On degradation functions in phase field fracture models

Charlotte Kuhn [a,*], Alexander Schlüter [a,b], Ralf Müller [b]

[a] Computational Mechanics, University of Kaiserslautern, P.O. Box 3049, D-67653 Kaiserslautern, Germany
[b] Institute of Applied Mechanics, University of Kaiserslautern, P.O. Box 3049, D-67653 Kaiserslautern, Germany

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ABSTRACT

Unlike the description of cracks as sharp surfaces which requires different criteria to predict the onset of crack propagation, the direction of crack growth, possible crack branching, and the nucleation of new cracks, the phase field approach provides a holistic description of all these fracture processes. The phase field order parameter is used to differentiate between broken and undamaged material, and the entire crack evolution is obtained implicitly by solving the evolution equation of the order parameter which is coupled to the mechanical field equations. A so called degradation function couples the order parameter to the elastic properties of the material in order to model the change in stiffness between fractured and undamaged material. The nucleation of a new crack in originally undamaged material is preceded by a localization of the fracture field. Before the onset of this localization the material response of the phase field fracture model is mainly controlled by the degradation function. However, the degradation function frequently found in the literature yields a pronounced softening behavior before the onset of fracture which is not desirable when modeling brittle materials. In this work we discuss the potential of alternative degradation functions in the context of crack nucleation and propagation.

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1. Introduction

The key objective of fracture mechanics is to predict the evolution of cracks in structural components under a given loading scenario. In order to model the entire fracture process, a fracture criterion must be able to predict the onset of the propagation of pre-existing cracks as well as the nucleation of new fractures in originally sound material. Additionally, the model must predict the crack path which requires criteria for the direction of crack extension and for the bifurcation of cracks.

The conceptual basis of the contemporary theory of brittle fracture was laid in the works of Griffith [1], who for the first time formulated an energetic fracture criterion. According to this criterion, crack propagation follows from the minimization of the sum of the elastic energy stored in the bulk material and the energy required to create new fracture surfaces. However, this criterion is only able to predict the onset of crack extension along a given crack path. Additional criteria are needed in order to predict the geometry of the crack path and the nucleation of new cracks. In the 2D case, there are numerous criteria available in the literature predicting different crack paths. Popular criteria are e.g. the maximum hoop stress criterion [2], the principle of local symmetry according to

[3] and the criterion of maximum energy release [4], only to name a few. However, no general consensus on which of these theories is the most adequate has been reached so far. Due to the manifold possible crack geometries, crack path prediction becomes even more difficult in 3D scenarios.

Further issues which have not been satisfactorily solved in fracture mechanics are the nucleation of new cracks in the absence of macroscopic initial cracks, and the transition from the phase of fracture nucleation to macroscopic crack extension.

Besides the development of physically sound fracture models, numerical strategies are needed to compute the fracture evolution and the elastic deformation of complex structures. The finite element method (FEM), where the structure is discretized into a set of elements, is a widely used tool for this purpose. The partial differential equations for the unknown field variables are recast into a finite dimensional set of equations for the values at the element nodes. Within the elements, the unknown field variables are usually interpolated from the nodal values by means of continuous finite element shape functions. Since the displacement field may have jump discontinuities where the material is broken, cracks within an element cannot be modeled well by this technique. Therefore, the finite element mesh needs to be adapted to the new crack geometry after every progression of fracture if this ansatz is used, see e.g. [5–7] for configurational force driven remeshing strategies. An alternative which allows to simulate

* Corresponding author.
  E-mail address: chakuhn@rhrk.uni-kl.de (C. Kuhn).

crack growth without adaptive remeshing is the extended finite element method (X-FEM) [8] where special enriched shape functions are used to model jumps in the displacement field and singularities in the stress field.

Regarding the numerical treatment of fracture a conceptually different modeling technique has gained importance in the recent past. So called phase field models, which base on the concepts introduced in [9], were originally used in [10,11] to model solidification processes. Applications of this modeling approach in the context of fracture mechanics have been introduced and discussed e.g. in [12–18]. In phase field fracture models, the phase field order parameter is also called the fracture field. The value 1 is used to characterize sound material, and 0 indicates fracture. The evolution of fracture can be regarded as a phase transition problem of the fracture field. At a fracture surface the order parameter varies smoothly between the values assigned to the different phases, avoiding discontinuous jumps. The width of this transition zone of the order parameter is controlled by a model inherent length scale. The entire evolution of fracture evolution is obtained implicitly by solving the coupled system of equations formed by the evolution equation of the order parameter and the mechanical field equations. As there are no jump discontinuities in the displacement field using this approach, phase field fracture models can be implemented very conveniently into standard finite element software. Standard finite element shape functions can be used and remeshing is not mandatory in order to simulate the propagation of fracture. Thus, finite element implementations of phase field fracture models are very powerful numerical tools to study topologically complex fracture problems.

If the nucleation of fracture in originally intact material is simulated with a phase field fracture model, the formation of a crack is preceded by a localization of the fracture field which is connected to the loss of stability of the unfractured solution. Before the onset of this localization process the material response of the phase field fracture model is mainly controlled by the interplay between the degradation function, which models the impact of the fracture field on the elastic properties, and the local part of the phase field fracture energy. During this phase, the quadratic degradation function which is frequently found in the literature yields a pronounced degradation of stiffness. However, this is not desirable when modeling brittle materials which are generally assumed to be linear elastic until the point of fracture. In this work we discuss alternative degradation functions and their potential to improve the modeling of fracture nucleation in brittle materials. Thus, a special focus is put on the pre-fracture behavior of the phase field model, but also the impact of the degradation function in the fractured state is considered. Also the crucial role of the phase field model's inherent length scale in the context of crack nucleation will be addressed.

The paper is organized as follows. In Section 2 the basic concept of phase field fracture models is introduced starting with the formulation of an appropriate phase field energy density, which approximates the elastic and fracture energy of the considered body in Section 2.1. Three different possible formulations of degradation functions which model the coupling between the mechanical fields and the phase field order parameter are proposed in Section 2.2 in order to improve the modeling of brittle material behavior before fracture. In order to provide the theoretical background a thermodynamically consistent derivation of the evolution equation of the phase field order parameter is presented in Section 2.3 and possible formulations of irreversibility constraints are discussed in Section 2.4. The impact of the choice of the degradation function is studied analytically in a simple 1D setting in Section 3. The results of numerical finite element simulations of fracture nucleation using models with different degradation functions are presented in Section 4. The simulations comprise a

reconsideration of the 1D setting and an extension to a more complex 2D scenario. A concluding discussion of the results is given in Section 5.

2. Formulation of phase field fracture models

2.1. Phase field energy

In a small strain setting, where the infinitesimal strain tensor $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla^T \boldsymbol{u} + \nabla \boldsymbol{u})$ is the symmetric part of the displacement gradient $\nabla \boldsymbol{u}$, the energy density functional ψ of a phase field fracture model is typically of the format

$$\psi(\boldsymbol{\varepsilon}, s) = \frac{1}{2}(g(s) + \eta)\boldsymbol{\varepsilon} : \mathbb{C}\boldsymbol{\varepsilon} + \frac{\mathcal{G}_c}{2c_w}\left(\frac{w(s)}{4\epsilon} + \epsilon|\nabla s|^2\right). \tag{1}$$

The elastic stiffness tensor $\mathbb{C}$ and the cracking resistance $\mathcal{G}_c$ describe the material properties. The parameter ϵ has the dimension of a length and is often referred to as regularization length, since it controls the width of the transition zone of the phase field order parameter between the broken state $s = 0$ and the undamaged state $s = 1$. However, an alternative interpretation of this parameter in the context of fracture nucleation will be discussed in Section 3. The so-called degradation function $g(s)$ with $g(1) = 1$ and $g(0) = 0$ models the release of elastic energy

$$\psi^e = \frac{1}{2}(g(s) + \eta)\boldsymbol{\varepsilon} : \mathbb{C}\boldsymbol{\varepsilon} \tag{2}$$

if the fracture field s becomes zero. A proper choice of the degradation function $g(s)$ and its impacts will be discussed in Section 2.2. The positive residual stiffness parameter $\eta \ll 1$ is needed to ensure numerical stability where $g(s) = 0$.

The function $w(s)$ models the local fracture energy. For a given function $w(s)$, the normalization constant c_w must be chosen such that the integral of $\left(w(s)/(4\epsilon) + \epsilon|\nabla s|^2\right)/(2c_w)$ over the fractured domain converges to the surface measure of the crack set as $\epsilon \to 0$. There are different formulations of $w(s)$ to be found in the literature, which split in basically two classes: Double well functions of type

$$w(s) = 16s^2(1 - s)^2, \tag{3}$$

as they are found in [12–15,18], and monotonous functions of the format

$$w(s) = (1 + \beta s)(1 - s) \tag{4}$$

with $\beta \in [-1, 1]$. Most commonly, the convex quadratic function with $\beta = -1$ is used, see e.g. [19–21]. But also the linear case $\beta = 0$ is found e.g. in [22,23]. For illustration, Fig. 1(a) shows plots of the double well function (3) and Fig. 1(b) shows the function (4) for distinct values of β. The vertical dotted lines indicate the relevant interval $s \in [0, 1]$.

The double well potential (3) provides an energy barrier between the broken and unbroken state and does therefore naturally model irreversibility of fracture processes to a certain extent. In contrast, local energy functions of the type (4) do not model irreversibility at all and additional constraints for the fracture field need to be formulated in order to model an irreversible evolution of fracture. This issue will be discussed in Section 2.3 in the framework of a thermodynamically consistent derivation of the evolution equation of the fracture field.

Despite the problems concerning irreversibility, in [24] the authors strongly advocate a monotonous potential. Besides mathematical issues, their skepticism towards the usage of a double well function as a local potential of a phase field fracture model is based on the fact that the broken ($s = 0$) and undamaged ($s = 1$) phases are equivalent from an energetic point of view.