases when our results should coincide with them, and we demonstrated how all our four advancements change solutions for these problems, introducing new features and mechanical effects.

The finite-element method with triangle Lagrangian elements and quadratic approximation were used to solve the governing equations in COMSOL Multiphysics code (see COMSOL 5.2a, 2016). Mathematics Application and Structural Application modules were utilized to solve the coupled elasticity and Ginzburg-Landau equations. For the order parameter \( \phi \) corresponding to the intact state and broken state extrema, we have \( \partial \psi / \partial \phi \approx 0 \) for large \( N \). Because of this, we include small deviations from the intact solid with \( \phi = 0.001 \) in the initial condition to avoid stacking the system in them. In our problems we do not have indeterminacy in \( m = \nabla \phi / |\nabla \phi| \) because for problems with surface stresses we have heterogeneous initial conditions for \( \phi \). In general, for homogeneous initial conditions for \( \phi \), we can add small heterogeneous fluctuations into initial conditions. The indeterminacy in the direction \( m \) of the gradient \( \nabla \phi \) when numerically \( \nabla \phi = \theta \) can generally be eliminated by the condition that, if \( \nabla \phi = \theta \), \( m \) is not calculated and \( \sigma_{\text{st}} = 0 \). To avoid numerical divergence, a small elastic energy is assumed to be sustained by the fully damaged state; thus, \( I(\phi) \) is changed to

\[
I(\phi) = (1-s)(1-\phi^2)[1+2\phi(1-e^{(1-N/\phi)})]+s, \tag{104}
\]

where \( s = 10^{-5} \). Surface stresses are excluded in our simulations except in Section 9.5, where they are specifically studied.

### 9.1. Center Cracked Tension Sample

A CCT (Center Cracked Tension) sample of size \( 2w \times 2l = 120 \times 50 \text{ nm}^2 \), with an initial crack of length \( 2a_0 = 30 \text{ nm} \) and with sharp crack tips (Fig. ), is treated. The plane strain problem is considered. The time-dependent displacement is symmetrically applied at the lateral edges. Displacement is linearly increased at a pace of 0.5 \( \text{nm/ps} \). Due to the symmetry, only one-quarter of the sample is considered for the solution of the coupled phase field and mechanics equations.
The following material properties were used: bulk modulus $K_0 = 112.62$ GPa, shear modulus $G_0 = 71.5$ GPa, and surface energy $\gamma = 1.0$ N/m. The value of the kinetic coefficient $L$ was chosen as $2500$ (Pa.s)$^{-1}$ so that the crack propagates in a quasi-static manner. Other parameters are $d_0 = 1$ nm, $A = 200$ MPa, $\beta = 6.12 \times 10^{-9}$ N, and $c = 5$. Parameter $d = 1$ nm corresponds to the width $\Delta = 1.14$ nm of the crack surface and the length $0.57$ nm of the process zone near the crack tip. The same material properties are used in all of the following examples unless otherwise stated.

To understand the effect of $N$ on global behavior, the sample length parameters $a_0$, $w$, $l$, $u(t)$, and $d$ are increased by a factor of $N$ at the fixed surface energy. The mesh is not changed.

For the CCT specimen, the analytical solution for the averaged normal stress for the onset of crack propagation, based on the Griffith energy balance (see e.g. Anderson (2017)), can be expressed as

$$\sigma_{\text{on}} = f\left(\frac{a_0}{w}\right)\sqrt{\frac{2\gamma E}{(1-v^2)\pi a_0}}, \quad (105)$$

and, when the sample length parameters are increased by a factor of $N$, as

$$\sigma_{\text{on}} = f\left(\frac{a_0}{w}\right)\sqrt{\frac{2\gamma E}{(1-v^2)\pi (Na_0)}}, \quad (106)$$

where

$$f\left(\frac{a_0}{w}\right) = \sqrt{\cos\left(\frac{\pi a_0}{2w}\right) \left[1 - 0.025(\frac{a_0}{w})^2 + 0.06(\frac{a_0}{w})^4\right]} = 1.00, \quad (107)$$

for our $a_0/w = 0.25$. With increasing $N$, $\sigma_{\text{on}} \propto 1/\sqrt{a_0 N}$, i.e. combination $\sigma_{\text{on}} \sqrt{N}$ is independent of $N$. 

Fig. 7. Schematics of the CCT sample with the boundary conditions
Fig. 8 shows the curve for the calculated averaged stress $\sigma_\text{N}$, which is the force over the initial area of the edge, multiplied by $\sqrt{N}$ vs. the averaged strain $u/l$ for various $N$. After reaching a peak point, crack propagation starts and the force drops. The critical stress $\sigma_\text{N}\sqrt{N}$ decreases while $N$ increases from 1 to 100, and then becomes independent of $N$, as is desired.

Our numerical results for $N=100$, 500, and 1000 yield $\sigma_\text{N}\sqrt{N} = 2.61$ GPa, which is close to 2.82 GPa, the analytical solution of Eq. (106). The coincidence of the crack propagation criteria within a generic phase field and the Griffith theories in the general case was justified in Hakim and Karma (2009).

For all remaining simulations in this Section, the sample size will be fixed when $N$ is increased. To obtain solutions comparable with the sharp-surface approach, the crack process zone will be kept much smaller than the characteristic size in the problem, e.g. the distance between the crack tip and the free sample surface. To compare the stress field for the sharp surface and phase field approaches, we solved the problem for the same geometry as in Fig. 8. The same boundary condition was applied, with the initial crack size of $a_0=16$ corresponding to $u=0.51$ for $N=10$. The crack tip location is chosen as the point for which $\phi=0.99$. As shown in Fig. 8, the maximum stress is restricted to the stress in the phase field approach, causing surface creation and crack propagation.
Fig. 9. Comparison of the stress field for crack with sharp surfaces and the phase field approach for different values of $N$ and the same sample size.

Although the length scale $N$ affects the stress field at the crack tip, the far-field stress is in agreement with the sharp-surface approach and independent of the length scale. An increase in $N$ increases the crack process zone proportionally and allows us to use a larger size of finite elements, thus obtaining a more economical solution.

The effect of the length scale on the maximum of $\sigma_x$, $\sigma_{x,\text{max}}$, within the fracture zone is shown in Fig. 9. Here, we keep the same geometry and change $N$. A linear relationship between $\sigma_{x,\text{max}}$ and $N^{0.5}$ for $N \geq 15$ with the slope of 29.4 GPa was found. This is in the agreement with the solution of the uniaxial problem in Eqs. (61) and (6), which predicts 26.6 GPa for the slope. The difference exists mainly because the stress field is three-dimensional (instead of only $\sigma_x$) in numerical simulations and because $N$ is not large enough. Still, the linear scale dependency in the maximum stresses is apparent.
Fig. 10. Maximum stress $\sigma_{x,\text{max}}$ in the fracture zone for different values of $N$.

Evolution of the order parameter. The order parameter profile along the crack direction $y$ is plotted for different time instants in Fig. 11. The order parameter evolves from 0 to the stress-free analytical solution before the crack starts to propagate. It subsequently propagates while keeping its shape, and the elastic stresses do not have much effect on the surface profile.

Fig. 11. Evolution of the profile of the order parameter along the crack direction $y$ for $N=10$.

Fig. also shows the evolution of the order parameter in two dimensions in the deformed state. We can see that there is no crack widening, which exists in the models with a double-well barrier (Aranson et al., 2000; Karma et al., 2001; Henry and Levine, 2004; Hakim and Karma, 2005).
Fig. 12. Evolution of the damage order parameter $\phi$ near the initial crack tip in the region: $[x,y]=[(-10),(30-50)]$ for $N=10$.

**Stress field.** The evolution of stress $\sigma_x$ distribution is shown in Fig. for $N=10$. An initial strong stress concentration at the crack tip prior to damage initiation drops to the maximum stress of 6.0 GPa. With the propagating crack, the pick stress grows slightly due to the increase in the crack length. The average of the maximum stress over the 4 different displacements ($u=0.52, 0.54, 0.56, 0.56$ nm) at the crack tip is 6.9 GPa, and the peak stress in the uniaxial stress-strain curve is 9.2 GPa, which shows that they are in the same range. The difference exists due to the complex stress state in the fracture zone and the significantly different behavior from the one-dimensional behavior, even in the opening direction.

Fig. 13. Evolution of the stress $\sigma_x$ distribution along the crack direction $y$ for $N=10$. 

\[ u=0.5 \quad u=0.54 \quad u=0.58 \]
9.2. Single Edge Notched Bending Sample

We applied the following boundary conditions on a single-edge notched bending sample as shown in Fig. 15a: the lower right corner is fixed in the vertical direction and the lower left corner is completely fixed. A displacement-controlled loading is applied at the middle point of the upper surface. Fig. shows the force-deflection curve for the sample.

![Diagram of force P-displacement v curve for different values of N.](image)

The contour plot of the order parameter is shown in Fig. b-d. Similar to the CCT specimen, Mode I crack propagation takes place. Thus, we refined the mesh along the straight crack trajectory.
Fig. 15. Schematic of bending problem (a) and evolution of the damage order parameter for the 20×20 square part of the sample and $N=1$ (b–d).

The crack path and stress-strain behavior are similar to the results in Miehe et al., (2010), Wu (2017). We use the analytical equation:

$$
\frac{P_{\text{crit}}}{B} = f\left(\frac{a_0}{w}\right) \frac{2E\gamma_{\nu}}{(1-\nu^2)a_0}w, \tag{108}
$$

where the thickness $B=1$ and

$$
f\left(\frac{a_0}{w}\right) = \frac{2(1+2\frac{a_0}{w})(1-\frac{a_0}{w})^{3/2}}{3\frac{S}{w}} \left[1.99 - \frac{a_0}{w}(1-\frac{a_0}{w}) \left\{2.15 - 3.93\left(\frac{a_0}{w}\right) + 2.7\left(\frac{a_0}{w}\right)^2\right\}\right]^{-1} = 0.075. \tag{109}
$$

Analytical solutions of Eq. (108) give $P_{\text{crit}}=13.00$ N, while the average of our numerical results for $N=10, 20,$ and $30$ leads to $13.43$ N.

9.3. Curved path L-shaped slab

To show the capability of the model in studying the curved-path crack, we turn our attention to the L-shaped slab. Two problem formulations will be considered: (a) when sizes of the sample increase proportionally to $N_1=N$ and (b) when size is fixed, i.e. $N_1=10^6$ but N varies. The geometry is shown in Fig. . All edges are free except the bottom edge, which is fixed, and the upward displacement of the point $A$ is increased linearly with time. The material properties are taken from Winkler (2001): elastic moduli $E_2=25.85$ GPa, Poisson ratio $\nu=0.18$, and fracture energy $\gamma=90$N/m. Such a large magnitude of $\gamma$ is often used at macroscale because it effectively includes plastic dissipation near the crack tip.
Fig. 16. Schematic of an L-shaped slab for which sample sizes vary proportionally to \( N \). The actual sample from Winkler (2001) corresponds to \( N_1 = 10^6 \).

We refined the mesh (see Fig. a) in the region that was expected as a crack path, according to the results in Wu (2017).

Fig. 17. Force-displacement curve for the point A for an L-shaped slab with \( N_1 = N \).

The effect of increasing both the length scale of the sample and \( d \) by increasing \( N_1 = N \) is shown in Fig. . As expected, the nanoscale treatment with \( N_1 = 1 \) shows a larger maximum force, which decreases with increasing \( N \) and grows weakly dependent on \( N \) for \( N > 100 \). The critical force \( F_{\text{max}} = 6.9 \text{ KN} \) is in good agreement with literature: \( F_{\text{max}} = 7.2 \text{ KN} \) (Wu, 2017), \( 6.4 \text{ KN} < F_{\text{max}} < 7.8 \text{ KN} \) (Winkler, 2001).
Fig. 18. Force-displacement curve for the point A for L-shaped slab with $N_1=10^6$ and several values of $N$.

The force-displacement curve for the actual sample is presented in Fig. , which corresponds to maintaining the same size for the actual scale sample but allowing different $N$. Increasing the phase field length scale $d$ by increasing $N$ from $2.5 \times 10^6$ to $10^7$ changes the peak force by 4% at most. The crack path is shown in Fig. b-c, which is almost identical to the crack path in Wu (2017).
For the same problem in Zhang et al. (2017), the crack also propagates in the region near the applied load and in the left side of the sample. This is not realistic because the material in these regions is under compression. Our model eliminates this drawback by properly treating the compressive stress states using Eq. (35), which will be elaborated upon in the next subsection.

9.4. Crack under compression

We solve a problem with a more pronounced crack under compression. A 100×50 µm² beam under bending stresses is considered. There are two 5-µm cracks on the top and bottom parts of the beam. The vertical displacement \( v \) of the right corner point is linearly increasing at a pace of 5 µm/ns. The left edge is the symmetry plane; all other edges are stress-free (see Fig. a). The solutions for the models without and with distinguishing between tension and compression are shown in Fig. b-c, respectively. Applying the same kinetic coefficient for both tensile and compressive stresses leads to growth of the crack in both regions (Fig. b), but the kinetic coefficient in Eq. (35) prevents crack propagation (initiation) in the region with compressive stresses.
Fig. 20. Propagation of cracks in the beam under applied displacement. (a) Schematic and boundary condition of the sample. (b) For a model with a constant (stress-sign independent) kinetic coefficient, the crack artificially grows in the region with compressive stresses. (c) When the kinetic coefficient from Eq. (35) is used, the crack does not propagate in the region with compressive stresses.

9.5. Surface tension

9.5.1. CCT specimen

Here, we consider surface stresses in our simulations for the CCT specimen. The only notable difference is that the initial crack is introduced by setting an initial value for the phase field order parameter based on the analytical solution in Eq. (85) for \( N=1 \):
\[
\phi(t = 0) = 0.99 \times \frac{3}{2} \left\{ 1 - (-1 + \frac{2}{1 + (2 - \sqrt{3})e^{\sqrt{\frac{\frac{\ddot{\phi}}{\ddot{\phi}_x}}{\ddot{\phi}_y}}})^2 \right\} a_0 > y \\
\frac{3}{2} \left[ 1 - (-1 + \frac{2}{1 + (2 - \sqrt{3})e^{\sqrt{\frac{\ddot{\phi}}{\ddot{\phi}_x}}})^2 \right] \times \left[ 1 - (-1 + \frac{2}{1 + (2 - \sqrt{3})e^{\sqrt{\frac{\ddot{\phi}}{\ddot{\phi}_y}}})^2 \right] \right\} a_0 \leq y
\]

and \( L_t \) was chosen as 10 \((\text{Pa.s})^{-1}\). Eq. (101) is considered to be the kinetic equation of damage. Note that, with such initial conditions, \( \nabla \phi \neq \mathbf{0} \) for the entire solution and the direction \( m \) is always defined.

**Surface tension evolution.** The evolution of all components of surface tension at the crack surface is presented in Fig. . During crack growth, the profile of the surface tension remains constant, as it does for the order parameter.
According to Eq. (27), the maximum of the surface tension occurs at the external layer of the crack surface, where both the order parameter and its gradient have their maximum value. While this layer represents a symmetry plane where shear stress is usually zero, the shear stress reaches 4.0 GPa near the crack tip due to the large gradient of the order parameter. The most important effect is expected from the normal to crack stress, which is also localized near the crack tip and reaches 4.0 GPa.

**Stress distribution.** Here, we show the effects of surface tension on stress distribution near the crack tip along the symmetry plane. Fig. shows the distributions of $\sigma_x$, $\sigma_y$, and $\sigma_z$ at three different times during the propagation of the crack. We see qualitatively that the local stress intensity factor has increased because of the surface tension.
with surface tension
without surface tension

\( \sigma_x (\text{GPa}) \)
\( u=0.6 \quad u=0.8 \quad u=1 \)

\( \sigma_y (\text{GPa}) \)
\( u=0.6 \quad u=0.8 \quad u=1.0 \)

(y (nm))

(a)

(b)
The maximum value of $\sigma_x$, $\sigma_{x,max}$, with surface tension and without surface tension are 15.9 GPa and 20.0 GPa, respectively. Although the $y$-component of the surface tension at the crack tip is zero, changes in $\sigma_y$ are observed. The surface stress in the $z$-direction has a maximum value and a constant within the constant $\phi$ surfaces. The effect of surface tension due to change in the stress distribution is more pronounced at the crack tip and negligible far from the crack tip.

**Effect of $N$ on surface stress effect.** It was shown in Eq. (91) that the surface width is proportional to $d$. This means that a larger $d$ leads to a more diffused surface and a smaller magnitude of the specific surface energy. Increasing $d$ reduces the maximum value of the surface stress; see Eq. (27).
It is shown in Error! Reference source not found. that the effect of surface stress is negligible for $N \geq 10$.

9.5.2. Crack nucleation and propagation near the notch

Crack nucleation is studied by solving the same problem for the geometry shown in Fig. 24a, which includes a notch with a stress concentrator rather than an initial crack.
Fig. 24. Crack nucleation and propagation for the sample with the notch. (a) Schematics of the sample with the notch and boundary conditions; (b) Distribution of the stress $\sigma_x$ for two different displacements $u$ corresponding to initiation of crack propagation for the case without and with surface tension; (c) Averaged stress $\bar{\sigma}_x$ - strain $u/l$ curves for the case without and with surface tension.

In the initial stage, during which the elastic stress is not sufficient for crack propagation, the surface stresses are negligible compared to the total stresses during propagation. Distribution of the stress $\sigma_x$ for two different displacements $u$ corresponding to the initiation of crack propagation for the cases without and with surface tension is shown in Fig. 24b. Surface stresses increase the maximum local total stress $\sigma_x$. As a result, crack propagation with surface tension starts at a smaller total displacement $u$ and, consequently, a smaller averaged stress $\bar{\sigma}_x$ (Fig. 24c). Thus, the maximum averaged stresses $\bar{\sigma}_x$ for the cases with surface stress and without surface stress are 2.87 GPa and 3.21 GPa, respectively.

To determine the effect of surface tension on crack propagation, we calculate the crack tip velocity by tracking the position of the crack tip, which we define as a point with $\phi=0.99$, against time for the range of prescribed displacements $u$. After reaching the corresponding maximum averaged stress $\bar{\sigma}_x$ in Fig. 24c, the crack velocity jumps from zero to the value, which is independent of $u$. For the displacements $u$ for which both crack velocities are nonzero, the crack propagates with the velocity 214.8 nm/ns with surface stress and 186.3 nm/ns without surface
stress, which shows a 15.3% increase. Consequently, surface tension promotes fracture by both increasing the local tensile stresses $\sigma_x$ in the fracture zone and increasing the thermodynamic driving force for crack propagation.

10. Conclusions

In this paper, a general thermodynamically-consistent phase field model for fracture was developed. The new points of the developed phase field model and the main results are listed and summarized below.

1) The thermodynamic procedure includes a traditional application of thermodynamic laws and additional conditions related to the thermodynamic equilibrium and its stability for homogeneous states. Similar conditions were formulated earlier for phase transformations (Levitas and Preston, 2002; Levitas, 2013a) and dislocation (Levitas and Javanbakht, 2015a). A general polynomial for a cohesive interpolation function that satisfies the formulated requirements is suggested. Analysis of the equilibrium stress-strain curves for all developed models is used, along with the above requirements, to choose the desired interpolation functions.

2) The free energy is formulated in a way that results in the desired expression for the surface stresses directly from the thermodynamical procedure. Thus, the surface stress represents the biaxial tension of the crack surface with the resultant force equal to the surface energy. To introduce such stresses, the cohesion and gradient energies, which produce the surface energy, are multiplied by the ratio of the areas of surfaces along the crack surface in the current and undeformed states. This is equivalent to consideration of the surface energy per unit deformed surface, as in traditional thermodynamic approaches for sharp interfaces, which are used to derive surface stresses. Thus, even for small strains, some geometric nonlinearities are required even within a geometrically-linear approach to introduce surface stresses. This approach is compared with approaches for introducing interfacial stresses in phase transformation theory (Levitas, 2013b, 2014; Levitas and Warren, 2016), and it is shown that the approaches in Levitas (2013b), Levitas and Warren (2016) are not applicable to fracture. Note that the Ginzburg-Landau equation includes several new terms related to the surface stresses, in contrast to the alternative approach in Levitas (2013b, 2014), Levitas and Warren (2016).

3) As a byproduct of the theory, we obtained a phase field model for the external surface. Since it is based on single-wall potential and does not involve the driving force for its propagation, it can be kept stationary. This is a significant advantage in comparison to the previous models for the external surfaces based on a double-well potential (Levitas and Javanbakht, 2011; Levitas and Samani, 2014; Levitas, 2018), in which it is difficult to keep the surface stationary due to the driving force that appears due to the surface energy and curvature. A finite-width external surface produces multiple interesting phase transformation effects and a more precise model is of great importance.
4) The theory is applicable from the atomistic to the macroscale. First, we developed two different limit-case models. One of these is valid at nano and atomic scales; it mimics atomistic behavior and can be calibrated using atomistic simulations. For the macroscale, we utilized the universal asymptotic form for the macroscopic cohesive law in the limit of large but finite number of atomic layers \( N \) in the cohesive zone (Nguyen and Ortiz, 2002) and transformed it into a corresponding phase field model. We then suggested an interpolation function for scale-dependent thermodynamic potential that matches both limit models. Note that in the simplest cases the scale parameter \( N \) in our model should be fixed for the chosen problem, i.e., the problem is solved at the chosen scale. However, when one develops any multiscale scheme, the models with different \( N \) can be used in different subregions, according to the chosen scaling up strategy.

5) Crack propagation in the region with compressive closing stresses is eliminated by including a stress-state-dependent kinetic coefficient in the Ginzburg-Landau equation. Thus, when normal-to-the-crack surface stresses are compressive, the kinetic coefficient is set to be zero and the damage does not evolve.

6) The coupled phase field and mechanics equations were implemented in the finite element code COMSOL Multiphysics. Various model problems were solved for straight and curved cracks to illustrate all of the novel features of our theory. Some known analytical solutions are well-reproduced. Local stresses decrease when all sample sizes and \( N \) increase proportionally while keeping the same mesh, and for large \( N \) they reduce proportionally to \( N^{-0.5} \); the averaged stresses slightly decrease for \( N<100 \) and are practically independent of \( N \) for \( N>100 \). When the sample size is fixed and \( N \) is increased along with a proportional increase of the finite element mesh, the local stress decreases again, but stresses away from the crack tip and, consequently, the averaged stress are unaffected by \( N \) for large \( N \). All of these results are desired and allow one, in particular, to increase the size of the finite elements to reduce the cost of simulations. With the chosen stress-state-dependent kinetic coefficient, crack propagation does not occur in the region of compressive closing stresses. Surface stresses increase the total stresses in the fracture zone and cause fracture initiation under smaller applied displacement and load, and also accelerate the crack velocity.

In future work, the following generalizations can be performed. Large deformation formulation is important, especially at nanoscale, where the strains during damage are large (Miehe et al., 2016). Anisotropic surface energy is another issue (Mozaffari and Voyiadjis, 2015; Hakim and Karma, 2009; Clayton and Knap, 2015) that should be incorporated. One of our main interests is generalizing the developed theory for the interaction between crack propagation and phase transformation (Zhao et al., 2016; Schmitt et al., 2015), dislocations (Mozaffari and Voyiadjis, 2016; Ruffini and Finel, 2015), and twinning (Clayton and Knap, 2013; Clayton and Knap, 2016).
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Appendixes

A. Asymptotic thermodynamic potential for the cohesive energy

At macroscale, the effective asymptotic thermodynamic potential for the cohesive energy for large \( N \) is found in Nguyen and Ortiz (2002) as follows:

\[
\Phi = \min \left\{ \frac{C}{2N} \delta^2, 2\gamma \right\} =\begin{cases} \frac{C}{2N} \delta^2 & \text{if } \delta < \delta_c; \\ 2\gamma & \text{otherwise,} \end{cases}
\]  

(A.1)

where \( C \) is deduced from the elastic moduli of the crystal, \( \delta \) is the crack opening and \( \delta_c \) is the interatomic distance at the peak point of the binding law:

\[
\delta_c = 2\sqrt{\frac{\gamma N}{C}}.
\]  

(A.2)

This potential results in the following macroscopic relationship between traction \( \bar{t} \) and crack opening \( \delta \):

\[
\bar{t} = \begin{cases} \frac{C}{N} \delta & \text{if } \delta < \delta_c; \\ 0 & \text{otherwise.} \end{cases}
\]  

(A.3)

The traction rises linearly from zero to a peak stress \( \bar{t}_{\text{max}} \)

\[
\bar{t}_{\text{max}} = \frac{C}{N} \delta_c = 2\sqrt{\frac{C\gamma}{N}}.
\]  

(A.4)

at a critical opening displacement \( \delta_c \), then \( \bar{t} \) drops to zero. Thus, the macroscopic critical opening displacement and peak traction scale as \( \delta_c \sim \sqrt{N} \) and \( \bar{t}_{\text{max}} \sim 1/\sqrt{N} \). Note that the fracture energy in Eqs. (A.1)-(A.3) \( \psi^\prime = 0.5\bar{t}_{\text{max}}\delta_c = 2\gamma \) is independent of \( N \).

B. Comparison with the previous approaches to surface stresses

As we mentioned, we are not aware of the treatment of the surface stresses for the phase field approach to crack propagation. Thus, we will focus here on interfacial stresses for phase
transformations. A very general treatment of the interfacial stresses (including anisotropic interface energy and tension) was suggested in Wheeler and McFadden (1997). The total energy was defined per unit deformed volume, and the gradient of the order parameter was defined in the current deformed configuration. Such assumptions and application of the principle of the least action (or Noether’s theorem) resulted in automatic appearance of interfacial stresses. As it was shown in Levitas (2013b, 2014), stresses obtained in Wheeler and McFadden (1997) were correct for the thermodynamically equilibrium isotropic interfaces but contained extra hydrostatic pressure, which was not localized at the interface but also contributed to the bulk stresses for propagating interfaces. Also, for anisotropic interface energy, interface stress tensor in Wheeler and McFadden (1997) is nonsymmetric, which (as shown in Levitas and Warren, 2016), violates moment of momentum principle and principle of material objectivity. Note that Hakim and Karma (2009) applied Noether’s theorem based approach to fracture, in which energy was determined per unit undeformed volume and the gradient of the order parameter was defined in the undeformed configuration. Such a formulation did not result in any surface stresses, which underlines importance of the utilization of the deformed configuration for such approaches. For an interface between two liquids (Lowengrub and Truskinovsky, 1998) and between a solid and liquid, when the solid is described as a highly viscous liquid (Anderson et al., 2001), the gradient energy was naturally defined in the current deformed configuration and some parts of the energy were determined per unit deformed volume. This led to some (not complete) expressions for the interfacial stresses. The most advanced theory for interfacial stresses during phase transformations is developed in Levitas and Javanbakht (2010), Levitas (2013b) for small strains and in Levitas (2014) and Levitas and Warren (2016) for large strains; in Levitas and Warren (2016) interfacial energy was anisotropic.

Let us compare in more detail the approach developed here with the approach used for phase transformations (Levitas, 2013b, 2014). It is sufficient to compare with results for small strains, isotropic surface energy, and the equilibrium phase interface, although none of these limitations are used in Levitas and Warren (2016). Thus, the free energy in Levitas (2013b, 2014) is postulated in the form

\[
\psi = \psi^d(\phi, \epsilon) + (1 + \epsilon_0)(\psi^s(\phi) + \psi^v(\nabla_d \phi)),
\]

where \(\psi^d\) is the double-well energy, \(\epsilon_0\) is the volumetric strain, and \(\nabla_d\) is the gradient operator in the deformed state. The term \(\psi^d(\phi) + \psi^v(\nabla_d \phi)\) defines the surface energy, similarly to the current approach, and the multiplier \(1 + \epsilon_0\) makes this term defined per unit current (deformed) volume. This equation results in the following expression for the stresses

\[
\sigma = \frac{\partial \psi^r}{\partial \epsilon} - \frac{\partial \psi}{\partial \nabla_d \phi} \otimes \nabla_d \phi = \frac{\partial \psi^r}{\partial \epsilon} + (\psi^d + \psi^v)I - \beta \nabla_d \phi \otimes \nabla_d \phi = \sigma_e + \sigma_s,
\]

where we took \(\psi^v = \frac{\beta}{2} |\nabla_d \phi|^2\) into account. The surface tension stress can be transformed to
\[ \sigma = \beta |\nabla \phi| (I - m \otimes m) + (\psi^d - \psi^\gamma)I. \]  \hspace{1cm} (B.3)

For the phase equilibrium interface, \( \psi^d = \psi^\gamma \) and the last term in Eq. (B.3) disappears. The surface stress then represents the biaxial tension, with the resultant force equal to the surface energy.

The current approach based on Eq. (19) directly corresponds to the traditional thermodynamic procedure of introducing surface stresses by defining surface energy per unit deformed surface (see, Porter et al., 2009) and seems more straightforward. In fact, this was our initial process in introducing surface stresses in the phase transformation theory, but we then switched to the approach based on Eq. (B.1) for two reasons:

(a) Eq. (B.1) does not involve interface (surface) normal \( m \) and can be applied for arbitrary initial conditions with e.g. homogeneous \( \phi = 0 \) and for arbitrary nonstationary distribution of the order parameter, which does not form an interface. For nonequilibrium distribution of the order parameter and for the critical nuclei, the interfacial stresses are not biaxial stresses but contain additional mean stress, which is the second term in Eq. (B.3). In contrast, Eq. (19) explicitly uses normal to the surface and produces biaxial tension even when the surface is not yet formed. Furthermore, one cannot use homogeneous initial conditions for the order parameter, and there must always be some perturbation in the initial conditions and in the region away from the surface to have nonzero \( \nabla \phi \) and to be able to determine \( m \) everywhere.

(b) Eqs. (B.1)-(B.3) are applicable to the interfaces and surfaces in liquids, in gases, and between liquid and gas because the gradient of the order parameter is defined in the current configuration. In contrast, Eq. (19) is not applicable to such cases because it is based on the gradient with respect to the fixed reference configuration, which does not make sense for liquids and gases.

(c) The Ginzburg-Landau equation does not change for the model based on Eqs. (B.1)-(B.3) but includes several sophisticated terms when Eq. (19) is used.

At the same time, we cannot use the approach based on Eq. (B.1) for fracture, at least for the known and current formulation. If energy had been defined per deformed volume, after the appearance of a crack or void, in addition to the surface energy, the finite energy \( A \) would be located at each point of the empty space between the crack or void surfaces, which is unphysical. In the reference state, empty space collapses to the line; thus, by defining energy per unit undeformed state, we avoid this contradiction.

C. Analysis of stress-strain curves of some known potentials

KKL model: The original free-energy function in the KKL model (Karma et al., 2001, Hakim and Karma, 2005) is given by \( \psi = \psi^\lambda + \psi^\gamma \). We change the order parameter \( \phi \) from (Karma et al.,
2001; Hakim and Karma, 2005) to $1 - \phi$ for consistency with the designation in the current paper. Then

$$
\psi^b = (1-\phi)^3 (1 + 3\phi) (\Psi^e - \Psi^c) + A \phi^2(1-\phi)^2,
$$

(C.1)
in which the last term represents the double-well energy with the magnitude $A$. Here, $\epsilon_c$ is defined as the critical strain magnitude such that the unbroken (broken) state is energetically favored for $|\epsilon| < \epsilon_c$ ($|\epsilon| > \epsilon_c$) and $\Psi^e$ is the corresponding elastic energy at $\epsilon_c$. The particular case of this model with $\Psi^c = 0$ was used in Hou et al. (2013) and Zhao et al. (2016). Error! Reference source not found. shows the dependence of $\psi^b$ on $\phi$ at different elastic energies and looks similar to a typical energy plot for materials with first-order phase transformations, e.g. in Levitas and Preston (2002) and Levitas (2014).

![Graph](C.1)

**Fig. C.1.** Bulk free energy vs. the order parameter for the KKL model at various $\epsilon = 6(\Psi^e - \Psi^c)/A$.

The equilibrium condition for the order parameter, $\partial \psi / \partial \phi = 0$, gives the following three roots

$$
\phi_1 = 0; \quad \phi_2 = 1; \quad \phi_3 = \phi_c = 1 - \frac{A}{2(A - 3(\Psi^e - \Psi^c))}.
$$

(C.2)
The first two roots correspond to the intact and fully damaged solids, respectively. The third root corresponds to the maximum of $\psi^b$, i.e. unstable state, for which $\phi$ is less than 1 and larger than 0 if $6(\Psi^e - \Psi^c) \leq A$. The difference between the maximum of the free energy and the energy at $\phi = 0$ represents the activation barrier for damage evolution. Relationship between the order parameter $\phi$ and the strain, Eq. (C.3), and linear elasticity rule, after exclusion of the order parameter, constitutes the unstable branch of the stress-strain curve after damage starts

$$
\sigma_e = (1-\phi)^3 (1 + 3\phi) E_2 \epsilon = \left(\frac{A}{2A - 3E_2 (\epsilon^2 - \epsilon_c^2)}\right)^3 \left(4 - \frac{3A}{2A - 3E_2 (\epsilon^2 - \epsilon_c^2)}\right) E_2 \epsilon.
$$

(C.3)
The stress-strain curves for the KKL model at several critical strains are shown in Fig. .

![Stress-strain curves for the KKL model](image)

**Fig. C.2.** Stress-strain curves for the KKL model for different values of $\epsilon_c$, which contains a stable branch for intact material for $3E_2(\epsilon^2-\epsilon^2_c)<A$ (solid line); unstable branch for damaged material with both decreasing stress and strain from the critical ones to zero $3E_2(\epsilon^2-\epsilon^2_c)<A$ (dashed lines) and nonequilibrium jump to zero stresses at $3E_2(\epsilon^2-\epsilon^2_c)=A$ (solid vertical lines) and zero stresses for $3E_2(\epsilon^2-\epsilon^2_c)>A$ (solid horizontal lines).

Initially, the solution $\phi=\phi_2=0$ holds, the material is intact and stable, and the slope of the stress-strain curve is equal to $E_2$. The instability condition Eq. (44) results in $6(\Psi'-\Psi') \geq A$, where the equality corresponds to $\phi_3=1$, the barrier between the intact and damage phases disappears, and “phase transition”, i.e. damage, occurs.

After $\phi_1=0$ loses its stability, two other equilibrium solutions $\phi_2$ and $\phi_3$ are possible.

(a) The solution for the fully damaged state $\phi_2=1$ can only appear in a non-equilibrium manner, and this is the only solution for $3E_2(\epsilon^2-\epsilon^2_c) \leq A$. For a solution with a crack, this solution localizes at the surface layer of a crack, and because it is non-equilibrium, it will propagate in the bulk material. This is a typical behavior for a non-equilibrium interface for phase transformation theory, which was used by the KKL model. Indeed, unphysical crack widening and lateral growth during crack propagation were observed and discussed in Bourdin et al. (2011).

(b) The behavior for another solution, $\phi_3$, is described by Eq. (44) and the lower unstable branch of the stress-strain curve. The unstable branch starts at the instability point and is tangent to the stable part, then decreases to the zero stress and strain. This behavior is not consistent with what occurs during bond breaking, when strain increases during damage evolution and reduction.
in stress. Another drawback is that the material is not completely broken after reaching zero stress and strain. Indeed, the final point in the unstable branch corresponds to \( \phi = 1 - A / (2(A + 3\Psi')) \) (in particular, \( \phi = 0.5 \) for \( \Psi' = 0 \)), with an elastic modulus of \( 0.3125E_2 \) for \( \Psi' = 0 \). The following loading corresponds to the lower stress-strain branch in Fig. with stable behavior, reducing damage, i.e. growing \( \phi \), and increasing the elastic moduli, i.e. the material is not broken and merely has lower elastic properties. The process repeats itself after reaching \( \phi = 1 \) and the main undamaged branch; the material loses its stability, \( \phi \) increases, and the stresses and strains are reduced to zero again. This solution only exists for \( 3E_2(e^2 - e_1^2) < A \), and only when the stresses and strains are both allowed to decrease after reaching instability. This solution is unphysical and should be avoided. However, such a solution may appear because stresses and strains are not controlled in the internal points during the solution of the boundary-value problems.

Thus, including a double-well barrier and phase transformation-like behavior in the description of fracture leads to unphysical effects and possible behavior. The above analysis shows the importance of analyzing the stress-strain curves for the models under study.

The KKL model in Hakim and Karma (2009) does not contain the double-well term. We utilized a generalized version of this model, with nonlinear elastic behavior and interfacial stresses, for our macroscale behavior. However, the model is not suitable for studying fracture at nanoscale because it does not reproduce the typical stress-strain curve from the atomistic studies.

D. Models with transformation strain.

An alternative way to describe the reduction in the slope of the stress-strain curve and the reduction of the stresses to zero during damage is to introduce transformation strain instead of the degradation function (Jin et al., 2001; Wang et al., 2002). However, analysis of the stress-strain curve in Levitas et al. (2011) for this model exhibited a reduction in the initial elastic modulus by a factor of 2 at the infinitesimal damage. The phase field model for dynamic fracture in liquid (Levitas et al., 2011) suggested local potential, which does not possess such a drawback. However, the gradient term is excluded in this model, and rate-type regularization of locally-unstable behavior and introduction of the characteristic spatial scale is performed instead of gradient-type regularization. This is in contrast to all other phase field models for fracture.

References


• A thermodynamically-consistent phase field approach for crack propagation which includes several novel features is presented.
• Scale dependency was included which makes the developed theory applicable from the atomistic to the macroscopic scales.
• The surface stresses (tension) are introduced by employing some geometrical nonlinearities even in small strain theory.
• Crack propagation in the region with compressive closing stresses is eliminated.
• The effect of the above novel features is analyzed with the finite element method for various model problems.