Discussion of hardening effects on phase field models for fracture

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Abstract. Phase field models have been successfully applied in recent years to a variety of fracture mechanics problems, such as quasi-brittle materials, dynamic fracture mechanics, fatigue cracks in brittle materials, as well as ductile materials. The basic idea of the method is to introduce an additional term in the energy functional describing the state of material bodies. A new state variable is included in this term, the so-called phase field, and enables to determine the surface energy of the crack. This approach allows to model phenomena such as crack initiation, crack branching and buckling of cracks, as well as the modelling of the crack front in three-dimensional geometries, without further assumptions. There is yet no systematic investigation of the influence of strain hardening on crack development within the phase field method. Thus, the aim of the paper is to provide an analysis of the effect of kinematic and isotropic hardening on the evolution of the phase field variable.

1 Introduction

In fracture mechanics, the description of complex crack phenomena such as initiation, propagation, kinking and branching of cracks is a very demanding task. For brittle materials, the concept of configurational forces e.g. is an appropriate framework to address these issues. However, this ansatz is not suitable in the case of ductile materials, cf. Tsakmakis et al. [1]. A different approach is given by phase field theories, which have been successfully introduced in fracture mechanics to capture complex phenomena in a unified framework. The applications include both elastic and plastic material behaviour, as well as extensions to fatigue crack propagation. The basic idea of the method is to introduce an additional term in the energy functional describing the state of material bodies. A new variable, the so-called phase field, as well as its spatial gradient, are accounted for in this term. The motivation for the introduction of such part in the state functional arises from a regularisation of the crack geometry in the context of the classical Griffith theory for brittle materials and enables the calculation of the surface energy during crack propagation.

From the point of view of continuum damage mechanics, the phase field variable can also be interpreted as the isotropic damage variable. Loss of ellipticity of the differential equations is a common problem in this theory, since damage evolution is often accompanied by softening of the material response. Introduction of the gradient of the

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damage variable is one possibility to ensure the well-posedness of the governing differential equations. Models of gradient damage mechanics are in principal the same as phase field models of fracture. In the present paper, a phase field model in common use is introduced by extension of a von Mises-plasticity model with the aid of the concept of energy equivalence known from continuum damage mechanics. Special attention in the context of the present problem needs to be paid to the thermodynamic consistency of the model. The framework of classical thermodynamics is in general not appropriate for material models, which deal with gradients of the state variables. Several approaches can be found in the literature addressing this issue. In Hofacker et al. [2], e.g., conventional thermodynamics is adopted while the gradient of the damage variable is incorporated in the postulated damage criterion and the associated damage dissipation function. This implies that crack propagation is modelled as a completely dissipative process. Another approach, followed e.g. by Borden et al. [3], is based on the postulated existence of microforces. Kuhn et al. [4], on the other hand, suppose an evolution equation of the Ginzburg-Landau type for the damage variable. In the present work, this issue is addressed in terms of the non-conventional thermodynamics proposed by Dunn and Serrin [5]. The introduced phase field model is finally investigated with regard to different types of hardening behaviour. Model responses for pure isotropic and pure kinematic hardening are examined for one- and two-dimensional problems.

2 Constitutive model

The constitutive model used is a von Mises-plasticity model coupled with damage. Further, the model exhibits kinematic or isotropic hardening. Assuming small deformations, the strain tensor is given by $\boldsymbol{\varepsilon} := \frac{1}{2}[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$, where $\mathbf{u}$ denotes the displacement vector and $\nabla(\cdot)$ is the spatial gradient of $(\cdot)$. As usual, the additive decomposition of $\boldsymbol{\varepsilon}$ into elastic and plastic parts, $\boldsymbol{\varepsilon}_e$ and $\boldsymbol{\varepsilon}_p$ respectively, is assumed. Following the concepts of continuum damage mechanics, the free energy density per unit volume ψ is decomposed into elastic-plastic and damage parts. The elastic-plastic part is further decomposed into an elastic part, and plastic parts due to isotropic and kinematic hardening, so that

$$\psi = \psi_{ep} + \psi_D = \psi_e + \psi_p^{iso} + \psi_p^{kin} + \psi_D. \quad (1)$$

The elastic part is supposed to obey the form $\psi_e = \psi_e(\boldsymbol{\varepsilon}_e, D)$. Several ways have been proposed in the literature to distinguish between tensile and compressive contributions in ψ . In the present work, the volumetric-deviatoric split of Amor et al. [6] is applied. Tensile and compressive contributions of the elastic part of the free energy, ψ_e^+ and ψ_e^- respectively, are distinguished. The influence of damage evolution is captured in terms of a positive, scalar valued degradation function $g(D)$ which affects only the tensile contributions. Therefore,

$$\psi_e(\boldsymbol{\varepsilon}_e, D) = \psi_e^+(\boldsymbol{\varepsilon}_e, D) + \psi_e^-(\boldsymbol{\varepsilon}_e) \quad (2)$$

with

$$\psi_e^+(\boldsymbol{\varepsilon}_e, D) = g(D) \left[\frac{1}{2} K (\text{tr}(\boldsymbol{\varepsilon}_e))^2 + \mu \boldsymbol{\varepsilon}_e^D \cdot \boldsymbol{\varepsilon}_e^D \right], \quad (3)$$

$$\psi_e^-(\boldsymbol{\varepsilon}_e) = \frac{1}{2} K (-\text{tr}(\boldsymbol{\varepsilon}_e))^2, \quad (4)$$

where K, μ are the compression modulus and shear modulus, respectively, $\text{tr}(\cdot)$ is the trace operator, $\langle \cdot \rangle$ are the Macaulay-brackets, $\mathbf{A}^D$ is the deviatoric part of $\mathbf{A}$ and $\mathbf{A} \cdot \mathbf{B}$ is the scalar product of the second-order tensors $\mathbf{A}$ and $\mathbf{B}$. The elasticity law is then given by

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}_e, D) = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} = K[g(D)\langle \text{tr}(\boldsymbol{\varepsilon}_e) \rangle - \langle -\text{tr}(\boldsymbol{\varepsilon}_e) \rangle] \mathbf{1} + g(D)2\mu \boldsymbol{\varepsilon}_e^D, \quad (5)$$

where $\mathbf{1}$ denotes the second-order unity tensor. Next, the forms for the plastic parts of the free energy density are specified. For that purpose, formulations based on the principle of energy equivalence are adopted (cf., e.g., Grammenoudis et al. [7]). For the aims of the present work, it is sufficient to confine to linear isotropic and linear kinematic hardening behaviour, with respective material parameters γ and c , so that

$$\psi_p^{iso}(s, D) = g(D) \frac{1}{2} \gamma s^2, \quad (6)$$

$$\psi_p^{kin}(\boldsymbol{\varepsilon}_p, D) = g(D) \frac{1}{2} c \boldsymbol{\varepsilon}_p \cdot \boldsymbol{\varepsilon}_p. \quad (7)$$

The accumulated plastic strain in Eq. (6) is given by the evolution equation

$$\dot{s} = \sqrt{\frac{2}{3} \dot{\boldsymbol{\varepsilon}}_p \cdot \dot{\boldsymbol{\varepsilon}}_p}. \quad (8)$$

Here, $(\dot{\cdot})$ denotes the derivative of $(\cdot)$ with respect to time t . The isotropic hardening R and the backstress tensor $\boldsymbol{\xi}$ are defined through

$$R(s, D) = \frac{\partial \psi}{\partial s} = g(D) \gamma s, \quad (9)$$

$$\boldsymbol{\xi}(\boldsymbol{\varepsilon}_p, D) = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} = g(D) c \boldsymbol{\varepsilon}_p. \quad (10)$$

Next, the von Mises-yield function is generalized to account for damage effects. Following Grammenoudis et al. [7], the yield function reads

$$F(\boldsymbol{\sigma}, R, \boldsymbol{\xi}, D) := g_f(D) f(\boldsymbol{\sigma}, \boldsymbol{\xi}, R) - k_0, \quad (11)$$

$$f := \sqrt{\frac{3}{2} (\boldsymbol{\sigma} - \boldsymbol{\xi})^D \cdot (\boldsymbol{\sigma} - \boldsymbol{\xi})^D} - R, \quad (12)$$

where k_0 represents the initial yield stress. Further, $g_f(D) = g^{-1}(D)$ is assumed for simplicity. In general, the two degradation functions need not to coincide. To complete the plasticity part of the model, an associated normality rule is assumed for the evolution equation of the plastic strain,

$$\dot{\boldsymbol{\varepsilon}}_p = \Lambda \frac{\partial F}{\partial \boldsymbol{\sigma}}, \quad (13)$$

together with the standard Kuhn-Tucker-conditions and the consistency condition

$$\Lambda \geq 0, \quad F \leq 0, \quad \Lambda F = 0, \quad \Lambda \dot{F} = 0, \quad (14)$$

where Λ denotes a scalar plastic multiplier.

For the damage part of the model, the form of ψ_D needs to be specified. In the context of phase field theories for fracture,

$$\psi_D(D, \nabla D) = G_c \left(\frac{1}{2l} D^2 + \frac{l}{2} |\nabla D|^2 \right) \quad (15)$$

is standard, cf, e.g., [2-4], with the material parameter G_c and the material internal length l .

3 Damage Law

3.1 Thermodynamic consistency

In the present work, the approach of non-conventional thermodynamics, proposed by Dunn and Serrin [5], is adopted to establish thermodynamic consistency. Accordingly, besides the heat flux vector $\bar{\mathbf{q}}$, the existence of an energy flux vector $\mathbf{q}'$ is assumed, which accounts for non-local effects. More precisely, the energy carriers responsible for this energy flux are assumed to be related to the initiation and evolution of damage effects. Assuming isothermal processes with uniformly distributed temperature, the second law of thermodynamics is postulated in the form

$$\boldsymbol{\sigma} \cdot \dot{\boldsymbol{\varepsilon}} - \operatorname{div} \mathbf{q}' - \dot{\psi} \geq 0. \quad (16)$$

Using standard arguments and incorporating Eqs. (5)-(7), (9), (10) and (15), inequality (16) finally reduces to

$$-\operatorname{div} \mathbf{q}' + (\boldsymbol{\sigma} - \boldsymbol{\xi}) \cdot \dot{\boldsymbol{\varepsilon}}_p - R\dot{s} - \frac{\delta\psi}{\delta D} \dot{D} - \operatorname{div} \left(\frac{\partial\psi}{\partial\nabla D} \dot{D} \right) \geq 0, \quad (17)$$

where the variational derivative

$$\frac{\delta\psi}{\delta D} := \frac{\partial\psi}{\partial D} - \operatorname{div} \left(\frac{\partial\psi}{\partial\nabla D} \right) \quad (18)$$

has been employed. Since $F = 0$ and $\dot{s} = g_f(D)\Lambda$ hold during plastic flow, it can be shown that

$$(\boldsymbol{\sigma} - \boldsymbol{\xi}) \cdot \dot{\boldsymbol{\varepsilon}}_p - R\dot{s} = \frac{k_0}{g_f(D)} \dot{s} \geq 0. \quad (19)$$

A sufficient condition to satisfy inequality (17) is to require

$$-\operatorname{div} \mathbf{q}' - \frac{\delta\psi}{\delta D} \dot{D} - \operatorname{div} \left(\frac{\partial\psi}{\partial\nabla D} \dot{D} \right) \geq 0. \quad (20)$$

Further, the energy flux vector is specified by the constitutive assumption

$$\mathbf{q}' = \frac{\partial \psi}{\partial \nabla D} \dot{D} + \mathbf{c} = -G_c l (\nabla D) \dot{D} + \mathbf{c} \quad (21)$$

where $\mathbf{c}$ is a divergence-free vector. Thus, inequality (20) becomes

$$\Omega \dot{D} \geq 0, \quad (22)$$

$$\Omega := -\frac{\delta \psi}{\delta D} = -\frac{\partial \psi_{ep}}{\partial D} - \frac{\delta \psi_D}{\delta D} \quad (23)$$

That means, Ω is the thermodynamic driving force for damage evolution. A common assumption for the degradation function is given by the quadratic function

$$g(D) = (1 - D)^2 + \kappa, \quad (24)$$

where $\kappa \ll 1$ is introduced for reasons of numerical stability. Denoting by ψ_{ep}^{0+} the sum of the undegraded parts of ψ_e^+ , ψ_p^{iso} and ψ_p^{kin} , the driving force is finally given by

$$\Omega = 2(1 - D)\psi_{ep}^{0+} - \frac{G_c}{l} (D - l^2 \Delta D). \quad (25)$$

3.2 Damage criterion

In analogy to the yield function in plasticity, a damage criterion can be formulated in terms of a damage function $F_D(\Omega) \leq 0$, where $F_D = 0$ only holds during damage evolution. An associated normality rule, the Kuhn-Tucker-conditions and the consistency condition are again assumed,

$$\dot{D} = \Lambda_D \frac{\partial F_D}{\partial \Omega}, \quad (26)$$

$$\Lambda_D \geq 0, \quad F_D \leq 0, \quad \Lambda_D F_D = 0, \quad \Lambda_D \dot{F}_D = 0 \quad (27)$$

where Λ_D is a scalar damage multiplier. A possible formulation for the damage function then reads

$$F_D := \Omega - k_D \leq 0. \quad (28)$$

The variable k_D can be used to model the counterpart of isotropic hardening in plasticity. It is assumed, that no constant value is included in k_D , so that

$$k_D = \beta \frac{\delta \psi_D}{\delta D} \quad (29)$$

is a possible ansatz as a pendant to isotropic hardening in gradient plasticity models, where β denotes a non-negative material parameter. With these definitions at hand, the damage criterion finally reads

$$2(1 - D)\psi_{ep}^{0+} - (\beta + 1) \frac{G_c}{l} (D - l^2 \Delta D) \leq 0 \quad (30)$$

Note, that thermodynamic consistency is guaranteed with the chosen approaches.

For later purposes of numerical implementation, it is convenient to introduce a so-called history field. Following Hofacker et al. [2], this is defined for every material point of the body, with respective location vector $\mathbf{x}$, as

$$\mathcal{H}(\mathbf{x}, t) := \max_{\tau \in [0, t]} \psi_{ep}^{0+}(\mathbf{x}, \tau). \quad (31)$$

Then, inequality (30) simplifies to the partial differential equation

$$2(1 - D)\mathcal{H} - (\beta + 1) \frac{G_c}{l} (D - l^2 \Delta D) = 0, \quad (32)$$

which needs to be solved now to obtain the solution of the phase field problem. This is the phase field model proposed by Hofacker et al. [2]. The remainder of the paper is concerned with an analysis of this model for the case of ductile fracture.

4 Numerical results

The aim of this section is to discuss the influence of the damage variable on the material behaviour for different types of hardening. Especially, pure isotropic or pure kinematic hardening will be addressed in the following. All material parameters are summarised in table 1. They are chosen so, that the stress-strain curves for monotonic uniaxial loading conditions are identical. Two cases are: one-dimensional tension/compression and a two-dimensional cracked specimen under plane strain conditions. Dimension and boundary conditions for the latter are depicted in Fig. 1. For both cases, harmonically varying, displacement controlled loading conditions are applied.

For numerical solutions by the finite element method, the above constitutive theory is implemented in ABAQUS. The phase field variable is treated as an additional degree of freedom and linear shape functions are used in all examples. The integration is performed in a staggered manner, as proposed in Hofacker et al. [2], i.e. the displacement problem and the phase field problem are solved separately. The advantage of this method is its numerical stability in comparison to a monolithic solution method. First, the phase field variable is held constant, and the displacement problem is solved, then the displacement is held constant and the phase field problem is solved. Both steps alternate until convergence is achieved in the respective time increment.

Fig. 1. Geometry and dimensions of the cracked plate.

Table 1. Material parameters

K	μ	k_0	$\gamma = 3c/2$	$(1 + \beta)G_c$	l
175000 MPa	80769 MPa	200 MPa	5000 MPa	2.7 N/mm	0.0075 mm

The first case to be discussed is that of pure kinematic hardening. The strain-stress-curve for the one-dimensional, uniaxial tension/compression model is depicted in Fig. 2(a). Cyclic, displacement-controlled loading conditions with vanishing mean value are applied. It can be seen, that after only one loading cycle a closed hysteresis loop is obtained as in the case of classic plasticity without damage. No further damage accumulation takes place after the first loading branch, cf. Fig. 2(b). The reason is that the maximum value of the history variable is obtained already at the end of the first loading branch. Hence, the material response after the first loading branch is purely elastic-plastic.

Fig. 2. Pure kinematic hardening. Displacement-controlled, uniaxial tension/compression loading with vanishing mean value. (a) Strain-stress-distribution. (b) Strain-damage-distribution.

The behaviour in the case of the cracked specimen is analogous. Harmonically varying, displacement-controlled loading conditions with positive mean value are applied for this case. The imposed displacement on the upper boundary varies between $u = 0$ mm and $u = 0.01$ mm, cf. Fig. 1. Again, no further damage accumulation takes place at the crack tip after the first loading branch. In other words, the damage distribution after one and after ten loading cycles is identical, see Fig. 3 (left), so that no crack propagation can be described with the model when only pure kinematic hardening is considered.

Fig. 3. Pure kinematic hardening (left) and pure isotropic hardening (right). Damage distribution in the cracked plate after (a) one loading cycle and after (b) ten loading cycles.

Fig. 4. Pure isotropic hardening. Displacement-controlled, uniaxial tension/compression loading with vanishing mean value. (a) Strain-stress-distribution. (b) Strain-damage-distribution.

In contrast, damage accumulates continuously in the case of pure isotropic hardening, cf. Fig 4, for uniaxial loading conditions. It can further be seen from Fig. 4(b), that damage evolution takes place equally in tension and in compression. This happens due to the strong influence of $\psi_p^{(iso)}$ on the history variable.

Again similar behaviour to the uniaxial case is observed for the cracked specimen. The damage distribution changes now in every cycle, cf. Fig. 3 (right), so that crack propagation can be captured in principle by the model with pure isotropic hardening. It is noteworthy, that a considerable part of the crack propagation takes place in the compression regime of the loading history.

5 Conclusions

In the present work, an analysis of a common phase field approach with respect to pure isotropic and pure kinematic hardening is given. A von Mises-plasticity model is extended to include damage effects and the associated damage law is derived with the aid of a non-conventional thermodynamics framework. The numerical investigation shows, that no crack propagation can be predicted by the model when only pure kinematic hardening is present. For the case of pure isotropic hardening on the other hand, crack propagation can be described in general. However, the influence of the modification of the elasticity law for tension/compression asymmetry is negligible, due to the strong influence of the plastic part of the free energy density. Moreover, it should be mentioned, that it is well known from classical plasticity theory, that linear isotropic hardening is not appropriate for the modelling of effects of cyclic plasticity. The results show, that the considered phase field model is generally not suitable to capture adequately effects of cyclic plasticity in fracture problems.

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