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Modelling of interfacial crack propagation in strongly heterogeneous materials by using phase field method

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Abstract.

Phase field model has been proved to be a useful tool to study the fracture behaviors in heterogeneous materials. This method is able to model complex, multiple crack fronts, and branching in both 2D/3D without ad-hoc numerical treatments. In this study, a new interfacial cracking model in the phase field framework is proposed. The effects of both stiff and soft interphases on the fracture response of composite materials are considered. A dimensional-reduced model based on a rigorous asymptotic analysis is adapted to derive the null thickness imperfect interface models from an original configuration containing thin interphase. The idea of mixing the bulk and interfacial energy within the phase field framework is then used to describe the material degradation both on the interface and in bulk. Moreover, in order to ensure the physical crack propagation patterns, a unilateral contact condition is also proposed for the case of spring imperfect interface. The complex cracking phenomena on interfaces such as initiation, delamination, coalescence, deflection, as well as the competition between the interface and bulk cracking are successfully predicted by the present method. Concerning the numerical aspect, the one-pass staggered algorithm is adapted, providing an extremely robust approach to study interfacial cracking phenomena in a broad class of heterogeneous materials.

Introduction

Study of interface failure has been the topic of an intense research in the last decades. Cohesive element [11] is a powerful method to model crack propagation along interface (situation where the crack path is known). Other techniques like XFEM [4] have been also used to study interfacial cracking in bi-materials [9], where the displacement jump can be accurately reproduced through the enrichment of the displacement field with discontinuous functions. The XFEM technique has been used along with the cohesive model to simulate delamination in composite materials [10]. However, XFEM methods can hardly handle triple junctions or complex interphases, such as those in polycristals. More recently, the interfacial cracking has been studied by using the phase field model [5].

This work is dedicated to developing a phase field framework for dealing with damage of a larger class of imperfect interfaces, i.e. exhibiting either displacement jump or traction jump across an interface. In order to avoid meshing the interphase, we employ an imperfect interface model of zero thickness (with appropriate jump conditions), which is derived from a dimensional-reduced model based on a rigorous asymptotic analysis. The jump conditions depend on the ratio of the stiffness of the interphase to those of the connected materials and lead to two well-known models in the literature: *coherent imperfect interface* for very stiff interphase, and *linear spring-layer imperfect interface* for very soft interphase [12, 13]. The framework proposed in [5] is extended by including these models within the phase field framework, so as to allow interaction between the damage in the thin interphase and the bulk cracks in an efficient and robust manner.

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1 Theoretical framework

The idea of mixing the bulk and interfacial energy within the phase field framework is used to describe the material degradation both on the interface and in bulk [5]. It implies the total energy in a standard framework of sharp discontinuity description as follows

$$E = \int_{\Omega/\Gamma_d,\Gamma_I} \psi^e \mathrm{d}\Omega + \int_{\Gamma_d} \psi^d \mathrm{d}\Gamma + \int_{\Gamma_{I,\alpha}} \psi^{ci} \mathrm{d}\Gamma + \int_{\Gamma_{I,\beta}} \psi^{si} \mathrm{d}\Gamma, \tag{1}$$

where ψ^e is the elastic energy density; ψ^d is the surface (fracture) energy density; ψ^{ci} and ψ^{si} are the densities of interfacial energy of stiff interface, and compliant interface, respectively.

We adapt here the regularized description to both crack and interface. Herein, the sharp crack is described by the smeared crack density function $\gamma_d(d, \nabla d)$, and the sharp interfaces are replaced by the smeared interfaces, i.e., $\gamma_\alpha(\alpha, \nabla\alpha)$ for stiff interphase and $\gamma_\beta(\beta, \nabla\beta)$ for compliant interphase, respectively. Furthermore, we substitute the displacement jump $[\![\mathbf{u}]\!]$ by a smeared displacement jump $\mathbf{v}(\mathbf{x})$ (see e.g. [5, 7] for more details). Then, the infinitesimal strain tensor $\boldsymbol{\varepsilon}$ in this framework can be decomposed into a part related to the bulk $\boldsymbol{\varepsilon}^e$ and a part induced by the smoothed jump at the interfaces $\tilde{\boldsymbol{\varepsilon}}$, implying $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \tilde{\boldsymbol{\varepsilon}}$. The aforementioned energy functional can be now rewritten as

$$E = \int_\Omega \psi^e \left(\boldsymbol{\varepsilon}^e, d\right) h_{\alpha,\beta}\ \mathrm{d}\Omega + \int_\Omega g_c \gamma_d(d, \nabla d)\ \mathrm{d}\Omega\ + \int_\Omega \psi^{ci}(\boldsymbol{\varepsilon}^s, d)\gamma_\alpha(\alpha, \nabla\alpha)\ \mathrm{d}\Omega + \int_\Omega \psi^{si}(\mathbf{v}, d)\gamma_\beta(\beta, \nabla\beta)\ \mathrm{d}\Omega, \tag{2}$$

in which, $h_{\alpha,\beta} = (1-\alpha)(1-\beta)$ is introduced to distinguish the elastic energy of bulk phases from the one of the interfaces; g_c here denotes the fracture resistance; the tangential strain $\boldsymbol{\varepsilon}^s$ is expressed by[†]

$$\boldsymbol{\varepsilon}^s = \mathbf{T}\boldsymbol{\varepsilon}^e\mathbf{T} = \mathbf{M}_t\boldsymbol{\varepsilon}^e, \quad \text{with} \quad \mathbf{M}_t = \mathbf{T}\underline{\overline{\otimes}}\mathbf{T}, \ \text{ and } \ \mathbf{T}(\mathbf{x}) = \mathbf{I} - \mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}), \tag{3}$$

where $n(\mathbf{x})$ is the unit normal vector field on the interface Γ_I, and $\mathbf{I}$ is the second order unit tensor.

The failure model for both bulk and interfacial crackings is constructed through the unilateral contact condition to maintain the physical crack propagation.

Bulk cracking

The model proposed by Miehe et al [3] with the assumption that damage induced by traction only is here used for the bulk cracking

$$\psi^e\left(\boldsymbol{\varepsilon}^e, d\right) = g(d)\ \psi^{e+}\left(\boldsymbol{\varepsilon}^e\right) + \psi^{e-}\left(\boldsymbol{\varepsilon}^e\right), \ \text{ with } \ \psi^{e\pm}(\boldsymbol{\varepsilon}^e) = \frac{\lambda}{2}\left[\,\langle \mathrm{tr}\,\boldsymbol{\varepsilon}^e\rangle_\pm\,\right]^2 + \mu\,\mathrm{tr}\left[\,\left(\boldsymbol{\varepsilon}^{e\pm}\right)^2\,\right], \tag{4}$$

where $g(d) = (1-d)^2 + \epsilon$ (with $\epsilon \ll 1$) is the degradation function, see [1, 3]); ε^{e+} and ε^{e-} are, respectively the extensive and compressive modes of the elastic strain tensor.

Interfacial cracking: coherent imperfect interface model

The interfacial cracking of the very stiff interface is assumed to be created by the whole tangential strains, implying

$$\psi^{ci} = g(d)\psi^{ci}_e = \frac{1}{2}\boldsymbol{\varepsilon}^s : \mathbb{C}^{ci}_s(d) : \boldsymbol{\varepsilon}^s, \quad \text{and} \quad \mathbb{C}^{ci}_s(d) = g(d)\left[\lambda^{ci}_s \mathbf{T}\otimes\mathbf{T} + 2\mu^{ci}_s \mathbf{T}\underline{\overline{\otimes}}\mathbf{T}\right]. \tag{5}$$

The Lamé's constants characterizing the interface, λ^{ci}_s, and μ^{ci}_s are given following [12].

Interfacial cracking: spring imperfect interface model

The interfacial cracking of the very soft interface is assumed to be created by the tangential displacement jump $\mathbf{v}_t$ and the positive part of normal displacement jump $\mathbf{v}^+_n$. This leads to a decomposition expressed by $\mathbf{v} = \mathbf{v}^+_n + \mathbf{v}^-_n + \mathbf{v}_t$, and ψ^{si} is postulated as

$$\psi^{si} = g(d)\left(\psi^{si}_{n+} + \psi^{si}_t\right) + \psi^{si}_{n-} = \frac{1}{2}g(d)\left[\mathbf{v}^+_n\cdot \mathbf{C}^{si}_s \cdot \mathbf{v}^+_n + \mathbf{v}_t\cdot \mathbf{C}^{si}_s\cdot \mathbf{v}_t\right] + \frac{1}{2}\mathbf{v}^-_n\cdot \mathbf{C}^{si}_s\cdot \mathbf{v}^-_n\,, \tag{6}$$

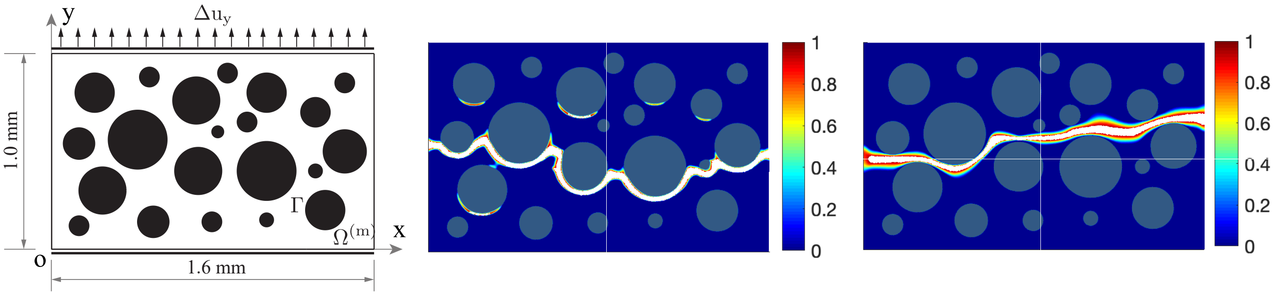
[†]The tensor product operation $\mathbf{A}\underline{\overline{\otimes}}\mathbf{B}$ is defined by $(\mathbf{A}\underline{\overline{\otimes}}\mathbf{B})_{ijkl} = \left(A_{ik}B_{jl} + A_{il}B_{jk}\right)/2$ for any two second-order tensors $\mathbf{A}$ and $\mathbf{B}$.

with the tangential interface stiffness $\mathbf{C}_s^{si}$ being defined following [13] as $\mathbf{C}_s^{si} = \lambda_s^{si} \mathbf{n} \otimes \mathbf{n} + \mu_s^{si} (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})$. The Lamé's constants characterizing the interface, λ_s^{si}, and μ_s^{si}, can be determined following [13].

The variational approach to fracture as proposed in Bourdin, Francfort and Marigo [2, 1] and developed in a convenient algorithmic setting by Miehe [3] is adopted here. It implies two problems: (i) phase field problem, corresponding to a minimization of the total energy with respect to the displacement field $\mathbf{u}$ and (ii) mechanical problem, corresponding to a minimization of the energy with respect to the scalar damage field d. The details of numerical implementation can be found in [6, 8].

2 Numerical examples: two dimensional simulation of a microstructure

A rectangular plate containing several inclusions is considered under tensile loading. The dimensions of the considered structure are $L \times B = 1 \times 1.6$ mm^2, while the inclusion diameters are taken to range from $d = 0.06$ mm to $d = 0.3$ mm. The detailed geometry and boundary conditions are provided in Fig. 1 (a).



(a) Geometry/boundary conditions (b) Soft interphase (c) Stiff interphase

Figure 1. 2D simulation of a microstructure containing multiple inclusions.

Both situations of very stiff interface (CI) and very soft interface (SI) are considered. The material properties are given in the Table. 1. The tangential Lamé's constants for the interface can be determined following [12, 13] with the interphase thickness $h = 1$ µm, we obtain $\lambda_{si}^s = 105$ GPa/mm, $\mu_{si}^s = 30$ GPa/mm and $\lambda_{ci}^s = 6.857$ GPa.mm, $\mu_{ci}^s = 8$ GPa.mm.

The displacements are prescribed along the $y-$direction for upper edge ($y = B$) while the displacements along x are free. On the lower edge ($y = 0$), the displacements along y are fixed to zero, while the displacements along x are free. The monotonic displacement increments of $\Delta u_y = 2 \times 10^{-5}$ mm have been prescribed via 1000 time steps. Plane strain condition is assumed.

Table 1. Material properties of the spring/coherent interface model.

Parameter	Matrix	Inclusion	Soft interphase	Stiff interphase	Unit
λ	18	60	4.5×10^{-2}	6×10^3	GPa
μ	12	32	3×10^{-2}	4×10^3	GPa
g_c	5×10^{-4}	3×10^{-3}	$g_c^{si,n} = 3.75 \times 10^{-5}$, $g_c^{si,t} = 3.18 \times 10^{-5}$	5×10^{-3}	[kN/mm]

The obtained results of crack propagation are shown in Fig. 1(b)(c). A strong impact of interfacial properties on the fracture behavior of the heterogeneous material is obtained. We capture that the soft interface provides a major interfacial cracking mode, while the stiff interface induces a main bulk cracking behavior.

The very complex behavior of the interfacial cracking is reproduced by the present model. The competition and interaction between bulk cracking and interfacial cracking are successively simulated. More interestingly, the proposed model can predict the poorly post-cracking properties of strongly bonded interface observed in the experiment. This demonstrated the performance of the present computational framework. It then constitutes a promising tool to evaluate the mechanical performance of complex composite materials.

3 Conclusion

In this work, we introduce a robust interfacial cracking model in the phase field framework based on the mixing of bulk energy with the energy of null-thickness interface. The proposed model is able to consider the complex interfaces with various properties, i.e, very stiff interphase and very compliant interphase. We apply the present model to study the interfacial cracking in composite materials and to understand the effects of thin interphase properties on the global behavior of advanced material and structures. The new model predict very well the complex cracking phenomena on interfaces such as initiation, delamination, coalescence, and deflection.

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