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Phase-Field Modelling of Interface Failure in Brittle Materials

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Abstract

A phase-field approach is proposed for interface failure between two possibly dissimilar materials. The discrete adhesive interface is regularised over a finite width. Due to the use of a regularised crack model for the bulk material, an interaction between the length scales of the crack and the interface can occur. An analytic one-dimensional analysis has been carried out to quantify this effect and a correction is proposed, which compensates influences due to the regularisation in the bulk material. For multi-dimensional analyses this approach cannot be used straightforwardly, as is shown, and a study has been undertaken to numerically quantify the compensation factor due to the interfaces between dissimilar materials, such that they are independent from the regularisation width of the interface. The method has been tested and validated on three benchmark problems. The compensation is particularly relevant for phase-field analyses in heterogeneous materials, where cohesive failure in the constituent materials as well as adhesive failure at interfaces play a role.

Keywords: phase-field modelling, brittle fracture, adhesive interface, diffuse interface model, interface failure

1. Introduction

The functionality of engineering structures may be compromised by cracks, and there has been a long-standing interest to predict crack initiation and propagation, i.e. the location at which a crack nucleates, under which conditions it propagates, and its propagating direction.

The work of Griffith [1] is a landmark contribution in the understanding of fracture. He introduced an energetic criterion to assess whether crack growth would occur or not. Herein, a central concept is the fracture toughness, which is an energetic threshold. Often, crack growth is a highly transient process, incorporating complex mechanisms like crack nucleation, propagation, branching and possibly crack arrest, i.e. such analyses can only be carried out numerically. Computational approaches can roughly be divided into two categories, namely methods in which the crack is represented in a discrete manner, and those in which a diffuse, or continuum, representation is employed, e.g. [2].

Herein, we will focus on a particular method within the class of diffuse representations, namely the phase-field approach to fracture. The phase-field model covers crack nucleation and crack propagation, yields qualitatively good results for homogeneous materials and is appealing due to its conceptual simplicity. Indeed, phase-field models are a powerful way of modelling cracks, especially when it comes to three-dimensional problems. Moreover, they can straightforwardly handle issues that may be complicated in discrete crack analyses, such as a priori unknown crack paths, crack arrest and branching. In this contribution we will show, however, that modelling adhesive failure along sharp interfaces is more complex and requires additional numerical treatment.

Starting from a Griffith approach, Francfort and co-workers [3] introduced an integral crack surface energy formulation where the total energy takes a minimum for the correct crack path. Subsequently, this formulation was regularised, resulting in a diffuse crack representation [4, 5]. The crack is now no longer described by a physical

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crack opening, but is rather represented by a scalar field over the entire domain. This, in principle, avoids the need for remeshing and is appealing for complex fracture processes. The auxiliary scalar variable, often referred to as the phase-field variable, regularises the boundary value problem and distributes the discrete crack over a finite width. In an extension of the above approach for brittle fracture to quasi-brittle and ductile fracture, Verhoosel and de Borst [6] incorporated the cohesive-zone model in the phase-field approach.

Engineering materials are often composed of several components, e.g. reinforced concrete, or fibre-reinforced composites, which consist of fibres and a matrix, or laminates with different plies. Often, the interfaces in such heterogeneous material systems are the weak spots where fracture initiates. A complete failure analysis of such composite materials or structures therefore requires that cracks can propagate within the matrix with an a priori unknown crack path, but also along interfaces between two dissimilar materials. Typically, the fracture toughness of an adhesive interface, say \mathcal{G}_c^{int} , is different from that in the bulk material, \mathcal{G}_c^{bulk} .

Schneider et al. [7] have presented a multiphase-field model which is capable of describing cracks within grains as well as along grain boundaries. The modification of the surface energy between the bulk materials allows for different interface properties. In a hybrid approach, Paggi et al. [8] incorporated a sharp interface by combining a phase-field model for brittle fracture with a cohesive-zone model for the interface. For a brittle, inclined interface, they achieved results comparable to linear elastic fracture mechanics derived by He and Hutchinson [9]. Nguyen et al. [10] extended the standard cohesive zone approach by introducing an interface regularisation similar to the crack phase-field, where the displacement jump over the interface takes a regularised form.

This work extends the findings of Hansen-Dörr et al. [11], who presented a method to incorporate an adhesive interface in the bulk material using a phase-field model for brittle fracture [12]. This qualitative study showed a significant interaction between the surrounding bulk material and the diffuse interface due to the different length scales of the crack and the interface. Indeed, the critical energy release rate at which the crack propagates is not only governed by the fracture toughness of the interface, but also by the fracture toughness of the bulk material.

Our aim is to correct the influence of the bulk material on crack propagation along an interface by modifying the fracture toughness of the interface. The testing environment to investigate the proposed modification should be such that:

- There is a steady, controllable crack growth along the interface;
- The method to calculate the energy release rate can be used to compare the results to the predefined values;
- There is an efficient spatial discretisation of the regularised crack surface.

The first requirement is met using a so-called surfing boundary condition, cf. [13, 14]. The second issue is addressed using the concept of configurational forces which exploits a generalised force acting on the crack tip [14, 15]. An accurate and efficient representation of the steep gradient of the regularised crack is obtained using isogeometric analysis, cf. [16], with local refinement [17, 18].

The paper is structured as follows. Section 2 gives a concise review of the phase-field model for brittle fracture. Section 3 introduces the idea of a diffuse interface and discusses the interaction of both length scales. An exact solution is derived for a proper compensation in a one-dimensional case. The next section shows that the one-dimensional approach cannot be taken over to two-dimensional configurations in a straightforward manner and presents a numerical study that provides compensation factors for two-dimensional cases. Section 5 presents numerical examples and a comparison with analytical results. Concluding remarks are drawn in Section 6.

2. Phase-field Model for Brittle Fracture

The phase-field approach introduces an additional scalar field c, which in a continuous manner separates fully intact material (c = 1) from fully broken material (c = 0), and is coupled to the mechanical part of the boundary value problem. Figure 1 illustrates the regularisation. The originally sharp crack Γ is regularised through a phase-field c, yielding a steep gradient near the original crack surface. Following [5], the total energy of a brittle, linear elastic (cracked) domain reads

$$\Psi = \Psi^{\rm el} + \Psi^{\rm c} = \int_{\Omega} \psi^{\rm el} + \psi^{\rm c} \, \mathrm{d}v = \int_{\Omega} (g(c) + \eta) \cdot \psi^{\rm el}_{+} + \psi^{\rm el}_{-} + \underbrace{\frac{\mathcal{G}_{\rm c}}{4l_{\rm c}} \left\{ (1-c)^2 + 4l_{\rm c}^2 c_{,i} c_{,i} \right\}}_{\operatorname{crack/dissipated energy}} \, \mathrm{d}v \,, \tag{1}$$

crack/dissipated energy



Figure 1: The discrete crack surface depicted on the left is regularised using an exponential function. The resulting distributed discontinuity, regularised using the length scale parameter l_c , is shown on the right.

where l_c is the characteristic length scale that governs the width of the crack phase and $(\bullet)_{,i} = \partial(\bullet)/\partial x_i$. The summation convention applies. For the specific elastic HELMHOLTZ free energy $\psi^{el} = \frac{1}{2}\varepsilon$: $E : \varepsilon$ a split is carried out into a tensile ψ^{el}_+ and a compressive ψ^{el}_- part to avoid cracking under compressive stresses [19]. The degradation function $g(c) = c^2$ fulfils the condition that the driving force of the phase-field c vanishes when c = 0. The fracture toughness \mathcal{G}_c is the material parameter within the energetic crack growth criterion of Griffith [1]. The residual stiffness $0 < \eta \ll 1$ prevents numerical instabilities.

The Euler-Lagrange equations, which describe the coupled problem, can be derived in a variational manner [12, 19]. Neglecting volume forces, they read

$$\sigma_{ij,i} = 0 \quad \text{and} \tag{2}$$

$$[1-c] + 4l_{\rm c}^2 c_{,ii} = \frac{2g'(c)l_{\rm c}}{\mathcal{G}_{\rm c}}\psi_+^{\rm el}, \qquad (3)$$

with
$$\sigma_{ij} = g(c) \frac{\partial \psi_+^{\text{el}}}{\partial \varepsilon_{ij}} + \frac{\partial \psi_-^{\text{el}}}{\partial \varepsilon_{ij}}$$
 (4)

subject to the boundary conditions

$$\sigma_{ij}n_i = \bar{t}_j \quad \text{on } \partial\Omega_t \,, \tag{5}$$

$$u_i = \bar{u}_i \quad \text{on } \partial \Omega_u \,, \tag{6}$$

of the momentum equation (2), and subject to

$$c_{,i}n_i = 0 \quad \text{on } \partial\Omega \,, \tag{7}$$

of the phase-field equation (3), where $\partial \Omega = \partial \Omega_t \cup \partial \Omega_u$ is the boundary of the body and $\emptyset = \partial \Omega_t \cap \partial \Omega_u$.

Irreversibility of the crack evolution can be enforced in different ways. In the damage mechanics interpretation of Miehe and co-workers [12, 19] the phase-field variable is similar to a gradient damage model with a smooth transition between the intact and fully broken state. While this damage-like interpretation of the phase-field approach to brittle fracture is appealing – for a further discussion on similarities and differences the reader is referred to Reference [20] – it turns out that the interpretation of the phase-field variable as a history parameter may compromise the convergence of the functional that describes the diffuse crack to that which describes the discrete crack [21, 22, 23], and that fixing the phase-field variable when it is very close to the value that indicates complete local failure, e.g. [24], is to be preferred. For this reason the latter approach, also known as fracture-like constraint

$$c = \begin{cases} c & c > c_{\rm th} \\ 0 & c < c_{\rm th} \end{cases},\tag{8}$$

is used here, with the threshold $c_{\text{th}} = 0.01$. In other words, as soon as the phase-field reaches a value below the very small threshold c_{th} , a Dirichlet boundary condition c = 0 is applied at the corresponding node in the finite element framework.



Figure 2: Interface failure: (a) Domain (l = 10a = 20h = 10 mm) and boundary conditions for the preliminary DCB test and red region with reduced $\mathcal{G}_{c}^{\text{int.}}$ (b) Influence of the choice of the interface half-width b on the material strength, while keeping $l_{c} = \text{const} = 50 \,\mu\text{m}$.



Figure 3: On the right, the detail describes a fully developed crack within the interface in the DCB. The solid red lines mark the original interface of width 2b as shown on the left. The fracture toughnesses of the interface and the bulk material differ. Reducing the interface width (dashed red lines) has an influence on the dissipated energy since the fracture toughness is heterogeneous in the domain of the regularised interfacial crack.

The weak form is discretised using locally refined Truncated Hierarchical B-splines (THB-splines) [17]. This allows for efficient computations with a high resolution of the steep gradient in regions where the crack develops. In the framework of isogeometric analyses (IGA), the control points of the splines, which are used to interpolate the field quantities, adopt the role of the nodes which are present in classical finite element analyses. The resulting non-linear equations are solved using a staggered scheme [12]. Iterations are carried out within this staggered scheme to ensure convergence of both fields at each load level. Displacement control has been used in all examples.

3. Phase-field Modelling of Interface Failure: The one-dimensional problem

3.1. Preliminary study

First, a study has been carried out on a Double Cantilever Beam (DCB), depicted in Figure 2a. The geometry and elastic properties are given in [25]. Within the diffuse interface (red area) the fracture toughness is fifty times smaller than that in the surrounding bulk material: $\mathcal{G}_{c}^{bulk} = 50\mathcal{G}_{c}^{int}$, *i.e.* the fracture toughness varies abruptly. For an internal length scale $l_{c} = 50 \,\mu\text{m}$ the interface half width *b* has been varied ($b = \{62.5, 31.25, 15.625, 7.8125\} \,\mu\text{m}$). The resulting

force-displacement curves are given in Figure 2b. A narrower interface clearly leads to a material strengthening and a higher energy dissipation.

This observation can be explained using Figure 3. In Figure 3, on the right, the phase-field for a fully developed crack has been plotted. As long as the crack fully lies within the interface, denoted by the solid (red) lines, the dissipation is only influenced by the fracture toughness of the interface, \mathcal{G}_{c}^{int} . When, however, the ratio between the half-width *b* and the internal length scale l_c , b/l_c , becomes smaller, and intersects the phase-field of a crack in the bulk material, denoted by the dashed (red) lines, the dissipation is no longer determined by \mathcal{G}_{c}^{int} alone, but is also influenced by \mathcal{G}_{c}^{bulk} . As a consequence, the results become dependent on *b*, the half width of the interface.

A straightforward solution would be to increase b/l_c either by increasing the interface length scale b or by lowering the phase-field length scale l_c . The former may not always be practical due to certain restrictions and topological requirements of the interface, while the latter is restricted because the phase-field length scale can be considered as a material parameter of the bulk. Moreover, it would be computationally expensive to numerically resolve the gradients which result from a very small value for l_c .

Table 1: Specifications of the one-dimensional bar

l	1 mm
E	210 GPa
$l_{\rm c}$	7.5 μm
Α	1 mm^2
$\mathcal{G}_{ ext{c}}^{ ext{bulk}}$	$5 \mathrm{N} \mathrm{m}^{-1}$
$\mathcal{G}_{ ext{c}}^{ ext{int}}$	$2.7 \mathrm{N} \mathrm{m}^{-1}$



Figure 4: One-dimensional bar: Red lines mark bulk interface with \mathcal{G}_{c}^{int} or $\hat{\mathcal{G}}_{c}^{int}$. Outside the interface, \mathcal{G}_{c}^{bulk} is applied.

3.2. Global dissipation equivalence

To quantify the influence of the bulk material on the crack propagation along the interface, the dissipated energy during crack growth is analysed. For this purpose, a cut perpendicular to a fully developed crack, see Figure 3, is considered. As long as the crack phase-field does not interfere with different fracture toughnesses (solid red lines), the energy per unit area dissipated for a fully developed crack within the interface reads

$$D = \frac{\mathcal{G}_{\rm c}^{\rm int}}{4l_{\rm c}} \int_{-b}^{b} (1-c)^2 + 4l_{\rm c}^2 c_{,x}^2 \,\mathrm{d}x \,. \tag{9}$$

The integral over the bulk material does not contribute to *D* because the crack phase-field takes a constant value of $c \equiv 1$. In other words, the ratio b/l_c is sufficiently large: $b/l_c \rightarrow \infty$. Substituting the analytical description of the crack phase-field, $c = 1 - \exp(-|x|/(2l_c))$, into Equation (9) and simplifying yields:

$$D = \mathcal{G}_{\rm c}^{\rm int} \,. \tag{10}$$

Since the interface is not infinitely wide for realistic applications, the bulk influence has to be accounted for (red dashed lines) and Equation (9) is replaced by:

$$\hat{D} = \frac{1}{2l_c} \left[\hat{\mathcal{G}}_c^{\text{int}} \int_0^b (1-c)^2 + 4l_c^2 c_{,x}^2 \, \mathrm{d}x + \mathcal{G}_c^{\text{bulk}} \int_b^\infty (1-c)^2 + 4l_c^2 c_{,x}^2 \, \mathrm{d}x \right]$$
(11)

with $\hat{\mathcal{G}}_{c}^{int}$ the modified fracture toughness of the interface, which is adjusted to account for the bulk influence. Evidently, the second term in brackets needs not to be taken into account in Equation (9) since *b* is then sufficiently large, $b/l_c \rightarrow \infty$. Elaboration of Equation (11) yields:

$$\hat{D} = \hat{\mathcal{G}}_{c}^{int} \left(1 - e^{-b/l_{c}} \right) + \mathcal{G}_{c}^{bulk} e^{-b/l_{c}} .$$
(12)

We now require that $D = \hat{D}$. Rearranging Equations (10) and (12) gives the modified interface fracture toughness:

$$\hat{\mathcal{G}}_{c}^{int} = \frac{\mathcal{G}_{c}^{int} - \mathcal{G}_{c}^{bulk} e^{-b/l_{c}}}{1 - e^{-b/l_{c}}} \quad \text{with} \quad \frac{b}{l_{c}} > \ln \frac{\mathcal{G}_{c}^{bulk}}{\mathcal{G}_{c}^{int}}$$
(13)

where the latter constraint ensures that $\hat{\mathcal{G}}_{c}^{int}$ does not take unphysical values, i.e. becomes smaller than zero. This approach would also work for an inverse correction, i.e. when $\mathcal{G}_{c}^{bulk} < \mathcal{G}_{c}^{int}$. Herein we have limited ourselves, however, to cases where $\mathcal{G}_{c}^{bulk} > \mathcal{G}_{c}^{int}$.

3.3. One-dimensional bar

One-dimensional numerical studies have been carried out to demonstrate the effect of the correction on the forcedisplacement curves. The test case is a one-dimensional bar $x \in [0, 1]$ mm with a reduced cross-sectional area in the centre to nucleate a crack, see Figure 4, while the material properties are given in Table 1. The reduced cross section has been accounted for by introducing a variable cross-sectional area in the derivation. The simulations have been carried out with a one-dimensional phase-field code which uses hierarchical B-spline basis functions. Quadratic shape functions have been used with reduced C^0 continuity at the centre of the bar. The spatial discretisation can be considered as sufficiently fine [23]. Now, the dissipated energy Ψ^c is compared to a reference value $\Psi^{c,ref}$ obtained from a 1-dimensional bar with \mathcal{G}_c^{int} . It is expected, that the dissipated energy is highly overestimated without the compensation, which is indeed the case: A comparison between the cases with and without the correction is shown in Table 2 with respect to the dissipated energy Ψ^c for the fully cracked bar. The correction clearly has the intended effect and brings down the deviation of more than 10% for the smallest ratio presented.

4. Phase-field Modelling of Interface Failure: Extension to two dimensions

4.1. Two-dimensional double cantilever beam

The testing geometry in two dimensions is a modified Double Cantilever Beam (DCB) with an initial notch, see Figure 5a. It differs from a classical DCB in the sense that the specimen is deformed using a so-called 'surfing boundary condition' [14, 13], which projects the near-field displacements $u(r, \varphi)$ of a mode-I crack obtained in linear elastic fracture mechanics to the IGA control points of the boundary edges. In this sense, an imaginary crack tip propagates along the *x*-axis and tears apart the upper and lower halves of the DCB. Figures 5c and 5d give the undeformed and the deformed meshes, respectively. In the two-dimensional simulations, there is not only crack initiation, but also crack propagation, and therefore the energy release rate is evaluated as well, and is compared with the fracture toughness. As will be demonstrated below, the surfing boundary condition yields steady crack growth and enables the accurate determination of the energy release rate. The diffuse interface, i.e. the grey shaded area in Figure 5a, is aligned with the *x*-axis and is incorporated by assigning different values \mathcal{G}_{c}^{bulk} and \mathcal{G}_{c}^{int} for the fracture toughness outside and inside the interface, *i.e.* the fracture toughness varies abruptly. The mesh is refined along the expected crack path. The initial crack is incorporated by setting the phase-field c = 0 (blue) along the straight notch, see Figure 5b. The averaged y-displacement \bar{u} of the nodes along the upper edge serves as abscissa for the following plots. The following values have been used for the material parameters: YouNG's modulus E = 210 GPa, Porsson's ratio $\nu = 0.3$ and $l_c = 15 \,\mu\text{m}$. Plane strain conditions are assumed. The values for the fracture toughness are set to $\mathcal{G}_{c}^{bulk} = 5.4 \,\text{N mm}^{-1}$ and \mathcal{G}_{c}^{int} has been calculated according to Equation (13).

Table 2: Dissipated energy for one-dimensional bar: For the setup where the original interface fracture toughness is used, the dissipated energy depends on the ratio b/l_c for small values. Using the compensated, artificially lowered interface fracture toughness the dissipated energy is almost equal for each case. The homogeneous case where $b/l_c \rightarrow \infty$ serves as reference $\Psi^{c,ref}$.

	$b/l_{\rm c}$	$\rightarrow \infty$	8.33	4.17	2.08
$\Psi^{c}/\Psi^{c,ref}-1$ using	$\mathcal{G}_{ ext{c}}^{ ext{int}}$	0	0	0.013	0.109
	$\hat{\mathcal{G}}_{ ext{c}}^{ ext{int}}$	0	0	-0.01	-0.011



(c) Undeformed geometry

(d) Deformed geometry

Figure 5: Geometry and boundary conditions: (a) The geometry with h = 2a = 1 mm is described. During the simulation, an imaginary crack tip (green circle) propagates along the *x*-axis and the near field K-concept displacements $u(r, \varphi)$ of a mode-I crack are assigned to all nodes on the purple edges. The grey stripe resembles the diffuse interface. (b) The predefined notch is initialised by setting the phase-field c = 0 (blue) along the red dashed line. The diffuse interface of width 2b is varied. In (c) and (d) the undeformed and deformed geometries are depicted. The displacements in (d) are exaggerated.

The energy release rate \mathcal{G} has been calculated using the concept of configurational forces [14], which is comparable to a generalised *J*-integral [26]. It is important to note that the predefined fracture toughness \mathcal{G}_c is not recovered numerically. Indeed, the discretisation and the choice of the length scale alter the predefined value [5] and the numerical fracture toughness

$$\mathcal{G}_{c,num} = \mathcal{G}_{c} \cdot \left(1 + \frac{\Delta h}{4l_{c}}\right) \tag{14}$$

governs the simulation. Herein, $\Delta h = 6.25 \,\mu\text{m}$ is the characteristic mesh spacing.

Figure 6 shows the increase of the dissipated energy from the point where the crack tip passes $x = x_c = 0.55$ mm. The value has been chosen slightly higher than the initial crack length to rule out differences due to the crack initialisation. The actual crack energy increase is compared with the theoretical value, i.e. the fracture toughness multiplied by the finite crack growth Δx_c . It is noted that the crack is an actual surface with h = 1 mm in the out-of-plane direction. As expected, the reference with $b/l_c \rightarrow \infty$ coincides with the theoretical increase represented by the (red) dashed line. For smaller ratios b/l_c similar to the case of the one-dimensional bar, the dissipated energy is overestimated due to the bulk material influence, which is evidenced from the increasing inclination of the curves in Figure 6a. For ratios up to $b/l_c \approx 2$, the correction suggested in the preceding section works fairly well, see Figure 6b. But for small ratios of b/l_c an increasing discrepancy occurs. One reason can be the discretisation of the phase-field which is considerably coarser compared to the one-dimensional case. Apart from this, the global compensation approach also yields a significant deviation for the critical energy release rate as will be pointed out in the following.

In the reference case, i.e. $b/l_c \rightarrow \infty$, the entire domain is assigned the interface fracture toughness $\mathcal{G}_c^{int} = 2.7 \text{ N mm}^{-1}$ and the bulk fracture toughness does not play a role. In contrast to a one-dimensional setting, the crack propagates for a two-dimensional situation, i.e. the *x*-position of the crack tip x_c changes when \mathcal{G} has reached a critical value, see Figure 7a. Again we observe an interaction between the values of the fracture toughness for the bulk



Figure 6: Crack energy: (a) Before the correction, the crack energy increases faster for smaller interface widths. (b) Applying the correction balances the crack energy increase to the same level. For small interface widths (red/blue curve) deviations occur. A closer look reveals that these curves are not linear, which implies that the crack length is overestimated.

material and for the regularised interface. For further illustration, the ratio b/l_c has been reduced gradually starting from the reference case. The resulting energy release rates are compared in Figure 7b. It is clear that \mathcal{G}_c attains higher values for smaller ratios b/l_c , which is consistent with the results reviewed in Sections 3.1 and 3.3.

Directly applying the compensation approach of Sec. 3.2 yields a significant underestimation of the energy release rate for crack propagation as is evident from Figure 7c. This is a drawback of the compensation method as it has been formulated for the one-dimensional case. Indeed, for $b/l_c \rightarrow 0$ the method can no longer be applied since the subsidiary condition formulated in Equation (13) is no longer fulfilled. A closer look at the compensation process illustrates the problem. The requirement of a global dissipation equivalence takes into account also areas where the crack has already propagated and is zero for intact parts of the body. However, the actual crack growth is governed by physical quantities in a region of the order l_c in front of the crack tip.

All in all, the global dissipation equivalence approach does not account for crack propagation, as it is the case for two-dimensional simulations, and is only valid for a one-dimensional setup where a crack emerges. However, it is essential to consider the energy release rate in order to predict crack growth. This raises the need for another compensation method.

4.2. Analytical implications using the concept of configurational forces

Kuhn and Müller [14] have derived a quantitative crack growth criterion, which accounts for heterogeneities in the vicinity of the crack tip. They showed that the *x*-component of the configurational force which contains the phase-field contributions \mathcal{G}^{fr} is equal to the fracture toughness when the crack starts propagating. It is noted, that the other contributions to the configurational force listed in [14] are zero for crack propagation within this contribution. The configurational force can be written as an integral over a finite area *A* around the crack tip of the divergence of the ESHELBY tensor:

$$\mathcal{G}_{j}^{\mathrm{fr}} = -\int_{A} \Sigma_{ij,i}^{\mathrm{fr}} \,\mathrm{d}A \,\,, \tag{15}$$

where

$$\Sigma_{ij}^{\rm fr} = \psi^{\rm c} \delta_{ij} - 2\mathcal{G}_{\rm c} l_{\rm c} c_{,i} c_{,j} \,. \tag{16}$$



Figure 7: \mathcal{G} and crack length: (a) The energy release rate \mathcal{G} and the crack tip position x_c are plotted as a function of the average displacement \bar{u} . As soon as \mathcal{G} reaches the numerical fracture toughness $\mathcal{G}_{c,num}^{int}$ the crack starts to propagate. The bumps in the \mathcal{G} curves are artefacts due to the phase-field initialisation. (b) The fracture toughness governing crack growth is between the bulk and the interface fracture toughness and increases for smaller ratios b/l_c because the bulk influence becomes more significant. It is noted, that the 3-dimensional plot layout has only been chosen for visualisation purposes because certain curves would not be differentiable in a 2-dimensional plot. (c) The global dissipation equivalence approach results in a large underestimation of the energy release rate of the crack propagating along the interface.

Making use of the analytical one-dimensional solution of the phase-field c, the integral over A can be split into two contributions $A = A_{crack} + A_{tip}$ and evaluated afterwards. For a crack propagating straight along the *x*-axis, the first contribution A_{crack} stems from the fully developed straight crack to the left of the crack tip. Here, the phase-field is homogeneous in the *x*-direction and follows the one-dimensional solution in the *y*-direction. Evaluating the *x*-component of the integral for A_{crack} in Equation (15) yields $\mathcal{G}_1^{fr} \equiv 0$, i.e. crack growth is not influenced by the tip history. Consequently, only the phase-field around the crack tip within A_{tip} contributes to \mathcal{G}_1^{fr} . The analytical evaluation of this contribution is challenging since the circumferential phase-field solution at the crack tip, which is attached to the straight crack path, is not known a priori. This also applies to the analytical solution of the two-dimensional HELMHOLTZ differential equation for this setup. For these reasons, a numerical approach is chosen below to quantify the influence of the fracture toughness of the interface and the bulk material, thus avoiding an analytical evaluation of Equation (15).

4.3. Numerical study for a local compensation approach

Figure 8a postulates a general relation between the ratios b/l_c , $\mathcal{G}_c^{\text{bulk}}/\mathcal{G}_c^{\text{int}}$ and the fracture toughness, which is numerically measured during the simulations. This fracture toughness is referred to as actual fracture toughness $\mathcal{G}_c^{\text{act}}$. The above observations suggest, that the ratio

$$\frac{\mathcal{G}_{c}^{act}}{\mathcal{G}_{c}^{int}} = g\left(\frac{\mathcal{G}_{c}^{bulk}}{\mathcal{G}_{c}^{int}}, \frac{b}{l_{c}}\right)$$
(17)

is a priori unknown. The function g will be referred to as the *exaggeration* function, *i.e.* the interface fracture toughness is exaggerated because of the bulk material influence and, for the most general case, one ends up with an actual fracture toughness not equal to the interface fracture toughness.

Now, two limiting cases will be discussed. For $b/l_c \rightarrow \infty$ the actual, numerically measured fracture toughness $\mathcal{G}_{c,num}^{act}$ equals the numerical interface fracture toughness $\mathcal{G}_{c,num}^{int}$:

$$\frac{\mathcal{G}_{c,num}^{act}}{\mathcal{G}_{c,num}^{int}} = \frac{\mathcal{G}_{c}^{act}}{\mathcal{G}_{c}^{int}} = 1.$$
(18)

This case is similar to the example in Figure 7a. Please note that the discretisation effect in Equation (14) cancels when considering relative values of the exaggeration function and is only relevant when interpreting absolute numerical values. For $b/l_c \rightarrow 0$ the actual, numerically measured value of the fracture toughness \mathcal{G}_c^{act} equals the fracture toughness of the bulk material \mathcal{G}_c^{bulk} :

$$\frac{\mathcal{G}_{c}^{act}}{\mathcal{G}_{c}^{int}} = \frac{\mathcal{G}_{c}^{bulk}}{\mathcal{G}_{c}^{int}} \,. \tag{19}$$

The range of the ratios $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ has been chosen such that it can be compared with analytical results from linear elastic fracture mechanics [9], cf. Figure 14a.

Figure 8b presents the semi-logarithmic plots for a large variety of different material parameters. Despite significant differences in the length scales of the regularisations and the corresponding values of the fracture toughnesses, a pattern can be observed for the non-dimensional results. All the results with the same ratio $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ form a group independent from the ratio b/l_c . This is emphasised by the three fits. The exaggeration function only depends on ratios of the values of the fracture toughnesses and the regularisation length scales, but not on the absolute values. The arrow in Figure 8b points at a representative example: The blue filled square, orange diamond and red non-filled square stand for simulations with different absolute values of the fracture toughnesses and the regularisation. This points at a general relationship for the exaggeration function g. Motivated by the exponential shape of the phase-field perpendicular to the crack path and the one-dimensional findings, the exaggeration function is chosen to be of an exponential type:

$$\frac{\mathcal{G}_{c}^{\text{act}}}{\mathcal{G}_{c}^{\text{int}}} = g\left(\frac{\mathcal{G}_{c}^{\text{bulk}}}{\mathcal{G}_{c}^{\text{int}}}, \frac{b}{l_{c}}\right) = Q \exp\left(-r \cdot \frac{b}{l_{c}}\right) + 1 , \qquad (20)$$

where the constants Q and r may depend on the ratios b/l_c and $\mathcal{G}_c^{\text{bulk}}/\mathcal{G}_c^{\text{int}}$.



Figure 8: Schematic illustration and numerical examples: (a) The sensitivity of the actual fracture toughness \mathcal{G}_{c}^{act} , which the material experiences, to the ratio b/l_c is shown. The exaggeration function g which describes the relationship is unknown, but an exponential relation is likely, since the phase-field follows such a description. (b) Simulation data reinforcing the use of g are presented. Over a wide range b/l_c the data behave linearly, independent from the absolute values of b and l_c . Importantly, the exponential fits show that the curve grouping only depends on the ratio $\mathcal{G}_{c}^{bill}/\mathcal{G}_{c}^{int}$.

4.4. Compensation procedure

To obtain crack propagation at the physical value \mathcal{G}_{c}^{int} , the interface fracture toughness is lowered to a new input value $\hat{\mathcal{G}}_{c}^{int}$. This new value has to satisfy

$$\hat{\mathcal{G}}_{c}^{int} \cdot g\left(\frac{\mathcal{G}_{c}^{bulk}}{\hat{\mathcal{G}}_{c}^{int}}, \frac{b}{l_{c}}\right) = \mathcal{G}_{c}^{act} = \mathcal{G}_{c}^{int}$$
(21)

in order to properly compensate for the influence of the fracture toughness of the bulk material. Rerarranging Equation (21) yields

$$\frac{\hat{\mathcal{G}}_{c}^{\text{int}}}{\mathcal{G}_{c}^{\text{int}}} = \left[g\left(\frac{\mathcal{G}_{c}^{\text{bulk}}}{\hat{\mathcal{G}}_{c}^{\text{int}}}, \frac{b}{l_{c}}\right)\right]^{-1} , \qquad (22)$$

where the right hand-side can be identified as the compensation factor. It is noted that Equation (22) cannot be solved directly because the exaggeration itself depends on $\hat{\mathcal{G}}_{c}^{int}$. This can be overcome by an interpolation between the results given in Figure 8b.

Figure 9a presents sets of curves for $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}} \equiv \text{const.}$ For a given ratio b/l_{c} the factor for lowering the interface fracture toughness is given by the ordinate. The curves are as expected: for large ratios of b/l_{c} there is no need for compensation, whereas larger ratios $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ call for smaller compensation factors when $b/l_{c} \rightarrow 0$. Another interesting aspect is the fact, that the curves in Figure 9b seem to converge towards a limiting case. The existence of a



Figure 9: Compensation of bulk influence: (a) Each curve is valid for a constant ratio $\mathcal{G}_{c}^{bulk}/\mathcal{G}_{c}^{int}$. For finite ratios b/l_c the bulk influence has to be compensated by artificially lowering the original interface fracture toughness \mathcal{G}_{c}^{int} by a certain factor depending on b/l_c . The factor can be determined from the ordinate. As mentioned, the bulk influence vanishes for large ratios b/l_c which can be seen from the curves converging to $\hat{\mathcal{G}}_{c}^{int}/\mathcal{G}_{c}^{int} = 1$. (b) For two examples with a ratio $\mathcal{G}_{c}^{bulk}/\mathcal{G}_{c}^{int} \equiv 2$ the compensation factor is determined. The thin dashed black lines indicate more curves belonging to the same family.



Legend for (a): $\Box b/l_c \equiv 0.625$ | $\Box b/l_c \equiv 1.25$ | $\diamondsuit b/l_c \equiv 1.875$ | $\bigtriangleup b/l_c \equiv 2.5$ | $\blacksquare b/l_c \equiv 3.125$

Figure 10: Influence of large ratios $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$: (a) For five ratios b/l_c , larger ratios $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ have been investigated. Both, the ratios from the regularisation length scales and from the fracture toughnesses, have a nonlinear influence on the exaggeration $g = \mathcal{G}_{c}^{\text{act}}/\mathcal{G}_{c}^{\text{int}}$. The black dashed line is the limit exaggeration which is reached for $b/l_c = 0$, *i.e.* the interface completely vanishes and $\mathcal{G}_{c}^{\text{act}} = \mathcal{G}_{c}^{\text{bulk}}$. (b) The results presented in (a) are plotted over b/l_c analogue to Fig. 8b. Despite the large ratios, the curves are still only vertically shifted, which verifies the assumption for the exponential fits in Fig. 8b. It can be seen, that the nonlinearity leads to a vanishing vertical shift of different curves for larger ratios. From the bottom to the top, the ratio $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ increases from 1.5 to 20 and takes values according to the abscissa in (a).



Figure 11: \mathcal{G} for two ratios b/l_c with and without compensation are compared to the reference calculation with $b/l_c \to \infty$. (a) The actual numerical energy release rate \mathcal{G}_{num}^{act} for crack propagation increases for smaller ratios b/l_c .(b) The crack propagates at equal \mathcal{G} for each compensated case. As expected, \mathcal{G} recovers the value of the numerical interface fracture toughness $\mathcal{G}_{c,num}^{int}$, *i.e.* $\mathcal{G}_{num}^{act} = \mathcal{G}_{c,num}^{int}$.

limiting compensation factor is reasonable, because the compensated fracture toughness would otherwise hit negative values eventually.

4.5. Larger ratios of $\mathcal{G}_{c}^{bulk}/\mathcal{G}_{c}^{int}$ and limitations of the approach

For five different ratios $b/l_c = \{0.625, 1.25, 1.875, 2.5, 3.125\}$, larger ratios of $\mathcal{G}_c^{\text{bulk}}/\mathcal{G}_c^{\text{int}} = \{1.5...20\}$ have been investigated. The corresponding exaggeration for every set of parameters is given in Fig. 10. Firstly, as already observed above, a variation of the fracture toughness ratio yields a nonlinear response of the exaggeration, which gets clearer when looking at large ratios $\mathcal{G}_c^{\text{bulk}}/\mathcal{G}_c^{\text{int}}$. The nonlinearity is reflected in Fig. 10b, where the curve families for larger ratios $\mathcal{G}_c^{\text{bulk}}/\mathcal{G}_c^{\text{int}}$ move more and more together. The exponential fits analogue to Fig. 8b are excluded for the sake of readability. Secondly, large ratios b/l_c reduce the exaggeration which can be seen from Fig. 10a. This is in line with Fig. 8b.

The computation of such large fracture toughness ratios showed a limitation of the approach: Due to the dramatic decrease of the fracture toughness within the interface, convergence was hard to reach, which made a local mesh refinement and smaller load increments necessary. This could have been avoided – at least partially – when using a smooth transition from the bulk to the interface material, which raises the need for alternative interface regularisations. The following selection of numerical examples demonstrates the general functionality of the interface model.

5. Numerical Examples

5.1. Crack propagation along interface aligned with mesh

As a first example, the compensation procedure is applied to two cases used in the parameter study. For the values $\mathcal{G}_{c}^{int} = 2.7 \,\mathrm{N}\,\mathrm{mm}^{-1}$ and $\mathcal{G}_{c}^{bulk} = 5.4 \,\mathrm{N}\,\mathrm{mm}^{-1}$, and the ratios $b/l_{c} = \{1.25, 2.08\}$ with $l_{c} = 15 \,\mu\mathrm{m}$, the results of the compensation are shown in Figure 9b by means of red and purple arrows. Since $\mathcal{G}_{c}^{bulk}/\mathcal{G}_{c}^{int} = 2$, the intersections of two vertical lines (red and purple arrows) at $b/l_{c} = \{1.25, 2.08\}$ with the orange curve are needed. From these intersections, two horizontal lines give the ordinate and thus, the compensation factors $\hat{\mathcal{G}}_{c}^{int}/\mathcal{G}_{c}^{int} \approx \{0.911, 0.958\}$ for the given cases. Instead of the original value for the interface fracture toughness \mathcal{G}_{c}^{int} , the corrected interface fracture toughness \mathcal{G}_{c}^{int} is applied together with the bulk fracture toughness \mathcal{G}_{c}^{bulk} .

Figure 11 presents the energy release rates before and after correction. Both cases are compared with the reference case. The compensation has the correct effect and eliminates the bulk influence.



(a) Geometry and boundary conditions

(b) Initial notch and prerefined mesh for $\varphi_{\text{mesh}} = 15^{\circ}$

Figure 12: Geometry and boundary conditions: (a) The geometry with h = 2a = 1 mm is described. As for the parameter study, surfing boundary conditions $u(r, \varphi)$ of a mode-I crack are assigned to all nodes on the purple edges. The grey stripe resembles the diffuse interface. (b) The predefined notch is initialised by setting the phase-field c = 0 (blue) along the red dashed line. The interface half width is set to $b = 25 \,\mu\text{m}$, the length scale to $l_c = 15 \,\mu\text{m}$.



Figure 13: Exaggeration for arbitrary mesh orientation: The black arrow points at the exaggeration data (black circle/cross) which has been extracted from the simulations with $\varphi_{mesh} = \{15, 20\}^\circ$. The mesh seems to be sufficiently fine in the vicinity of the abrupt change in the fracture toughness since the points perfectly match the data from the parameter study. For details on colouring, the reader is referred to Figure 8b.

5.2. Crack propagation along interface not aligned with mesh

In the simulations that have been presented up to this point, the interfaces were aligned with the given mesh and the interface half width b was chosen such that it was a multiple of the element edge Δh . Of course, the orientation of the interface within the mesh can be arbitrary. Therefore, the second example features an interface which is inclined with the mesh lines. The geometry and the mesh are depicted in Figure 12. Again, surfing boundary conditions have been applied to all edges. Two orientation angles $\varphi_{mesh} = \{15, 20\}^\circ$ have been investigated. The Young's modulus E = 210 GPa and the Poisson's ratio v = 0.3 are the same as in the previous simulations. Plane strain conditions have



$$\hat{G}_{c}^{int} = 2.459 \,\mathrm{N \, mm^{-1}} \& b/l_{c} = 1.25 \,| \diamond \hat{G}_{c}^{int} = 2.586 \,\mathrm{N \, mm^{-1}} \& b/l_{c} = 2.08$$

Figure 14: Relation between deflection and penetration for an inclined interface: (a) Analytic relationship according to linear elastic fracture mechanics. The black curve is given in Equation (23) and describes the limiting case between penetration and deflection for the given parameters. It is noted that the interface fracture toughness \mathcal{G}_{c}^{int} is achieved by assigning the compensated interface fracture toughness $\hat{\mathcal{G}}_{c}^{int}$ in the simulations. (b) For different inclination angles the measure *s* prescribes how long the crack follows the interface before penetrating into the opposite bulk material. Contour plots for the simulations represented by the orange diamond can be found in Figures 15b – e.

been adopted.

For both cases, a reference calculation with a homogeneous fracture toughness $\mathcal{G}_{c}^{int} = 2.7 \,\mathrm{N \, mm^{-1}}$ has been carried out. In Figure 13, the exaggeration functions from Figure 8b are recapped and the results for different angles φ_{mesh} are added (marked by a black arrow). Even though the numerical integration near the (abrupt) change in the fracture toughness may be slightly inaccurate due to the distorted mesh, the ratios perfectly match the results where the numerical integration errors have been eliminated. Thus, the model allows for arbitrary mesh orientations as long as the discretisation near the interface with a crack is sufficiently fine.

5.3. Crack impinging on an interface

In linear elastic fracture mechanics, a crack impinging on an interface which is inclined compared to the crack path, has been considered analytically in [9]. Depending on the fracture toughness ratio $\mathcal{G}_{c}^{\text{bulk}}/\mathcal{G}_{c}^{\text{int}}$ and the interface inclination angle φ_{int} , a crack impinging on an interface is either deflected, or penetrates into the bulk material [8, 9]:

$$\frac{\mathcal{G}^{\text{int}}}{\mathcal{G}^{\text{bulk}}} = \frac{1}{16} \left\{ \left[3\cos\left(\frac{\varphi_{\text{int}}}{2}\right) + \cos\left(3\frac{\varphi_{\text{int}}}{2}\right) \right]^2 + \left[\sin\left(\frac{\varphi_{\text{int}}}{2}\right) + \sin\left(3\frac{\varphi_{\text{int}}}{2}\right) \right]^2 \right\}.$$
(23)

For a ratio

$$\frac{\mathcal{G}_{c}^{\text{int}}}{\mathcal{G}_{c}^{\text{bulk}}} < \frac{\mathcal{G}^{\text{int}}}{\mathcal{G}_{c}^{\text{bulk}}}, \qquad (24)$$

the crack is deflected [9]. Otherwise, it penetrates into the bulk. The limiting curve between deflection and penetration is plotted in Figure 14a. It is noted that the inverse of Equation (23) is shown in line with the other ratios presented herein. The limiting curve has to be understood as a tendency of what will happen, rather than a prediction.

For the two cases in Section 5.1 simulations for different inclination angles have been carried out to demonstrate the capability of the model. The different configurations are included in Figure 14a. The geometry is similar to Figure 5a except for the domain size in the *y*-direction, which is enlarged by a factor of 1.8 in a symmetric manner. The



Figure 15: Geometry and results for different inclination angles: (a) The initial phase-field and the inclination of the interface are depicted. The material parameters are chosen similar to the previous examples. A surfing boundary condition is applied similar to Figure 5a. (b) – (e) The resulting phase-fields for different inclination angles φ_{int} (black lines) and $b/l_c = 2.08$ are plotted. It can be seen that there is absolutely no deflection for $\varphi_{int} = 70^{\circ}$. Starting from $\varphi_{int} = 60^{\circ}$ deflection occurs. This is consistent with Figure 14a where the transition from deflection to penetration happens between these inclination angles.

orientation of the inclined interface is shown in Figure 15a. Surfing boundary conditions are applied as well as plane strain conditions. It is noted that the compensated interface fracture toughness, $\hat{\mathcal{G}}_{c}^{int}$, is used to satisfy Equation (21), as also discussed in Section 5.1. Adaptive local refinement has been used in all the simulations.

Figure 14b shows how long the crack follows the interface before it penetrates into the bulk material. For $\varphi_{int} = 30^{\circ}$ no penetration occurred. For larger inclination angles, the crack started to penetrate the bulk after being deflected. As expected, no deflection occurred for $\varphi_{int} = 70^{\circ}$, which is consistent with the analytical result. There is no significant difference in the results for the two values for b/l_c . The contour plots in Figure 15 can be compared to those obtained for a brittle interface in [8], Figure 9. The crack lengths following the interface match well qualitatively. Differences occur for the cracking behaviour after penetrating into the bulk material. Different from here, a cohesive-zone model is introduced in [8] which influences the direction of the crack after penetrating into the bulk material. The crack does not propagate horizontally as in Figures 15b – e. From Figures 15b – e, which show the resulting phase-field for $b/l_c = 2.08$, it also becomes clear that adaptive refinement is most useful for this kind of phase-field simulations. Without adaptive refinement, the complete region below the interface and above the *x*-axis would have had to be refined a priori.

6. Conclusions and Outlook

In this work, a phase-field model has been introduced for interface failure. The standard phase-field model can describe bulk failure, but is not able to describe adhesive interfacial failure without a modification. Herein, the interface was distributed over a finite length and assigned an interface fracture toughness \mathcal{G}_{c}^{int} .

An interaction between the width of the interface and the characteristic length scale of the phase-field model for the bulk can occur for certain ratios of the smearing widths of interface and the bulk fracture zones. For one-dimensional simulations, an analytical expression was derived to compensate for this effect. For two dimensions, a numerical correction approach was developed motivated by a theoretical reasoning and several simulations which suggest that a compensation, herein named exaggeration function, can be described by an exponential decay. Numerical simulations underpinned this assumption. Moreover, it was shown that the exaggeration function is independent of absolute values of the fracture toughnesses of the interface or the bulk, as it only depends on ratios which makes the relation universal.

Numerical examples demonstrate the basic functionality of the compensation approach and the applicability to arbitrary mesh orientations, which is a main feature and advantage over models which exploit interface elements. Finally, a crack impinging on an interface was simulated. The results compare well with analytical relations from linear elastic fracture mechanics.

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