



Phase field modeling of cracks in quasi-brittle and elastoplastic micro-structured materials: topology optimization, 3D printed materials and image-based models

Pengfei Li

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THÈSE DE DOCTORAT DE L'UNIVERSITÉ PARIS-EST

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Phase field modeling of cracks in quasi-brittle and elastoplastic micro-structured materials : topology optimization, 3D printed materials and image-based models

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And I would like to acknowledge ...

Abstract

The objective of this thesis is to develop numerical modeling and simulation techniques to describe the damage in quasi-brittle and elastoplastic composites, which can be obtained by additive manufacturing processes like 3D-printing. We develop phase field methods to fracture and propose several extensions and applications to composites. First, after validating available elastoplastic phase field models on experimental results, we extend these models to interfacial damage, which is central in composites. In a second part, we develop design methodologies for composite microstructures to increase the resistance to cracking, for quasi-brittle and elastoplastic composites. For this purpose, we combine the phase field method and topology optimization (SIMP and BESO techniques). Then, models are proposed to describe cracking in polymer-glass fiber composites obtained by 3D printing, and which are characterized by a strong anisotropy. For this purpose, we develop an original anisotropic elastoplastic phase field model for the macro scale. Finally, experimental images obtained by X-Ray micro tomography are used to model the complex cracking process at the microscale of the composites.

Résumé

Cette thèse a pour objectif de développer des méthodologies de modélisations numériques pour représenter l'endommagement dans les composites quasi-fragiles et élastoplastiques, possiblement obtenus par des procédés de fabrication additive comme l'impression 3D. Nous développons des approches de champ de phase pour modéliser la fissuration et proposons plusieurs nouvelles extensions et applications aux composites. Premièrement, après avoir validé des modèles de champs de phase élastoplastiques sur des résultats expérimentaux, nous étendons ces modèles à l'endommagement aux interfaces, qui est primordial dans les composites. Dans une deuxième partie, nous développons des méthodes de design des microstructures en vue de résister à la fracturation, pour des composites quasi-fragiles ou élastoplastiques. Pour cela, nous combinons la méthode de champ de phase avec des techniques de type optimisation topologique (BESO et SIMP). Ensuite, des modèles sont présentés pour représenter la fissuration dans les composites élastoplastiques polymère-fibres de verres imprimés en 3D, caractérisés par une forte anisotropie du fait de leur texture par couche. Pour cela, nous développons un modèle original de fissuration anisotrope basée sur la méthode champ de phase dans un cadre élastoplastique pour l'échelle macroscopique. Enfin, des images expérimentales de composites imprimés en 3D obtenues par micro tomographie sont directement utilisées pour modéliser les phénomènes complexes de fissuration à l'échelle de la microstructure.

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Chapter 1

Introduction and literature review

1.1 Background and motivations

Modeling the brittle/ductile fracture process in homogeneous/heterogeneous materials is of extreme importance in engineering, since it covers several major applicative fields such as civil engineering materials, biomechanics materials (bones), metallic materials, or architected materials obtained by 3D printing, as shown in Fig. 1.1.

Recently, several advances in formulations, numerical methods and computer capabilities have opened the route to analyze damage of composites and heterogeneous materials directly from their microstructure, by simulating microcracking initiation, propagation and merging up to global failure. Such analyses offer new possibilities in material design, such as optimization of the constituents composition/morphologies [152, 65, 176, 49], or investigation of microcracking mechanisms directly from realistic microstructures, such as the ones arising from experimental micro-CT images [129, 126].

However, several challenges are related to microstructure-based damage analyses: (i) the development of appropriate formulations and related numerical methods to handle initiation, propagation and interactions of micro cracks in complex geometrical domains related to heterogeneous microstructures; (ii) the computational complexity, which warrants describing all heterogeneities in the whole sample; (iii) the presence of interfaces which may involve different damage mechanisms as compared to the bulk cracks.

More recently, design of structures and materials with enhanced resistance to damage and fracture has emerged as a new challenging and exciting topic in computational mechanics. With the quick development of 3D printing and additive manufacturing techniques [120], new technological solutions which were not possible a few years ago can now be considered, like on-demand geometries of multi-materials structures and microstructures. More specifically, 3D printed bi-materials [170, 75, 13] offer new exciting possibilities such as designing

composites with non-trivial periodic microstructures and ad-hoc functionalities. Among them, particle-matrix composites able to increase the fracture resistance as compared to existing composites is of industrial and technological critical importance, for applications in aircraft, automotive or biomechanics, among many others. One central ingredient for this task is the use of topology optimization.

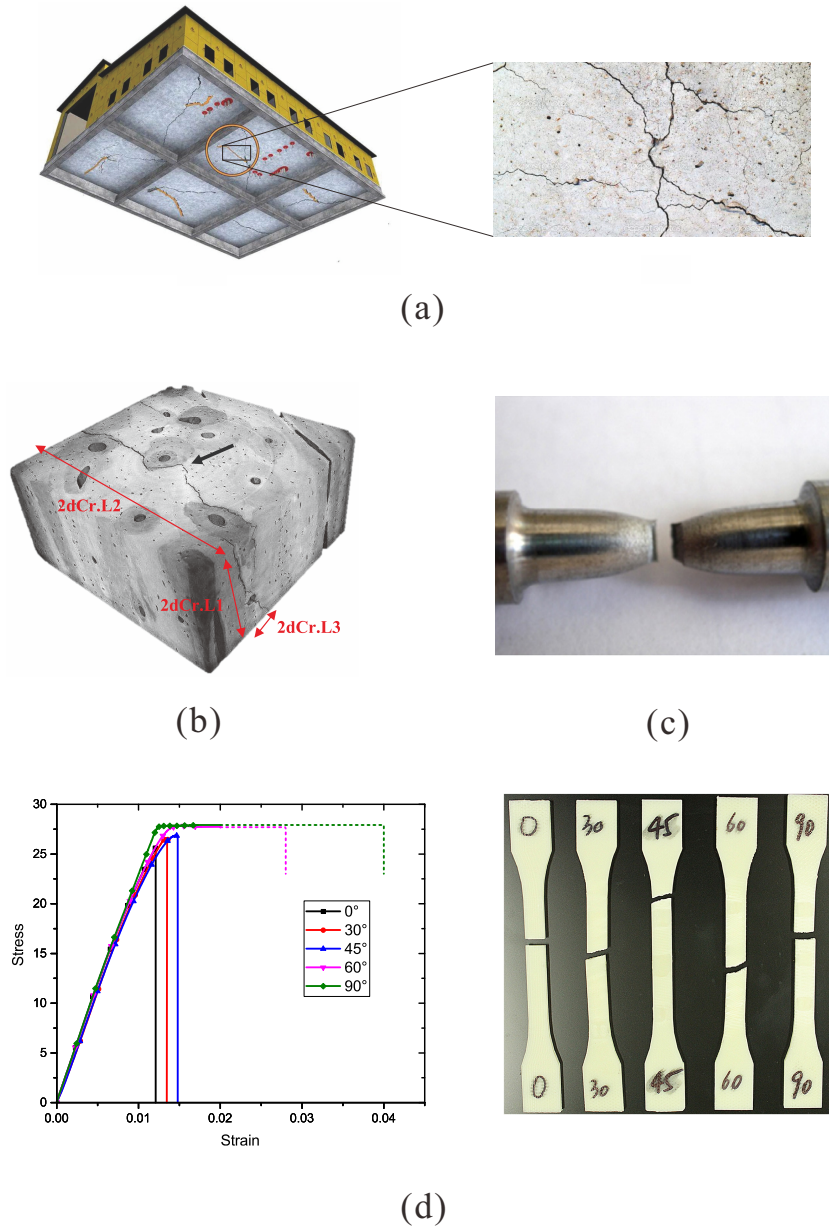


Fig. 1.1 Damage phenomena in (a) civil engineering material [123]; (b) biomechanics material (bone) [59]; (c) metallic material [34]; (d) 3D printed elastoplastic brittle materials [194].

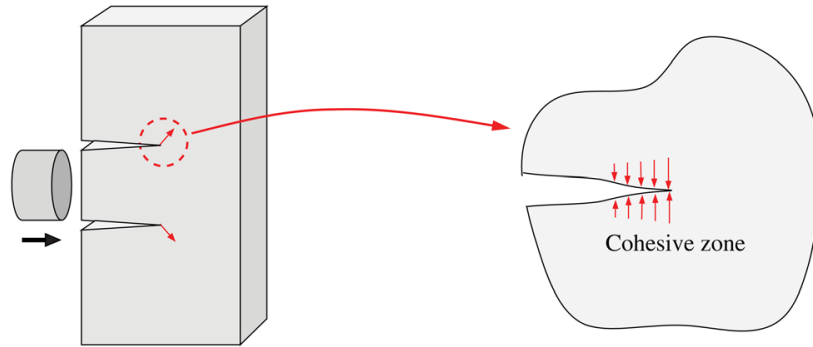


Fig. 1.2 Schematics of the cohesive zone model [138].

In the above background, the motivations of this PhD work are listed as follows:

- Simulate the initiation and propagation of micro cracks in elastoplastic brittle homogeneous materials and compare with the experimental datas, then extend this model to heterogeneous materials with taking into account the interfacial damage.
- Develop a topology optimization framework for maximizing the fracture resistance of quasi-brittle and ductile composites.
- Develop an anisotropic damage model for 3D printed elastoplastic materials, which can simulate the cracks following preferential directions and cracks in 3D printed layer. This strongly anisotropic damage phenomenon can be found in Fig. 1.1(d).
- Simulate the initiation and propagation of micro cracks in realistic models of microstructures obtained from 3D imaging techniques.

1.2 Literature review

1.2.1 Numerical modeling of damage and cracks

1.2.1.1 Cohesive Zone Models

The concept of the Cohesive Zone Models (CZMs) goes back to the 60's and was originally developed from Dugdale [54] and [21]. The principal idea of cohesive cracks is shown in Fig. 1.2. The cohesive model is used in the so-called process zone, sometimes also called cohesive zone. The complex stress state around the crack tip is lumped into a single surface. A surface energy term which controls the displacement jump along a known surface where a nonlinear traction-displacement jump relation must be introduced to describe the failure.

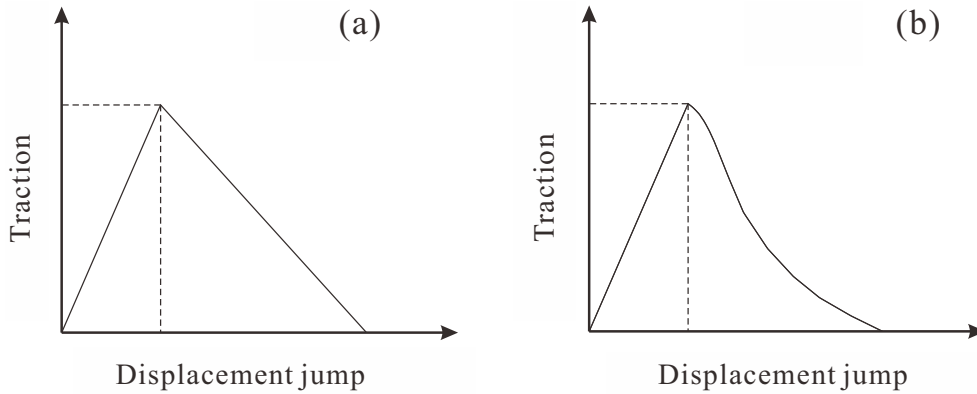


Fig. 1.3 (a) Bilinear traction-separation law; (b) Exponential law.

The method usually associates with finite elements in which the damageable interface is discretized by surfaces where the nodes are doubled to allow jump displacements [68]. An important material parameter of the CZMs is the fracture energy G_c which is related to the energy dissipation during crack opening.

In cohesive cracks, a traction-separation model is applied across the crack surface that links the cohesive traction transmitted by the discontinuity surface to the displacement jump, characterized by the separation vector. Fig. 1.3 shows two popular types of traction-separation law in brittle materials: the bilinear softening law [22, 66, 139] and the exponential softening law [181, 46]. The intrinsic form of CZMs employs cohesive surface elements in the potential fracture area before computational simulations [71, 180]. Alternatively, cohesive surfaces elements can be inserted during the simulation when a criterion is satisfied. In this way, the model is so-called "extrinsic" (sometimes also called initially rigid models) [81, 136, 137]. The drawback of the intrinsic CZM is the requirement of a priori fracture zone while the extrinsic version needs to be employed with an adaptive mesh. It has been shown that the extrinsic models cause numerical difficulties when elastic unloading occurs at an early stage such that the stiffness for the unloading case tends to infinity [144]. It is believed that extrinsic models are better suited particularly in the context of dynamic fracture. In general, cracks in CZMs propagate by following the boundary of elements, leading to strong mesh-dependency issues.

1.2.1.2 Embedded Finite Element Method

The basic idea of Embedded Finite Element Method (EFEM) is to introduce discontinuous enrichment inside elements, which vanishes at the boundaries of elements, see Fig. 1.4. This class of methods are much more flexible than schemes that allow discontinuities only

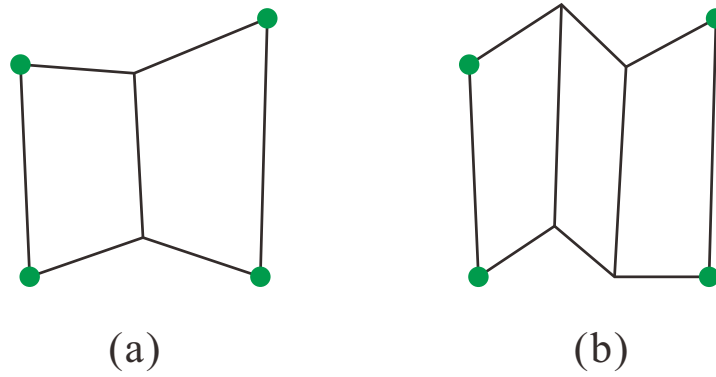


Fig. 1.4 Element with (a) one weak discontinuity and (b) two weak discontinuities.

at element interfaces, and it eliminates the need for continuous remeshing. One major advantage of the EFEM (compared to XFEM discussed in the next section) is that the additional unknowns could be condensed on the element level, so that discontinuities could be captured with very small changes of the existing code. The computation costs of XFEM and EFEM have been compared in [135]. First contributions to E-FEM can be found in [160, 100], in which discontinuities have been assumed to be fixed. The drawbacks of EFEM lies on unexpected approximation errors due to the lack of the continuity of the displacement field between two elements leading to the strong mesh-dependency as well as the lack of convergence of the solution with respect to the mesh size. More detail about EFEM, one can find in [174].

1.2.1.3 Extended Finite Element Method

The eXtended Finite Element Method (XFEM) aims at avoiding the remeshing step in crack propagation process within Finite Elements and linear fracture mechanics. This method employs the local partition of unity concept [105, 164, 163] and introduces additional nodal parameters for the elements cut by the crack. Hence, the additional unknowns cannot be condensed on the element level as in EFEM. The displacement discontinuity depends only on the additional nodal parameters. The basic idea of XFEM is to decompose the displacement field into a continuous part $\mathbf{u}^{cont}$ and a discontinuous part $\mathbf{u}^{disc}$:

$$\mathbf{u}^h(\mathbf{x}) = \mathbf{u}^{cont}(\mathbf{x}) + \mathbf{u}^{disc}(\mathbf{x}). \quad (1.1)$$

The continuous part is the standard FE interpolation and additional information is introduced into the FE interpolation through the local partition of unity approach by adding an enrichment $\mathbf{u}^{disc}$. The approximation of the displacement function for n_c cracks with m_l crack tips takes

the following form:

$$\mathbf{u}^h(\mathbf{x}) = \sum_{I \in \Theta} N_I(\mathbf{x}) \mathbf{u}_I + \sum_{N=1}^{n_c} \sum_{I \in \Theta_c} N_I(\mathbf{x}) \Phi_I^{(N)} \mathbf{a}_I^{(N)} + \sum_{M=1}^{m_t} \sum_{I \in \Theta_t} N_I(\mathbf{x}) \sum_{K=1}^{N_k} \phi_{KI}^{(M)} \mathbf{b}_{KI}^{(M)}, \quad (1.2)$$

where Θ is the set of nodes in the entire discretization, Θ_t is the set of nodes around the crack tip, and Θ_c is the set of nodes associated to elements completely cut by the crack. $\Phi_I^{(N)}$ is the enrichment function of crack N , and $\phi_{KI}^{(M)}$ is the enrichment function for the crack tip M . $\mathbf{a}_I$ and $\mathbf{b}_{KI}$ are additional degrees of freedom that needs to be solved.

In XFEM, cracks can propagate in an arbitrary direction without dependence to the underlying mesh. Nevertheless, in the classical XFEM, two additional issues remain: (i) the difficulties to deal with many cracks, due to associated level-set functions which must be constructed to describe the position of the crack front; (ii) initiation of cracks cannot be dealt with as the method is based on classical fracture mechanics. Despite these drawbacks, XFEM is a good alternative when dealing with fixed cracks and interface problems. Applications and developments of XFEM can be mentioned, such as, among many others: dynamic fracture [132, 18], hydraulic fracture [116] and ductile fracture [39].

1.2.1.4 Continuous damage model without regularization

Kachanov [73] pioneered the concept of the effective (undamaged) configuration and introduced the basis for the continuum damage mechanics theories. The model characterizes damage induced by the formation of micro-cracks. In this context, an isotropic degradation function was introduced and involves a scalar damage parameter $d \in [0, 1]$. The constitutive equation relating the stress field $\boldsymbol{\sigma}$ and the strain field $\boldsymbol{\varepsilon}$ of an isotropic damage model is written as:

$$\boldsymbol{\sigma} = (1 - d) \mathbb{C} : \boldsymbol{\varepsilon}, \quad (1.3)$$

where $\mathbb{C}$ is the stiffness matrix of the elastic material. In the case of anisotropic damage effects, a damage tensor $\mathbb{D}$ must be introduced. In addition, an evolution law is necessary for d . This damage law should be chosen in order to reflect the behavior of the considered material. For example, for quasi-brittle materials, a popular damage law is written as [140]:

$$d = \begin{cases} 0 & \text{if } \kappa < \kappa_0 \\ 1 - \frac{\kappa_0}{\kappa} ((1 - \alpha) + \alpha \exp[-\beta(\kappa - \kappa_0)]) & \end{cases} \quad (1.4)$$

In (1.4), the scalar parameter β describes the softening behavior; α is a scalar which controls the residual state in the post peak stage; κ_0 is the threshold for the initiation of damage and κ

is a history scalar parameter which takes the largest value of an equivalent strain $\tilde{\epsilon}$ which is a function of ϵ . The reader is referred to [140] for detailed definition of $\tilde{\epsilon}$. Damage evolution is governed by the Kuhn-Tucker inequalities as follows:

$$\dot{d} \geq 0, \quad f(\tilde{\epsilon}, \kappa) \leq 0, \quad \dot{d}f(\tilde{\epsilon}, \kappa) = 0, \quad (1.5)$$

where $f(\tilde{\epsilon}, \kappa) = \tilde{\epsilon} - \kappa$ is the loading function driving the evolution of damage. Early developments in the context of numerical methods can be found in [79, 42].

The well-known drawbacks of this model are twofold mesh sensitivities: (i) dependence on the alignment of the mesh, see the results in [64] and (ii) a non-convergence of the response with respect to mesh density, see the results in [72]. The underlying reason is that the dissipated energy vanishes with the size of the elements. When accumulated damage gets to an extent, the governing equations become ill-posed. Various techniques have been proposed in the literature to remedy for aforementioned mesh sensitivity issues, such as:

- A cosserat continuum or micropolar model e.g. [50, 82], where the governing field equations are regularized by adding an internal length scale.
- An artificial viscosity technique [56].
- Gradient Enhanced Damage (GED) models [141].
- Nonlocal techniques using weight functions to regularize the damage fields [72, 24].
- Adding higher order gradient of deformation [118, 119].

Pros and cons of these methods have been discussed in [33]. Among those, the last two methods are the most used in computational analysis and are called regularization techniques. A very popular method in this context is the so-called phase field method to fracture [36, 76, 108], which will be detailed in Section 1.2.2 and used in this thesis.

1.2.1.5 Non-local damage models

Nonlocal damage models are based on regularization through a convolution of strain, where the localization of damage is kept in a zone defined by a given internal length, as firstly developed in [24]. This model does not suffer from lack of mesh dependence as in local models. Then, the driving force is a function of a nonlocal term $\bar{\epsilon}$, as:

$$f(\bar{\epsilon}_{eq}, \kappa) = \bar{\epsilon}_{eq} - \kappa, \quad (1.6)$$

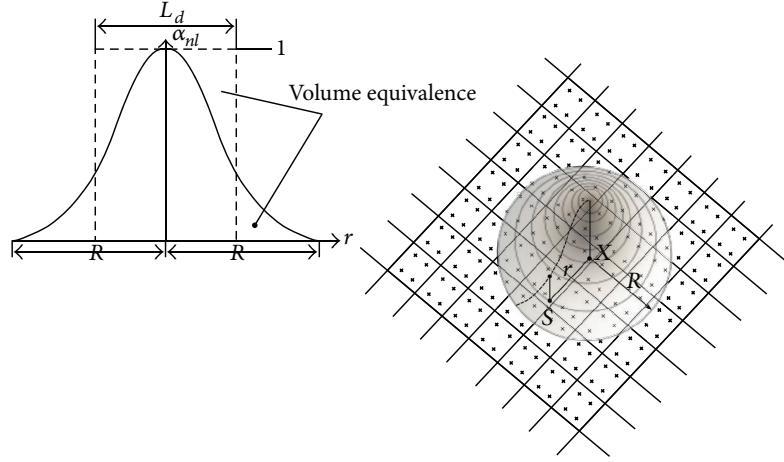


Fig. 1.5 Principle of nonlocal constitutive models with the typical bell-shaped function [144].

where $\bar{\epsilon}$ is defined by:

$$\bar{\epsilon}_{eq}(x) = \frac{\int_{\Omega} g(s) \epsilon_{eq}(x+s) dV}{\int_{\Omega} g(s) dV}, \quad (1.7)$$

where the weight function $g(s)$ satisfies $\int_{\Omega} g(s) dV = 1$. A popular choice is the Gauss weighting function, as:

$$g(s) = \exp \left[-\frac{\|x+s\|^2}{\alpha \ell^2} \right]. \quad (1.8)$$

In (1.8), α has to be chosen by the users, ℓ is the length of the model, and s denotes the relative position vector of a point in Ω . Another alternative is the bell-shaped function, where the regularization occurs at a finite distance from one point through a cut-off distance $r = \|\mathbf{x} - \mathbf{s}\|$:

$$g(s) = \begin{cases} 1 - \frac{r^2}{R^2} & \text{if } r \leq R, \\ 0 & \text{if } r > R. \end{cases} \quad (1.9)$$

This nonlocal damage model is also referred to in the literature as the integral damage model, see Fig. 1.5. For this types of nonlocal models, changing the dimensions of the problem requires recalibration of the parameters of the non-local model, where the parameters can be obtained by an inverse analysis. An excellent overview on non-local models of the integral types and physical motivations can be found in [23].

1.2.1.6 Gradient enhanced model

Gradient-enhanced models [141, 140], or briefly called gradient models, are typically described by differential equations that contain higher order spatial derivatives. Gradient models

are usually mentioned as a differential type nonlocal models (weakly non-local models), and use another regularization definition of the strain field, estimated by:

$$\bar{\varepsilon}_{eq} - c\nabla^2 \bar{\varepsilon}_{eq} = \varepsilon_{eq} \quad (1.10)$$

with an additional boundary condition [85, 117]:

$$\nabla \bar{\varepsilon}_{eq} \cdot \mathbf{n} = 0. \quad (1.11)$$

(1.10) is obtained from a Taylor expansion of the term ε_{eq} in (1.7).

Both integral-type and differential-type model can solve the mesh-dependence issues in presence of localization, nevertheless, induce an incorrect crack initiation, as reported in [161]. Improvements to these problems have been proposed in later works, e.g. [62, 122].

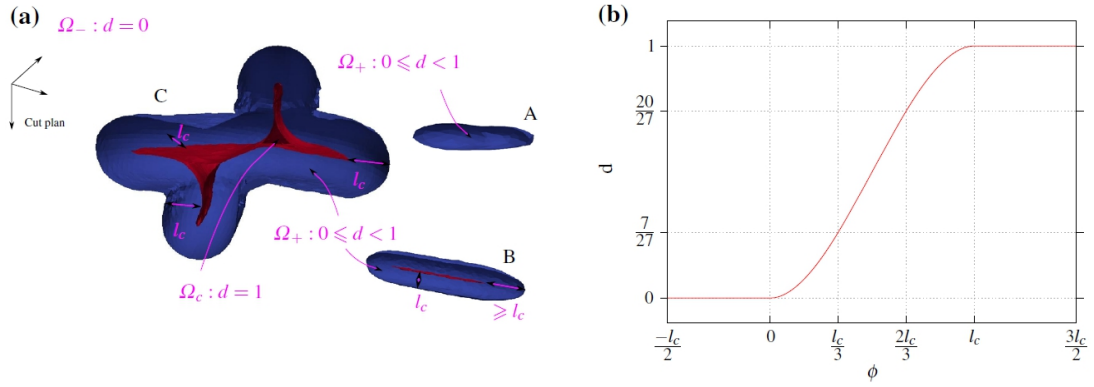


Fig. 1.6 (a) Damage domain and (b) damage function $d(\phi)$ [151].

1.2.1.7 Thick level set method

The thick level set model was introduced in [115, 27] for modelling damage as a propagating level set front. As a constitutive model, it allows capturing complex morphology cracks from the initiation, branching and merging. In these models, a level-set function ϕ is used to separate the undamaged zone from the damaged one, and d which depends on the level set must be

- Equal to 1 when $\phi(x) \geq l_c$ (the fully damaged zone Ω_c shown in Fig. 1.6(a)).
- Equal to 0 when $\phi(x) \leq 0$ (Ω_- shown in Fig. 1.6(a)).
- $d'(\phi) \geq 0$ when $0 \leq \phi \leq l_c$.

l_c is a mesh-size-independent characteristic length leading to the non-local effect of the model. However, TLS induces spurious oscillations in mechanical responses as well as complexity related to self-contact within the crack. In [151], A. Salzman et al. gave a function for d as:

$$d(\phi) = \left(\frac{\phi}{l_c}\right)^2 \left(3 - 2\frac{\phi}{l_c}\right) \quad (1.12)$$

which can be found in Fig. 1.6(b).

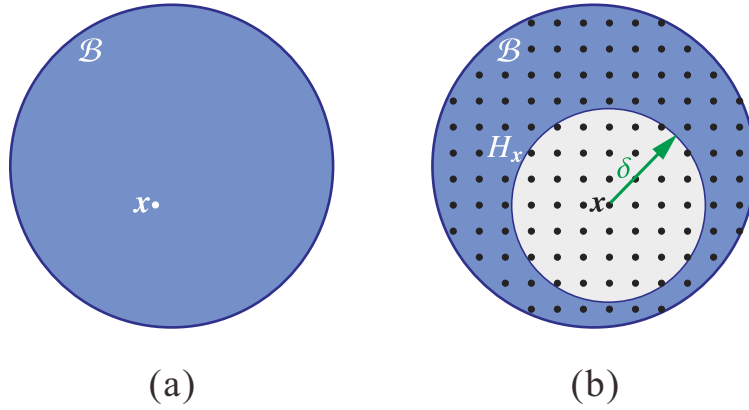


Fig. 1.7 (a) Classical continuum mechanics and (b) peridynamics.

1.2.1.8 Peridynamics

This technique was originally developed from [158]. It assumes that the material is described by discrete particles which represent the continuous matter. The core of the Peridynamics (PD) formulation is that the behavior of each material point is governed by its interaction with other material points located within its neighborhood. The PD equation can be understood as an integral expression of the linear momentum balance in classical continuum mechanics, but the integral domain is within the neighborhood H_x with the distance δ of a material point at $\mathbf{x}$ as shown in Fig. 1.7. The equation of motion of a material point in an elastic material can be expressed as

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H_x} \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})dV' + \mathbf{b}(\mathbf{x},t), \quad (1.13)$$

where $\mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x})$ is a pairwise force density vector function and $\mathbf{u}$ is the displacement of the material point at $\mathbf{x}$. The interaction between the material points at $\mathbf{x}$ and $\mathbf{x}'$ corresponds to the “bond” term [134, 193]. In this method, the rupture criterion is based on a threshold elongation $(\mathbf{u}' - \mathbf{u})$ between two particles. When this link breaks up there is no more

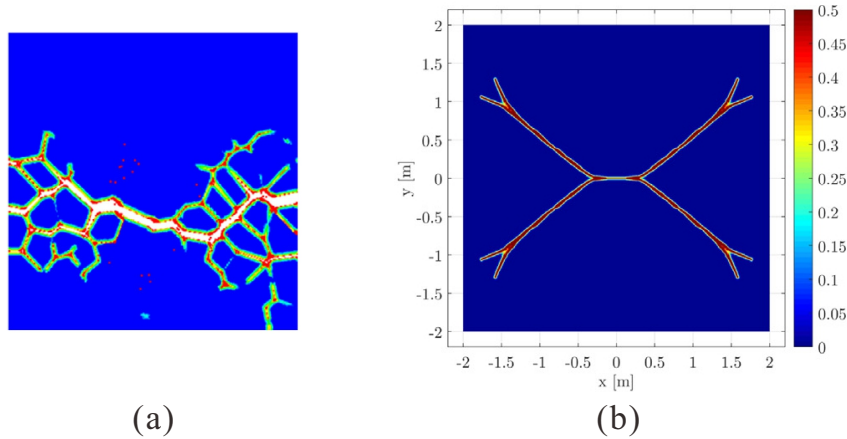


Fig. 1.8 Peridynamic simulation of (a) dynamic fracture in orthotropic media [61] and (b) hydraulic fracture [133].

interaction and the forces are redistributed on the neighborhood links. It can easily model complex cracks patterns (see Fig. 1.8) but has several drawbacks, such as ambiguous definition and calibration of interaction models to reproduce general mechanical behavior, spatial convergence issues, etc.

1.2.2 Phase field models for fracture

The development of the variational approach to fracture [57, 37, 108, 112, 32, 10], also called phase field method in the literature, offers several advantages in this context, like: the possibility to initiate cracks from undamaged configurations; the possibility to handle arbitrary crack networks (including branching, merging, in both 2D and 3D) without specific treatment and use of classical finite elements; a variational framework allowing to include many models or mechanisms, and a mesh-independence due to an appropriate regularization process. The method requires a fine mesh along the crack path and a suitable definition for regularization parameters (see a discussion in [128] and recent internal length-insensitive formulations in [175, 102]). However, due to the above-mentioned advantages, the phase field method has been widely developed and applied to many problems, such as, among many others: brittle fracture [10, 167, 189, 95], composite delamination [147], dynamic fracture [38, 52, 98], hydraulic fracture [171, 110, 179, 55], topology optimization for resistance to cracking [176, 49], anisotropic material fracture [125, 28, 187], elastoplastic brittle/ductile fracture [9, 8, 107, 30, 6, 185], ductile/fragile transition [44], fracture in micro tomography image-based models of microstructures [126, 129, 127] and more recently adapted in machine learning strategies in [63]. In the following, we review in detail different methods which

will be central to this work: (a) quasi-brittle fracture models, (b) elastoplastic brittle/ductile fracture models, and (c) anisotropic fracture models.

1.2.2.1 Quasi-brittle fracture models

To overcome the failure of Griffith's theory to predict the initiation of cracks in the case a crack tip is absent, Francfort and Marigo in [57] proposed a variational approach in which the total potential energy of a cracked body is written as the sum of a buck energy E_u and a surface energy E_s , as

$$E(\mathbf{u}, \Gamma) = E_u(\mathbf{u}) + E_s(\Gamma) = \int_{\Omega} \psi(\mathbf{u}, \Gamma) d\Omega + g_c \int_{\Gamma} ds, \quad (1.14)$$

where $\mathbf{u}$ is the displacement field, and Γ refers to an admissible crack surface. The variational approach does not involve any crack tip or predefined path and allows the initiation, the branching of cracks, as long as the crack set is the solution of the minimization problem. However, the crack set Γ is unknown, and solving this problem is nontrivial. In [36], Bourdin et al. gave a specialization of (1.14) with a regularized version as:

$$E(\mathbf{u}, v) = \int_{\Omega} (g(v) + k) \psi(\mathbf{u}) d\Omega + g_c \int_{\Omega} \gamma(v, c) d\Omega, \quad (1.15)$$

where

$$\gamma(v, c) = \frac{(1 - v^2)}{4c} + c \nabla v \cdot \nabla v \quad (1.16)$$

is the crack density function, and g_c is the energy release rate, and v is the crack field parameter which varies smoothly from 1 (undamaged state) to 0 (totally damage state), $g(v)$ is the degradation function and k is a small numerical parameter to prevent loss of definite posedness of the elastic tensor in case of full damage. Note that in the absence of the second right-hand term in (1.16), a local damage model is found, with well-known related non-convergence issues with respect to the mesh discretization.

The total energy in (1.15) does not distinguish between fracture behavior in tension and compression, which could induce unrealistic crack patterns in compression, see [36]. To avoid such situations, H. Amor in [16] proposed a decomposition of the elastic energy density ψ_0 into volumetric and deviatoric contributions, as:

$$\psi_0^+(\varepsilon) = \frac{1}{2} \kappa \langle \text{Tr}(\varepsilon) \rangle_+^2 + \mu \varepsilon^{\text{dev}} : \varepsilon^{\text{dev}}, \quad (1.17)$$

$$\psi_0^-(\varepsilon) = \frac{1}{2} \kappa \langle \text{Tr}(\varepsilon) \rangle_-^2, \quad (1.18)$$

where κ and μ denote bulk modulus and shear modulus, respectively, $\langle x \rangle_{\pm} = \frac{1}{2}(x \pm |x|)$ and $\boldsymbol{\varepsilon}^{\text{dev}} = \boldsymbol{\varepsilon} - \frac{1}{3}\text{Tr}(\boldsymbol{\varepsilon})\mathbf{1}$.

Miehe in [112] proposed another expression for the potential energy of the cracked solid as:

$$E(\boldsymbol{\varepsilon}, d) = \int_{\Omega} [g(d)\psi_0^+(\boldsymbol{\varepsilon}) + \psi_0^-(\boldsymbol{\varepsilon})] d\Omega + g_c \int_{\Omega} \gamma(d) d\Omega, \quad (1.19)$$

where d denotes the damage variable and $\gamma(d)$ is the crack density function which regularizes the crack. The free energy is split into positive and negative parts using the spectral decomposition of the strain tensor:

$$\psi_0^{\pm} = \frac{1}{2}\lambda \langle \text{tr}[\boldsymbol{\varepsilon}] \rangle_{\pm}^2 + \mu \text{tr}[\boldsymbol{\varepsilon}^{\pm}]^2 \quad (1.20)$$

with

$$\boldsymbol{\varepsilon}^{\pm} = \sum_{i=1}^3 \langle \boldsymbol{\varepsilon}^i \rangle_{\pm} \mathbf{n}^i \otimes \mathbf{n}^i, \quad (1.21)$$

where $\boldsymbol{\varepsilon}^i$ and $\mathbf{n}^i$ are the eigenvalues and eigenvectors of $\boldsymbol{\varepsilon}$. Then in [108], a staggered manner was introduced to decouple and solve the minimization problem with a history function

$$\mathcal{H}(\boldsymbol{\varepsilon}) = \max_{s \in [0, t]} \psi_0^+(\boldsymbol{\varepsilon}, s). \quad (1.22)$$

It is considered as a robust algorithm since it overcomes the convergence difficulty of the monolithic scheme.

In order to avoid damage occurring at low stress levels, Miehe in [111] proposed a strain criterion with threshold by a new surface energy density function as:

$$\psi_{\text{frac}} = 2\psi_c \left[d + \frac{\ell^2}{2} \nabla d \cdot \nabla d \right]. \quad (1.23)$$

Here, ψ_c is a specific fracture energy density. After some simple algebraic manipulation, a new history function can be obtained as

$$\mathcal{H}(\boldsymbol{\varepsilon}) = \max_{s \in [0, t]} \left[\langle \psi_0^+(\boldsymbol{\varepsilon}, s) - \psi_c \rangle_+ \right] \quad (1.24)$$

which ensures a linear behavior at low stress levels.

In [31], Borden et al. proposed a fourth-order phase field formulation which improves the convergence of the fracture problem. The potential energy of the cracked solid is as:

$$E(\boldsymbol{\varepsilon}, c) = \int_{\Omega} [c^2 \psi_0^+(\boldsymbol{\varepsilon}) + \psi_0^-(\boldsymbol{\varepsilon})] d\Omega + g_c \int_{\Omega} \gamma(c) d\Omega, \quad (1.25)$$

where c is the crack field parameter which varies smoothly from 1 (undamaged state) to 0 (totally damage state), and the fourth-order crack density function $\gamma(c)$ is defined as:

$$\gamma(c) = \frac{(1-c^2)}{4\ell} + \frac{\ell}{2} \nabla c \cdot \nabla c + \frac{\ell^3}{4} (\Delta c)^2. \quad (1.26)$$

In order to keep the benefit of Miehe's model in the decomposition of the free energy and save the computational cost, a hybrid model has been proposed in [10]:

$$\begin{cases} \sigma(\mathbf{u}, d) = (1-d)^2 \frac{\partial \psi(\epsilon)}{\partial \epsilon}, \\ -\ell^2 \delta d + d = \frac{2\ell}{g_c} (1-d) \mathcal{H}, \\ \forall \mathbf{x} : \psi_0^+ < \psi_0^- \Rightarrow d := 0. \end{cases} \quad (1.27)$$

This model saves the computing time, however it fails to capture cracks in compressive loading where the negative energy is dominant.

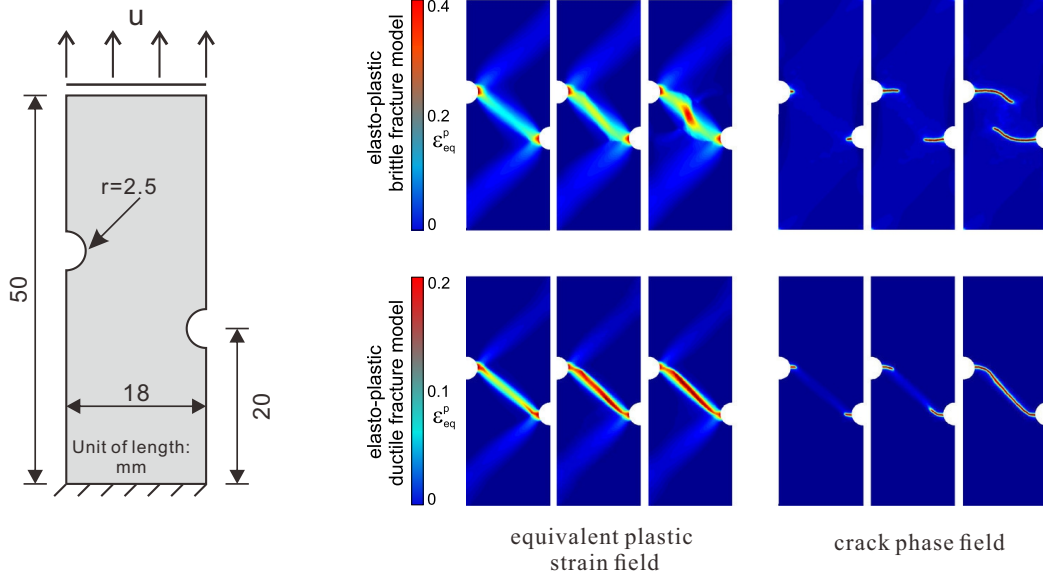


Fig. 1.9 The different performance for elastoplastic brittle/ductile fracture models [9].

1.2.2.2 Elastoplastic brittle/ductile fracture models

In most of elastoplastic phase field models, the total energy density ψ per unit volume can be written as the sum of elastic energy density ψ^e , plastic dissipative potential ψ^p and damage

dissipative potential ψ^d as:

$$\psi(\varepsilon, \varepsilon^p, p, d) = \underbrace{g(d)\psi_0^e(\varepsilon - \varepsilon^p)}_{\psi^e} + \underbrace{h(d)\psi_0^p(p)}_{\psi^p} + \psi^d(d), \quad (1.28)$$

where ε^p is the plastic strain, and p is the equivalent plastic strain.

In these elastoplastic phase field models, according to the difference of damage mechanism, there are two main categories of elastoplastic fracture models as: (a) elastoplastic brittle fracture model, where the fracture is driven primarily by the elastic strains; (b) elastoplastic ductile fracture model, where the fracture is driven mainly by the plastic strains. The different performance for these two categories of models can be found in Fig. 1.9.

In [53], F.P. Duda et al. proposed an elastoplastic brittle fracture model, here the specialization of (1.28) is as follows:

$$g(d) = (1 - d)^2, \quad h(d) = 1, \quad (1.29)$$

$$\psi_0^p = \frac{\sigma_y^2}{E(n+1)} \left(1 + \sqrt{\frac{2}{3}} \frac{Ep}{\sigma_y} \right)^{n+1} - \sqrt{\frac{2}{3}} \sigma_y p, \quad (1.30)$$

$$\psi^d = g_c \left(\frac{1}{2\ell} d^2 + \frac{\ell}{2} \nabla d \cdot \nabla d \right), \quad (1.31)$$

where σ_y is the yield stress, and n is the strain hardening exponent. This model fits in the variational framework, however there is no coupling between damage and plasticity.

In [9], Ambati et al. proposed an elastoplastic ductile fracture model based on the work in [53]. This model employed

$$g(d) = (1 - d)^{2\zeta}, \quad h(d) = 1, \quad (1.32)$$

$$\psi_0^p = \sigma_y p + \frac{1}{2} H p^2, \quad (1.33)$$

where H is the hardening modulus, and $\zeta = \frac{p}{p_{\text{crit}}}$ where p_{crit} as a threshold value. The variable ζ accounts for accumulation and localization of plastic strains, the increase of the order of ζ is expected to slow down the accumulation of damage before reaching the threshold value p_{crit} ($\zeta < 1$), and to accelerate it when the threshold is exceeded ($\zeta > 1$). This model has a good performance, however there is no real coupling between damage and plasticity.

Kuhn in [80] proposed a new ductile fracture model within the variational framework. The specialization of (1.28) is as follows:

$$g(d) = (1 - d)^2, \quad h(d) = g(d), \quad (1.34)$$

ψ_0^p and ψ^d are the forms in (1.33) and (1.31), respectively. This model has a real coupling between damage and plasticity, however the obtained yield criterion in this model is analogous to classical plasticity and not explicitly coupled to the fracture field (see [80] for more details). Thus, the evolution of the accumulated plastic strain becomes independent on the phase field.

In [30], Borden et al. proposed a ductile model with the same ψ_0^p and ψ^d in (1.33) and (1.31), but a new $g(d)$ and $h(d)$ as

$$g(d) = (1 - d)^2 (1 + d(2 - k)), \quad h(d) = g(d), \quad (1.35)$$

where $k > 0$, for $k = 2$ it recovers the model in [80]. This model meets the same problem to [80].

Alessi in [4–6] proposed a new coupling model within the variational framework. The specialization of (1.28) is as follows:

$$g(d) = \frac{(1 - d)^2}{k - (k - 1)(1 - d)^2}, \quad h(d) = (1 - d)^{2n}, \quad (1.36)$$

$$\psi_0^p = \sigma_y p, \quad (1.37)$$

$$\psi^d = \frac{3g_c}{8} \left(\frac{1}{\ell} d + \ell \nabla d \cdot \nabla d \right). \quad (1.38)$$

In this model, no plastic hardening effects are considered. By our best knowledge, this model also meets the problem that the evolution of the accumulated plastic strain is independent on the phase field, as in [80], even if $g(d) \neq h(d)$ here.

Recently in [110], Miehe proposed a new ductile fracture model within the variational framework, which is based on a gradient-extended plasticity-damage theory. The specialization of (1.28) is as follows:

$$\psi_0^p = \frac{1}{2} H p^2 + (\sigma_\infty - \sigma_y) \left(p + \frac{1}{\eta} e^{-\eta p} \right) + \frac{1}{2} \ell_p^2 \nabla p \cdot \nabla p, \quad (1.39)$$

$$\psi^d = (1 - (1 - d)^2) \omega_c + \frac{\omega_c}{\xi} \ell \left(\frac{d^2}{\ell} + \ell \nabla d \cdot \nabla d \right), \quad (1.40)$$

with

$$\eta > 0, \sigma_{\infty} > \sigma_y, \omega_c > 0, \xi > 0. \quad (1.41)$$

The $g(d)$ and $h(d)$ are same to (1.34). This formulation includes an additional internal length scale ℓ_p to regularize the plastic response, and to ensure that the damage zones of ductile fracture are contained within plastic zones. It guarantees on the computational side a mesh objectivity in post-critical ranges. However, it seems here the evolution of the accumulated plastic strain is also independent on the phase field.

More recently in [184], B. Yin and M. Kaliske proposed a new ductile fracture model, whose ideas in some ways are similar to [9]. This model is based on a hardening degradation function $f(\zeta)$ which works on the fracture toughness as

$$g_c = f(\zeta)g_c^0, \quad (1.42)$$

where g_c^0 is a material constant representing fracture toughness for brittle fracture, and ζ is the equivalent plastic strain, and $f(\zeta)$ is defined as

$$f(\zeta) = \begin{cases} 1 & \zeta < \zeta_{cr}, \\ \frac{1-b}{a^2} (\zeta - \zeta_{cr} - a)^2 + b & \zeta_{cr} \leq \zeta < a + \zeta_{cr}, \\ b & \zeta \geq a + \zeta_{cr}, \end{cases} \quad (1.43)$$

where a and b are two key parameters to control the profile of the degradation function f , see Fig. 1.10. This model has good performances in several benchmarks, however there is also no real coupling between damage and plasticity.

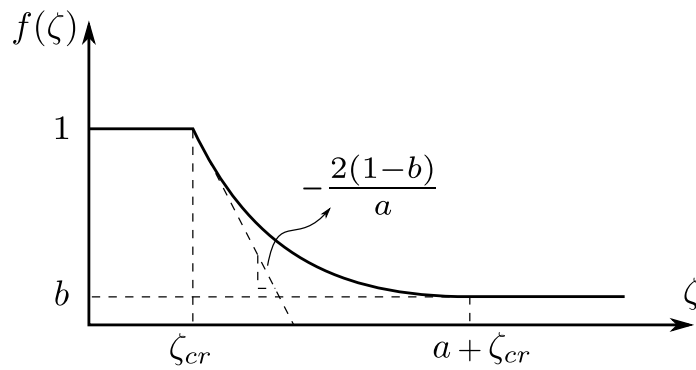


Fig. 1.10 The hardening degradation function $f(\zeta)$ [184].

1.2.2.3 Anisotropic fracture models

Phase-field models based on the variational formulation for anisotropic fracture have recently gained popularity, for example in [89], where an anisotropic fracture energy was employed to simulate crack propagation in polycrystals [45, 125]. The anisotropic crack surface density function is written by the following expression:

$$\gamma(d, \nabla d, \omega) = \frac{1}{2\ell} d^2 + \frac{\ell}{2} \omega : (\nabla d \otimes \nabla d), \quad (1.44)$$

where ω is a second order structural tensor, being invariant with respect to rotations, and is defined by:

$$\omega = \mathbf{1} + \xi (1 - \mathbf{M} \otimes \mathbf{M}), \quad (1.45)$$

where $\mathbf{M}$ denotes the unit vector normal to the preferential cleavage plane, $\xi \gg 0$ is used to penalize the damage on planes not normal to $\mathbf{M}$. This type of fracture energy anisotropy shows good performances in controlling the crack direction, however it is still not clear what such a gradient energy contribution does physically represent. A higher-order anisotropic crack surface density function can be found in [168, 88].

In [3], R. Alessi and F. Freddi proposed a phase field to simulate the unidimensional behavior of hybrid laminates, including a competition between fracture of both layers and debonding of the adhesive interface.

Recently in [28], J. Bleyer and R. Alessi proposed an anisotropic brittle fracture model to simulate the longitudinal/transverse damage in unidirectional fiber-reinforced composites. The total energy density for this model is given as:

$$W(\varepsilon, d_1, d_2) = \frac{1}{2} \varepsilon^T \mathbf{C}(d_1, d_2) \varepsilon + \frac{3g_c^1}{8\ell} (d_1 + \ell^2 \nabla d_1 \cdot \nabla d_1) + \frac{3g_c^2}{8\ell} (d_2 + \ell^2 \nabla d_2 \cdot \nabla d_2), \quad (1.46)$$

where d_1 and d_2 are longitudinal damage and transverse damage, respectively. The symmetric damage-dependent elasticity matrix is defined for 2D case as:

$$\mathbf{C}(d_1, d_2) = \begin{bmatrix} (1-d_1)^2 \mathbf{C}_{11} & (1-d_1)(1-d_2) \mathbf{C}_{12} & 0 \\ (1-d_1)(1-d_2) \mathbf{C}_{12} & (1-d_2)^2 \mathbf{C}_{22} & 0 \\ 0 & 0 & (1-d_1)(1-d_2) \mathbf{C}_{66} \end{bmatrix}, \quad (1.47)$$

where (1.47) is given by an empirical manner, thus this model can not accurately represent all the complex constitutive behaviors of such materials but rather to capture specific features of crack propagation in anisotropic materials in terms of elastic and/or fracture properties.

1.2.3 Topology optimization for fracture resistance

Recently, Topology Optimization (TO) has been applied to enhance the mechanical resistance of structures and materials subjected to damage and cracking.

One pioneering work combining TO and fracture mechanics can be traced back to Challis et al. [43], where the level-set TO method has been used to maximize fracture resistance of structures, defined here as the elastic energy released by the crack that are in tension and was calculated using the virtual crack extension. J-integral calculation was employed and crack propagation within the structure was not taken into account. Another related technique can be found in [74], where pre-defined cracks were inserted and TO used to minimize the J-integral as a fracture criterion.

An important progress was made by optimizing the topology while taking into account the incremental damage response of the structure during a full load, from initiation to damaged/cracked structures. A first series of works have been proposed where damage mechanics was considered during the TO problem. In [15, 14], Amir and Sigmund used a gradient enhanced model to define the truss topology and optimal cross sections of reinforcement bars, and where the external work was maximized as an evaluation of the fracture energy. In [77], Kato and Ramm investigated optimal placement and shape of reinforcement in composites with respect to damage criterion to optimize the structural ductility during a full incremental procedure. In [67], Hilchenbach and Ramm optimized the position and shapes of stiff inclusions during the nonlinear loading of a structure. Even though not implying TO, the work shares similarities with the procedures developed in TO in this context. In [70], James and Waisman developed TO within a nonlocal damage framework using SIMP (Solid Isotropic Material with Penalization) where TO was performed with respect to a maximum damage criterion during the whole nonlinear load of a structure while minimizing the quantity of material within the structure as an objective. In [99], Liu et al. investigated TO with respect to damage induced by debonding at the interfaces between two materials in a structure during an incremental loading with Level-set TO and XFEM description of interfaces location. In [90–92], Li et al. proposed SIMP TO using an elastoplastic-damage model where TO was performed to find the optimal structural topologies with high energy absorption capacity while constraining the damage indicator.

An important recent step was to include brittle fracture propagation [173, 154] within TO. In [191] Zhang et al. used TO with XFEM and took into account full crack propagation to optimize several indicators such as tensile stress during loading of a structure. One issue with XFEM as a crack propagation simulation tool is its complexity in 3D and its inability to initiate the cracks, as well as handling multiple, complex crack networks which may connect and merge during the process. The development of the variational approach to fracture

[57, 35, 108, 112, 29, 11, 129, 126, 192], also called phase field method in the literature, offers several advantages in the context of crack propagation simulation, like: the possibility to initiate cracks from undamaged configurations; the possibility to handle arbitrary crack networks (including branching, merging, in both 2D and 3D) without specific treatment and use of classical finite elements; a variational framework allowing to include many models or mechanisms, and a mesh-independence due to an appropriate regularization process. This point is of special interest in TO approach where the use of a fixed mesh is required.

In [153], San and Waisman combined phase field and genetic algorithms to find the optimal location of particles in order to maximize indicators such as the peak force, maximum deformation at failure point and maximum fracture energy during an incremental procedure. The first works to our knowledge combining phase field and TO was introduced in Xia et al. and Da et al. in [176, 49], where the BESO TO [69] was used to optimize the fracture resistance of two-phase structures with respect to inclusions shapes, including cracks in both bulk and interfaces. In [148, 149], Russ and Waisman developed a SIMP TO combined with phase field to optimize the fracture energy in one-phase material structures, and Wu et al. [172] developed a Level-Set TO-phase field approach to optimize the fracture resistance of composites.

1.2.4 Fracture in image-based microstructures

X-ray computed tomography (XRCT) is a nondestructive characterization technique which provides images of the bulk of the materials. The benefits of 3D maps with high spatial resolution to characterize internal structures led to a rapid adaptation of this technique to many fields including materials science (e.g. investigation of the pore geometry, water flow and water distribution at the microscopic scale in porous media [58, 60, 78, 87]), in particular for the study of damage phenomena (e.g. brittle fracture [129, 126, 183] and ductile fracture [155, 41]).

Because X-ray tomography is a non-destructive technique, many scans of the same sample can be made under different conditions. As a consequence, a wide variety of mechanical tests have been coupled with X-ray tomography characterization [165]. In order to investigate the evolutions of a material under mechanical load, three popular procedures can be considered, as follows:

- **Post-mortem characterization:** This procedure consists in performing the same test on many specimens and stopping these test at different stages to follow evolution of the material. It assumes that the material does not change from one specimen to another.

- Ex-situ characterization: A unique specimen is tested up to a given level of deformation. It is thereafter unloaded and imaged. It is then mounted again on the testing device, loaded up to a next deformation level, unmounted and imaged again. This procedure assumes that the unloading process and interruption of the deformation do not influence the test.
- In-situ characterization: This procedure is similar to ex-situ, but the sample is here loaded in a device, which is placed on the X-ray beam. Thus during scanning, the state of sample is kept constant (deformation is stopped and maintained constant). This procedure can prevent the influence of unloading process, e.g. the closure of crack, which might be observed in ex-situ.

The combination of XRCT with the above testing procedure has been applied to study damage phenomena in many works. Babout in [19] introduced the detection of damage initiation in metallic materials. This technique was used to examine damage in civil engineering materials [83, 84, 101], which were observed under mechanical loading. Crack evolutions under fatigue loading conditions, including closure phenomena, have also been studied by XRCT combined with in-situ fatigue testing, e.g. in [162, 96, 97]. XRCT is particularly interesting when most of the damage development occurs within the bulk of the studied material (e.g., nucleation, growth and coalescence of damage in 3D experiments). Many techniques have been developed in literature to characterize quantitatively damage. Among these techniques, Digital Volume Correlation (DVC) is more and more used. By measuring the displacement field, this technique is used to evaluate crack crack closure and crack propagation [96]. It can also be used to extract fracture parameters, e.g. stress intensity factors [146] and energy release rates [103]. Calibration of elastoplastic parameters and choice of boundary conditions via DVC analyses for the simulation of ductile damage have been reported in [155, 41].

To date, the simulation of cracking phenomena in strongly heterogeneous materials, especially in elastoplastic polymer composites with realistic microstructures is still a very challenging problem. In this work, crack propagation in elastoplastic polymer composite microstructures, which are obtained by segmenting XRCT images of real materials, is investigated for the first time by means of an elastoplastic phase field model.

1.3 Outline of the thesis

The content of this thesis is organized as follow:

In Chapter 2, we first review the elastoplastic brittle phase field method developed in [53, 9] and then extend this method to model interactions between interfacial damage and brittle fracture in elastoplastic composites. In Chapter 3, we extend our previous BESO framework [176] to a combined SIMP and phase field for maximizing the fracture resistance of two-phase quasi-brittle materials. In Chapter 4, we introduce a topology optimization framework for maximizing the fracture resistance of elastoplastic ductile composites, where interfacial damage is taken into account through a regularized description of interfaces. In Chapter 5, we propose a phase field anisotropic damage model able to describe the behavior of polymer structures obtained by 3D printing processes, and which are formed by a layered structure. In Chapter 6, crack propagation in elastoplastic polymer composite microstructures, which are obtained by segmenting XRCT images of real materials, is investigated for the first time with the model in Chapter 2. Finally, conclusions and perspectives are drawn in Chapter 7.

Chapter 2

Phase field modeling elastoplastic brittle fracture

The main content of this chapter has been adapted from our published paper [94].

2.1 Introduction

In this chapter, we first review the elastoplastic brittle phase field method developed in [53, 9] in Section 2.2. An efficient and robust staggered scheme is adopted by decoupling the fracturing phase field and displacement field. With this numerical scheme, a three-dimensional phase field model to simulate crack initiation and propagation in elastoplastic brittle solids is implemented. Several comparisons with available experimental results are proposed to validate this method.

In Section 2.3, we extend the elastoplastic brittle phase field method proposed in Section 2.2 to model interactions between interfacial damage and brittle fracture in elastoplastic composites. We follow the framework developed in [130, 121] to interfacial damage in composites. To introduce interfacial damage between inclusions and the matrix, a strain density function depending on the jump due to decohesion is added to the total energy. To maintain the regularized character of the approximation, smooth indicator functions are used to weight the different terms in the energy with respect to the vicinity of interfaces. Then, the different problems (mechanical and phase field problems) are derived and an algorithmic procedure is described. The performance of the proposed framework is demonstrated using several numerical examples.

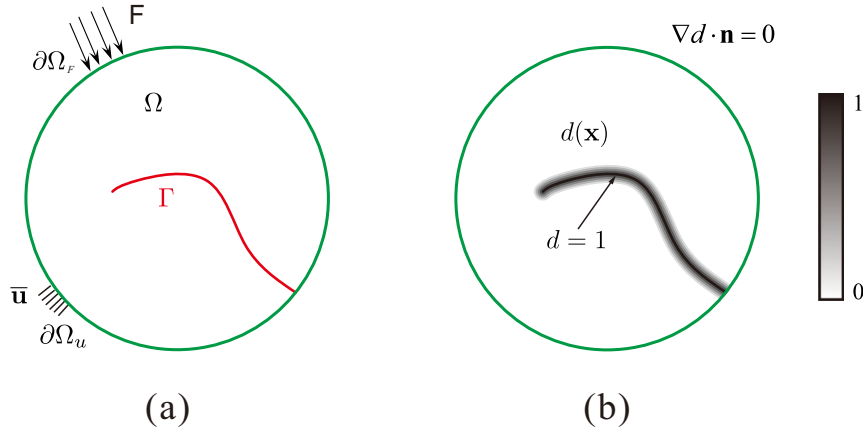


Fig. 2.1 Phase field approximation of a sharp crack discontinuity. (a) A sharp crack surface Γ embedded into the solid Ω . (b) The regularized representation of the crack by the phase field $d(\mathbf{x})$.

2.2 Phase field modeling elastoplastic brittle fracture in homogeneous materials

This section is organized as follows. In Section 2.2.1 and 2.2.2, we briefly review the elastoplastic brittle phase field method developed in [53, 9]. Section 2.2.3 provides FEM discretization and numerical implementation. Finally, numerical examples and applications are presented in Section 2.2.4.

2.2.1 Phase field approximation of crack

Let $\Omega \subset \mathbb{R}^D$ be an open domain with $D = 2, 3$, describing a cracked solid as depicted in Fig. 2.1. The external boundary of Ω is denoted by $\partial\Omega \in \mathbb{R}^{D-1}$. Cracks which may propagate within the solid are collectively denoted by Γ . In this work, we adopt the framework proposed in [112, 108, 111, 12] for a regularized representation of discontinuities. In this regularized framework, the crack is approximately represented by a scalar phase field $0 \leq d(\mathbf{x}, t) \leq 1$ (see Fig. 2.1(b)), such that when $d = 0$ the material is undamaged, and when $d = 1$ the material is fully broken.

The scalar phase field $d(\mathbf{x}, t)$ can be determined through solving the following boundary value problem subjected to Dirichlet boundary conditions $d = 1$ on the crack (see [108] for

more details):

$$\begin{cases} d(\mathbf{x}, t) - \ell_d^2 \Delta d(\mathbf{x}, t) = 0 & \text{in } \Omega, \\ d(\mathbf{x}, t) = 1 & \text{on } \Gamma, \\ \nabla d(\mathbf{x}, t) \cdot \mathbf{n} = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.1)$$

where $\Delta(\cdot)$ and $\nabla(\cdot)$ are the Laplacian and gradient operator respectively, ℓ_d is a length scale parameter that governs the width of the regularization zone and gives for $\ell_d \rightarrow 0$ the exact sharp crack in Fig. 2.1(a), and $\mathbf{n}$ the outward normal on $\partial\Omega$. It can be shown that (2.1) is the Euler-Lagrange equation associated with the variational problem:

$$d = \text{Arg} \left\{ \inf_{d \in S_d} \Gamma^d(d) \right\}, \quad \Gamma^d(d) = \int_{\Omega} \gamma_d(d) d\Omega, \quad S_d = \{d \mid d(\mathbf{x}) = 1, \forall \mathbf{x} \in \Gamma\}, \quad (2.2)$$

where $\Gamma^d(d)$ represents the total length of the crack in 2D and the total crack surface area in 3D, and $\gamma_d(d)$ is the crack surface density function per unit volume defined by:

$$\gamma_d(d) = \frac{d^2}{2\ell_d} + \frac{\ell_d}{2} \nabla d \cdot \nabla d, \quad (2.3)$$

where the second term in $\gamma_d(d)$ penalizes high values of $\nabla d(\mathbf{x})$ and where d varies between 0 and 1. Note that in the absence of the second right-hand term in (2.3), a local damage model is found, with well-known related non-convergence issues with respect to the mesh discretization.

It must be noted that, ℓ_d does not represent physically the exact crack width, but a parameter which is used to regularize the discontinuities. It has been shown that this parameter can be treated as a material parameter related to the Young's modulus, the tensile strength, and the critical energy release rate of the material in [128, 16, 190]. In our previous work [126], an inverse approach was developed to identify this parameter, by combining simulations and experiments.

2.2.2 Review of the elastoplastic brittle phase field method

In this section, we briefly review the elastoplastic brittle phase field method using the variational framework for fracture as introduced in [6, 145].

First, we introduce the total strain as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad (2.4)$$

where ε^e and ε^p are the elastic strain and plastic strain, respectively. The plastic incompressibility is assumed, i.e. $\text{Tr}(\varepsilon^p) = 0$, $\text{Tr}(\cdot)$ being the trace operator. The cumulated plastic strain is defined as:

$$\dot{p} = \sqrt{\frac{2}{3}} \|\dot{\varepsilon}^p\| \quad (2.5)$$

where $(\dot{\cdot})$ denotes time derivative. In the following, we introduce the deviatoric parts of the stress and of the elastic strain tensors as $\mathbf{s} = \text{dev}(\boldsymbol{\sigma})$ and $\mathbf{e}^e = \text{dev}(\varepsilon^e)$, respectively, with $\text{dev}(\cdot) = (\cdot) - \frac{1}{3}\text{Tr}(\cdot)\mathbf{1}$, $\mathbf{1}$ being the first-order identity operator. Finally, we define the directional derivative as:

$$D_{\mathbf{v}}f(\mathbf{u}) = \left[\frac{d}{dh}f(\mathbf{u} + h\mathbf{v}) \right]_{h=0}. \quad (2.6)$$

The damage variable d is introduced to penalize the stiffness of the material.

2.2.2.1 Total energy

Let us consider a solid whose phase is elasto-plastic with possible damage. Small strains are assumed. In the present regularized framework, the total energy of the solid is defined by

$$W(\mathbf{u}, p, d) = \int_{\Omega} [\psi^e(\varepsilon(\mathbf{u}), p, d) + \psi^p(p) + \psi^d(d)] d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\Omega, \quad (2.7)$$

where ψ^e , ψ^p and ψ^d denote the elastic strain density function, the plastic and damage dissipative potentials, respectively. Above, $\mathbf{f}$ and $\mathbf{F}$ are body forces and prescribed traction over the boundary $\partial\Omega_F$, respectively. Note that the total energy is a function of 3 state variables $\mathbf{u}$, p and d .

2.2.2.2 Variational framework

We follow the framework presented in [6] to construct the variational principle, which involves: irreversibility condition, stability condition and energy balance. In this framework, stability condition provides mechanical balance equation, damage and plastic criteria. The energy balance provides damage consistency and plastic flow rule.

Irreversibility condition

The irreversibility condition is imposed on the damage variable to disallow material regeneration. It can be expressed as

$$\dot{d} \geq 0, \quad 0 \leq d \leq 1. \quad (2.8)$$

In the present work, the irreversibility condition is implemented by using an appropriate history function [108].

First-order stability condition

The first order stability condition (see [113, 114, 143]) is expressed by:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d) + D_{\delta p} W(\mathbf{u}, p, d) + D_{\delta d} W(\mathbf{u}, p, d) \geq 0. \quad (2.9)$$

Applied to (2.7), it yields:

$$\begin{aligned} & \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} + \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega + \\ & \int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega \geq 0 \end{aligned} \quad (2.10)$$

where

$$\boldsymbol{\sigma} = \frac{\partial \psi^e}{\partial \boldsymbol{\varepsilon}^e} \quad (2.11)$$

and $\hat{\mathbf{n}}$ is a unit tensor in the direction of the plastic flow. From (2.4):

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p \quad (2.12)$$

and then:

$$D_{\delta \mathbf{u}} \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) = \boldsymbol{\varepsilon}(\delta \mathbf{u}). \quad (2.13)$$

The following results stem out:

- For $\delta p = \delta d = 0$ we obtain:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (2.14)$$

which is the weak form of the equilibrium equation.

- For $\delta d = 0$ and $\delta \mathbf{u} = \mathbf{0}$:

$$\int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} + \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega \geq 0. \quad (2.15)$$

For J_2 -plasticity, this expression leads to

$$\int_{\Omega} \left(\sqrt{\frac{3}{2}} \|\mathbf{s}\| - \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega \leq 0, \quad (2.16)$$

which is the weak form of the plasticity yield criterion. The local form of the plastic yield criterion can be expressed as

$$F^p(p) = \sqrt{\frac{3}{2}} \|\mathbf{s}\| - \frac{\partial \psi^p}{\partial p} \leq 0 \text{ in } \Omega \quad (2.17)$$

which is the classical von Mises yield criterion.

- For $\delta p = 0$ and $\delta \mathbf{u} = \mathbf{0}$:

$$\int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega \geq 0 \quad (2.18)$$

which is the weak form of the damage criterion. In local form, it can be expressed as:

$$F^d(d) = - \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \leq 0 \text{ in } \Omega. \quad (2.19)$$

Energy balance

The energy balance represents the need for the total energy to remain constant as the state variables evolve. Following a procedure analogous to the treatment of the stability condition, this condition leads to

$$\begin{aligned} \int_{\Omega} \left[-\boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\dot{\mathbf{u}}) + \left(\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} - \frac{\partial \psi^p}{\partial p} \right) \dot{p} - \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \dot{d} \right] d\Omega \\ + \int_{\partial\Omega_F} \mathbf{F} \cdot \dot{\mathbf{u}} dS + \int_{\Omega} \mathbf{f} \cdot \dot{\mathbf{u}} d\Omega = 0. \end{aligned} \quad (2.20)$$

The following cases are analyzed:

- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{d} = 0$, and using (2.17), the plasticity consistency condition is obtained:

$$F^p(p) \dot{p} = 0. \quad (2.21)$$

- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{p} = 0$, and using (2.19), the damage consistency condition is obtained:

$$F^d(d) \dot{d} = 0. \quad (2.22)$$

Alternate minimization

In this section, a staggered alternate minimization algorithm is applied, which naturally stems out from the energetic principles. This procedure takes advantage of the fact that

although the global energy is non-convex, it is convex with respect to $\mathbf{u}$, p and d individually [2]. With the total energy (2.7) at hand, the alternate minimization follows.

- Minimization with respect to the displacement field:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d) = 0 \quad (2.23)$$

leads to

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (2.24)$$

which corresponds to the weak form of the mechanical problem to be solved for $\mathbf{u}$, given d .

- Minimization with respect to the equivalent plastic strain:

$$D_{\delta p} W(\mathbf{u}, p, d) = \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} + \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega = 0 \quad (2.25)$$

which is the weak form of the plastic yield criterion (2.15) which has to be satisfied for $\dot{p} \geq 0$. In the present work, this condition is handled by a return-mapping algorithm (see [159]). In [145] a regularization term was introduced in the total energy and the above equation was verified through solving a global problem for p . Here we do not adopt this approach and treat this criterion as a local one (at Gauss integration points). Eqs. (2.24) and (2.25) are solved together using the return-mapping algorithm (see Algorithm 1).

- Minimization with respect to the damage field:

$$D_{\delta d} W(\mathbf{u}, p, d) = \int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega = 0, \quad (2.26)$$

which corresponds to the global problem to be solved to find the field $d(\mathbf{x})$ (phase field problem), given $\mathbf{u}$ and p . Note that if ψ^d does not include the gradient of damage ∇d , then (2.26) leads to a local relationship to define the damage evolution, leading to well-known issues like non-convergence with respect to the mesh size, or dependence of the crack paths to the mesh structure and orientation.

2.2.2.3 Specialization

We now specialize the energy components introduced in (2.7). From [9], we define the different strain density functions as follows:

$$\psi^e(\mathbf{u}, d) = g(d) \psi_0^{e+}(\boldsymbol{\varepsilon}^e(\mathbf{u})) + \psi_0^{e-}(\boldsymbol{\varepsilon}^e(\mathbf{u})), \quad (2.27)$$

with [16]

$$\psi_0^{e+}(\boldsymbol{\varepsilon}^e) = \frac{1}{2} \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_+^2 + \mu \mathbf{e}^e : \mathbf{e}^e, \quad (2.28)$$

$$\psi_0^{e-}(\boldsymbol{\varepsilon}^e) = \frac{1}{2} \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_-^2. \quad (2.29)$$

Above, κ and μ denote bulk modulus and shear modulus, respectively, $\langle x \rangle_{\pm} = \frac{1}{2} (x \pm |x|)$.

$$g(d) = (1 - d)^2 + k, \quad (2.30)$$

where k is a small numerical parameter to prevent loss of definite posedness of the elastic tensor in case of full damage,

$$\psi^p(p) = \sigma_Y p + \frac{1}{2} H p^2, \quad (2.31)$$

$$\psi^d(\beta, d) = g_c \left(\frac{d^2}{2\ell_d} + \frac{\ell_d}{2} \nabla d \cdot \nabla d \right). \quad (2.32)$$

In (2.31), σ_Y and H are yield stress and hardening modulus, respectively. In (2.32), g_c is the fracture toughness.

Using the aforementioned constitutive specialization results, we can re-write (2.11), (2.17) and (2.5) as:

$$\boldsymbol{\sigma} = g(d) \boldsymbol{\sigma}_{\text{eff}}^+ + \boldsymbol{\sigma}_{\text{eff}}^-, \quad (2.33)$$

$$F^p(p) = \sqrt{\frac{3}{2}} \|\mathbf{s}\| - (\sigma_Y + H p) \leq 0, \quad (2.34)$$

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\|\mathbf{s}\|} \text{ with } \dot{p} \geq 0 \quad (2.35)$$

where $\boldsymbol{\sigma}_{\text{eff}}^+$ and $\boldsymbol{\sigma}_{\text{eff}}^-$ are the effective tensile and compressive stresses defined as

$$\boldsymbol{\sigma}_{\text{eff}}^+ = \frac{\partial \psi_0^{e+}}{\partial \boldsymbol{\varepsilon}^e} = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_+ \mathbf{1} + 2\mu \mathbf{e}^e, \quad \boldsymbol{\sigma}_{\text{eff}}^- = \frac{\partial \psi_0^{e-}}{\partial \boldsymbol{\varepsilon}^e} = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_- \mathbf{1}. \quad (2.36)$$

The associated Euler-Lagrange equations to (2.24) are given by:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} & \text{in } \Omega, \\ \mathbf{u} = \bar{\mathbf{u}} & \text{on } \partial\Omega_u, \\ \boldsymbol{\sigma} \mathbf{n} = \mathbf{F} & \text{on } \partial\Omega_F. \end{cases} \quad (2.37)$$

Using (2.26) and the property:

$$(\Delta d) \delta d = \nabla \cdot (\nabla d \delta d) - \nabla d \cdot \nabla (\delta d) \quad (2.38)$$

as well as the divergence theorem and $\nabla d \cdot \mathbf{n} = 0$, we obtain the weak form of the phase field problem as:

$$\int_{\Omega} \left(\left\{ -2(1-d) \psi_0^{e+} + \frac{g_c d}{\ell_d} \right\} \delta d + g_c \ell_d \nabla d \cdot \nabla (\delta d) \right) d\Omega = 0. \quad (2.39)$$

To prescribe irreversibility, we employ the strain history functional introduced in [108]:

$$\mathcal{H}(\boldsymbol{\varepsilon}^e) = \max_{s \in [0, t]} \psi_0^{e+}(\boldsymbol{\varepsilon}^e, s). \quad (2.40)$$

Then, the corresponding Euler-Lagrange equations to (2.39) are given by:

$$\begin{cases} \frac{g_c}{\ell_d} (d - \ell_d^2 \Delta d) = 2(1-d) \mathcal{H}(\boldsymbol{\varepsilon}^e) \\ \nabla d \cdot \mathbf{n} = 0 & \text{on } \partial\Omega, \\ d = 1 & \text{on } \Gamma. \end{cases} \quad (2.41)$$

The different equations of the model are summarized in Table 2.1. The weak forms of the problems to be solved alternatively are summarized in Table 2.2.

Table 2.1 Governing equations of the elastoplastic brittle phase field model.

Irreversibility	$\dot{d} \geq 0, \quad 0 \leq d \leq 1$
Mechanical balance	$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} \text{ in } \Omega$ $\mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial\Omega_u, \quad \boldsymbol{\sigma} \mathbf{n} = \mathbf{F} \text{ on } \partial\Omega_F$
Constitutive law	$\boldsymbol{\sigma} = g(d) \boldsymbol{\sigma}_{\text{eff}}^+ + \boldsymbol{\sigma}_{\text{eff}}^-$ $\boldsymbol{\sigma}_{\text{eff}}^+ = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_+ \mathbf{1} + 2\mu \mathbf{e}^e, \quad \boldsymbol{\sigma}_{\text{eff}}^- = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_- \mathbf{1}$
Damage criterion	$\frac{g_c}{\ell_d} (d - \ell_d^2 \Delta d) - 2(1-d) \mathcal{H}(\boldsymbol{\varepsilon}^e) \geq 0$ $\mathcal{H}(\boldsymbol{\varepsilon}^e) = \max_{s \in [0, t]} \psi_0^{e+}(\boldsymbol{\varepsilon}^e, s)$
Damage consistency	$\left(\frac{g_c}{\ell_d} (d - \ell_d^2 \Delta d) - 2(1-d) \mathcal{H}(\boldsymbol{\varepsilon}^e) \right) \dot{d} = 0$
Plastic yield criterion	$F^p(p) = \sqrt{\frac{3}{2}} \ \mathbf{s}\ - (\sigma_Y + Hp) \leq 0,$
Plastic flow rule	$\dot{\boldsymbol{\varepsilon}}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\ \mathbf{s}\ } \text{ with } \dot{p} \geq 0$

Table 2.2 Problems to be solved in the staggered procedure

Mechanical problem: given d , solve for $\mathbf{u}$:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0$$

$$F^p(p) = \sqrt{\frac{3}{2}} \|\mathbf{s}\| - (\sigma_Y + Hp) \leq 0$$

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\|\mathbf{s}\|} \text{ with } \dot{p} \geq 0$$

Phase Field problem: given $\mathbf{u}$, solve for d :

$$\int_{\Omega} \left[\left(2\mathcal{H}(\mathbf{u}) + \frac{g_c}{\ell_d} \right) d \delta d + g_c \ell_d \nabla d \cdot \nabla(\delta d) \right] d\Omega = \int_{\Omega} 2\mathcal{H}(\mathbf{u}) \delta d d\Omega.$$

2.2.3 Discretization and numerical implementation

In this section, we detail the weak forms and FEM discretizations for displacement and damage problems, and finally provide the different algorithms.

2.2.3.1 Weak forms the linearized mechanical problem

We can re-write the associated weak form for the displacement problem (2.24) as:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\boldsymbol{\delta u}) d\Omega = \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\delta u} d\Omega + \int_{\partial\Omega_F} \mathbf{F} \cdot \boldsymbol{\delta u} dS, \quad (2.42)$$

where $\boldsymbol{\sigma}$ is given in (2.33). We can rewrite the balance equation (2.42) as

$$\mathbf{R} = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\boldsymbol{\delta u}) d\Omega - \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\delta u} d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \boldsymbol{\delta u} dS = 0. \quad (2.43)$$

In a standard Newton method, the displacements are updated for each loading increment by solving the tangent problem:

$$D_{\Delta u} \mathbf{R}(\mathbf{u}^{(k)}, d) = -\mathbf{R}(\mathbf{u}^{(k)}, d) = 0, \quad (2.44)$$

where $\mathbf{u}^{(k)}$ is the displacement solution known from the previous iteration. The displacement corrections are obtained as

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta \mathbf{u}. \quad (2.45)$$

In (2.44),

$$D_{\Delta u} \mathbf{R}(\mathbf{u}^{(k)}) = \int_{\Omega} \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}^e} : \boldsymbol{\varepsilon}^e(\Delta \boldsymbol{\varepsilon}) : \boldsymbol{\varepsilon}^e(\boldsymbol{\delta \varepsilon}) d\Omega, \quad (2.46)$$

with

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}^e} = \mathbb{C}_s(\mathbf{u}, d). \quad (2.47)$$

Using (2.41), we can re-write the associated weak form for the damage problem (2.26) as:

$$\int_{\Omega} \left[\left(2\mathcal{H} + \frac{g_c}{\ell_d} \right) d \delta d + g_c \ell_d \nabla d \cdot \nabla(\delta d) \right] d\Omega = \int_{\Omega} 2\mathcal{H} \delta d d\Omega. \quad (2.48)$$

2.2.3.2 Discretization of the displacement problem

In this work, for the sake of clarity, only 2D FEM discretization is detailed. The vector form of second-order tensors are introduced as $[\boldsymbol{\varepsilon}] = [\varepsilon_{11}, \varepsilon_{22}, \sqrt{2}\varepsilon_{12}]^T$, $[\boldsymbol{\sigma}] = [\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12}]^T$, as well as the FEM approximations $\mathbf{u} = \mathbf{N}_u \mathbf{u}^e$, $\boldsymbol{\delta u} = \mathbf{N}_u \boldsymbol{\delta u}^e$, and $\Delta \mathbf{u} = \mathbf{N}_u \Delta \mathbf{u}^e$ where $\mathbf{u}^e$, $\boldsymbol{\delta u}^e$, $\Delta \mathbf{u}^e$ and $\mathbf{N}_u$ are nodal displacement components in one element, nodal trial function components, nodal incremental displacement components and a matrix of displacement shape function, respectively. Then we obtain:

$$[\boldsymbol{\varepsilon}](\mathbf{u}) = \mathbf{B}_u \mathbf{u}^e, \quad [\boldsymbol{\varepsilon}^e](\Delta \mathbf{u}) = \mathbf{B}_u \Delta \mathbf{u}^e, \quad [\boldsymbol{\varepsilon}^e](\boldsymbol{\delta u}) = \mathbf{B}_u \boldsymbol{\delta u}^e, \quad (2.49)$$

where $\mathbf{B}_u$ is a matrix of displacement shape function derivatives.

After discretization, the linear system (2.44) with the displacement corrections (2.45) reduces to a standard Newton-type iteration:

$$\mathbf{K}_{\text{tan}} \Delta \mathbf{u} = -\mathbf{R}(\mathbf{u}^{(k)}), \mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta \mathbf{u}, \quad (2.50)$$

where $\mathbf{u}^{(k)}$ is the displacement field known from the previous (k -th) Newton-Raphson iteration,

$$\mathbf{K}_{\text{tan}} = \int_{\Omega} \mathbf{B}_u^T \mathbf{C}_s \mathbf{B}_u d\Omega, \quad (2.51)$$

and

$$\mathbf{R}(\mathbf{u}^{(k)}) = \int_{\Omega} \mathbf{B}_u^T \boldsymbol{\sigma}^{(k)} d\Omega - \int_{\Omega} \mathbf{N}_u^T \mathbf{f} d\Omega - \int_{\partial\Omega_F} \mathbf{N}_u^T \mathbf{F} dS, \quad (2.52)$$

and where $\mathbf{C}_s$ is the matrix form corresponding to the fourth-order elastoplastic consistent tangent operator $\mathbb{C}_s$ in (2.47), which is determined by the classical elastic predictor and plastic corrector (return-mapping) algorithm outlined in [51]. It should be noted that an accurate evaluation of the operator $\mathbb{C}_s$ is crucial to guarantee the convergence of the Newton-Raphson iterative solution scheme. The analytical form of $\mathbb{C}_s$ for a J_2 -plasticity yield function can be found in [8]. The iterative update (2.50) is performed until convergence is achieved in the sense $\|\Delta \mathbf{u}\| / \|\mathbf{u}^{(k+1)} - \mathbf{u}^{(0)}\| \leq \text{tol}$.

2.2.3.3 Discretization of the phase field problem

We solve alternatively the damage problem and then the mechanical problem within a staggered procedure [108]. The damage and damage gradient are approximated in one element by

$$d = \mathbf{N}_d \mathbf{d}^e, \quad \nabla d = \mathbf{B}_d \mathbf{d}^e, \quad (2.53)$$

where $\mathbf{N}_d$ and $\mathbf{B}_d$ are matrices of damage shape function and of damage shape function derivatives, respectively, and $\mathbf{d}^e$ denote nodal damage in one element.

The discretization of damage problem (2.48) results into the following discrete system of equations:

$$\mathbf{K}_d \mathbf{d} = \mathbf{F}_d \quad (2.54)$$

in which

$$\mathbf{K}_d = \int_{\Omega} \left[\left(2\mathcal{H} + \frac{g_c}{\ell_d} \right) \mathbf{N}_d^T \mathbf{N}_d + g_c \ell_d \mathbf{B}_d^T \mathbf{B}_d \right] d\Omega \quad (2.55)$$

and

$$\mathbf{F}_d = \int_{\Omega} 2\mathbf{N}_d^T \mathcal{H} d\Omega, \quad (2.56)$$

where $\mathcal{H}$ is given in (2.40).

2.2.3.4 Numerical implementation

In the present work, a staggered scheme is employed following [108], where at each load increment the displacement problem is solved for fixed damage field which is known from the previous time step. The damage problem is then solved with the new displacement field. The overall algorithm is illustrated in Algorithm 1. The flowchart for return-mapping algorithm on one Gauss point is provided in Algorithm 2.

Algorithm 1: Overall algorithm for elastoplastic brittle fracture model

Initialize $\mathbf{u}_0$, d_0 , $\boldsymbol{\varepsilon}_0^p$, and p_0 with assumption of not plasticised and undamaged state.

Loop over load increments n

for $i = 1, \dots, n$ **do**

Displacement problem

Newton-Raphson iterative solution scheme

$k = 1, err = 1, tol = 10^{-5}, \mathbf{u}_i^{(0)} = \mathbf{u}_{i-1}$

while $err > tol$ **do**

$\boldsymbol{\varepsilon} = \mathbf{B}_u \mathbf{u}_i^{(k-1)}$

Return-mapping algorithm

Given $(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_{i-1}^p, p_{i-1}, d_{i-1})$, Compute $(\mathbf{C}_s, \boldsymbol{\varepsilon}_i^{p,(k)}, p_i^{(k)})$ from Algorithm 2

Compute $\mathbf{K}_{tan}$ and $\mathbf{R}(\mathbf{u}_i^{(k-1)})$ from (2.51) and (2.52)

Compute $\Delta \mathbf{u}$ from (2.50)

Update $\mathbf{u}_i^{(k)} = \mathbf{u}_i^{(k-1)} + \Delta \mathbf{u}$

$\mathbf{u}_i = \mathbf{u}_i^{(k)}, \boldsymbol{\varepsilon}_i^p = \boldsymbol{\varepsilon}_i^{p,(k)}, p_i = p_i^{(k)}$

$err = \|\Delta \mathbf{u}\| / \|\mathbf{u}_i - \mathbf{u}_{i-1}\|, k = k + 1$

end

Damage problem

Compute $\mathcal{H}$ with $\mathbf{u}_i$ and $\boldsymbol{\varepsilon}_i^p$ from (2.40)

Compute $\mathbf{K}_d$ and $\mathbf{F}_d$ from (2.55) and (2.56)

Compute the damage field d_i from (2.54)

$i = i + 1$

end

2.2.4 Numerical examples and applications

In this section, all numerical computations are performed within the finite element framework and assuming plain strain conditions for 2D cases. Both damage and displacement fields are

discretized with 4-node quadrilateral elements for 2D cases and tetrahedron elements for 3D case.

Algorithm 2: Return-mapping algorithm

Input: $\varepsilon, \varepsilon_{i-1}^p, p_{i-1}, d_{i-1}$

Output: $\mathbf{C}_s, \varepsilon_i^{p,(k)}, p_i^{(k)}$

Elastic prediction

$$\varepsilon^{e \text{ trial}} = \varepsilon - \varepsilon_{i-1}^p$$

Compute σ^{trial} and $F^p(\sigma^{trial}, p_{i-1}, d_{i-1})$ from (2.33) and (2.34)

if $F^p \leq 0$ **then**

$$\varepsilon_i^{p,(k)} = \varepsilon_{i-1}^p, p_i^{(k)} = p_{i-1}$$

else

Plastic correction

Compute Δp from $F^p(\sigma, p_{i-1} + \Delta p, d_{i-1}) = 0$

$$\Delta \varepsilon^p = \Delta p \sqrt{\frac{3}{2}} \frac{\mathbf{s}^{trial}}{\|\mathbf{s}^{trial}\|}$$

Update the variables

$$\varepsilon_i^{p,(k)} = \varepsilon_{i-1}^p + \Delta \varepsilon^p$$

$$p_i^{(k)} = p_{i-1} + \Delta p$$

end

$$\varepsilon^e = \varepsilon - \varepsilon_i^{p,(k)}$$

Compute σ from (2.33)

Compute $\mathbf{C}_s$ with the analytical form in [8]

2.2.4.1 Asymmetrically notched specimen

In the first example, we validate the present numerical implementation introduced in section 2.2.3.4. For this purpose, an asymmetrically notched specimen introduced in [9], as described in Fig. 2.2(a), is considered. The lower end ($y = 0$) of the domain is blocked along x - and y - directions. On the upper end ($y = 50$), the displacement along x is fixed to zero, while y -displacement are prescribed to an increasing value of u with $\Delta u = 0.002$ mm during the simulation. The spatial discretization of the model comprises 23277 4-node quadrilateral elements, with refinement in the central region where the crack is expected to propagate (see Fig. 2.2(b)). The material parameters from [9] are: $\kappa = 27.28$ GPa, $\mu = 71.66$ GPa, $\sigma_Y = 0.345$ GPa, $H = 0.25$ GPa and $g_c = 9.31$ N/mm. The length scale parameter is chosen as $\ell_d = 0.2$ mm.

The evolution of the crack phase field and the equivalent plastic strain field are shown in Fig. 2.3(a) and (b), the final results from [9] are presented in 2.3(c). Fig. 2.4 shows

the load-displacement curve. As can be observed from Fig. 2.4, our results have a good agreement with the reference results.

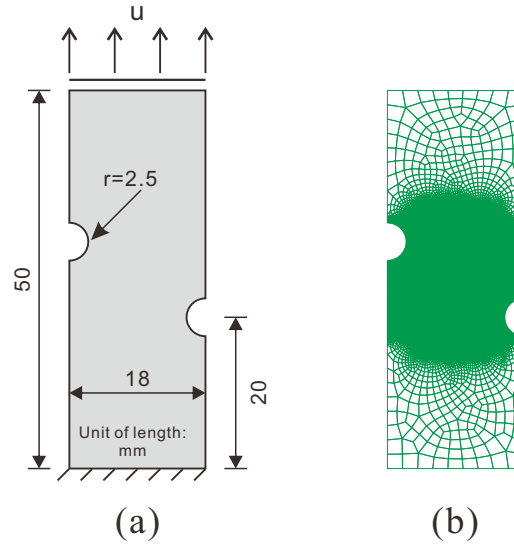


Fig. 2.2 Asymmetrically notched specimen: (a) geometry and boundary conditions; (b) finite element model.

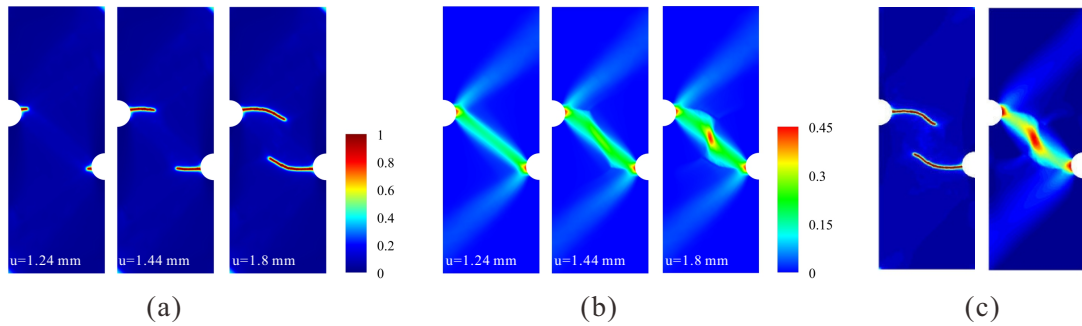


Fig. 2.3 Asymmetrically notched specimen: (a) elastoplastic brittle crack fields; (b) equivalent plastic strains; (c) reference [9].

2.2.4.2 Three-point bending test

In this example, three-point bending test is conducted and compared with available experimental results in [142]. The geometry and boundary conditions are illustrated in Fig. 2.5(a). The finite element model with a refinement in the central region where the crack is expected to propagate is shown in Fig. 2.5(b), where 11163 4-node quadrilateral elements are used.

Young's modulus is $E = 48.3$ GPa as reported in [142], and Poisson's ratio is assumed to be $\nu = 0.2$.

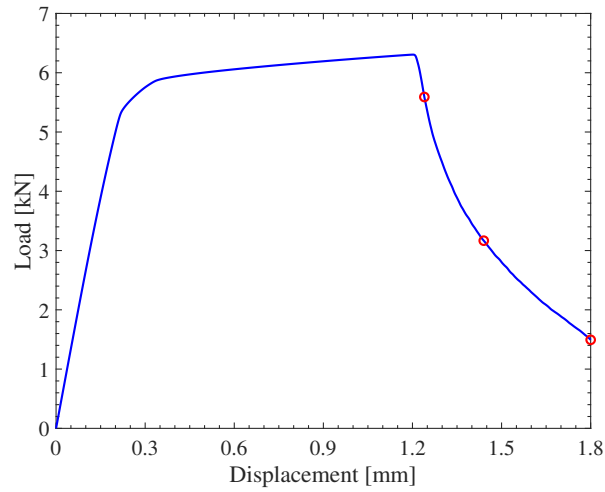


Fig. 2.4 Asymmetrically notched specimen. Load-displacement curve.

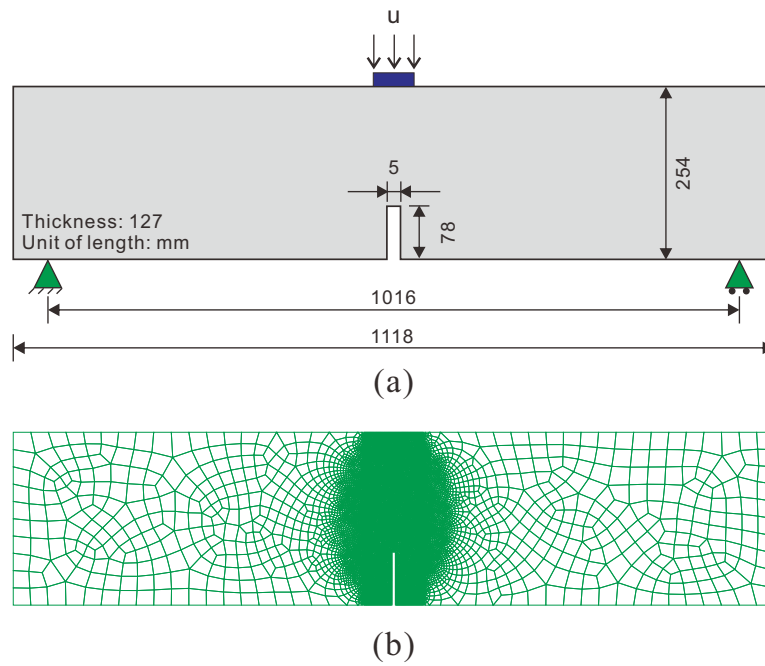


Fig. 2.5 Three-point bending test: (a) geometry and boundary conditions; (b) finite element model.

Elastic brittle fracture

In a first test, we try simulating the available experimental results with the elastic brittle fracture model. For this purpose, two simulations are performed: in the first one $g_c = 0.029$ N/mm and $\ell_d = 13$ mm, in the second one $g_c = 0.045$ N/mm and $\ell_d = 20$ mm. External loading is applied by displacement control through a series of load increments with a fixed step value $\Delta u = 0.001$ mm. Fig. 2.6 shows the comparison of load-displacement curves for the two simulations and the experimental data. As can be observed from this figure, the peak load in the first simulation with $g_c = 0.029$ N/mm and $\ell_d = 13$ mm shows a better agreement with the experimental data, and the second simulation with $g_c = 0.045$ N/mm and $\ell_d = 20$ mm has better performance after the peak load. However, the simulated reaction forces both drop much faster than the experimental data after reaching the peak load. These deviations on one aspect stem from the fact that a linear fracture model is used in the simulation whereas the real fracture is nonlinear; the model neglects any plastic deformation. The evolution of the crack phase fields for these two simulations are shown in Fig. 2.7.

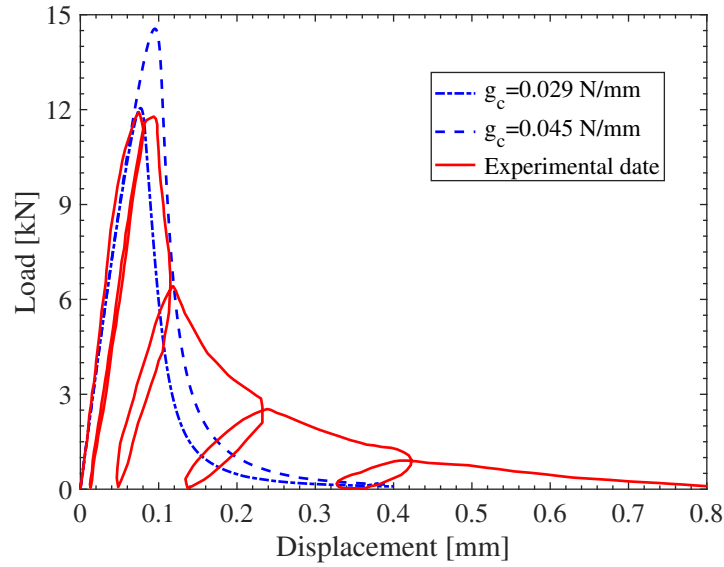


Fig. 2.6 Load-displacement curves of elastic brittle fracture for two value of g_c .

Fig. 2.8 shows the load-displacement curves for cyclic loading case and non cyclic loading case, here $g_c = 0.045$ N/mm and $\ell_d = 20$ mm are used. In this figure, we can observe that no residual deformation is maintained in the simulation after unloading which is typical when using phase field models for elastic brittle fracture [10, 108], whereas residual deformation is observed at the end of each unloading in the experimental data. This disparity is mainly caused by the fact that we do not consider other dissipated process, e.g. plastic

deformation. Thus, in the next test we use the model introduced in this section to take into account the plastic deformation process.

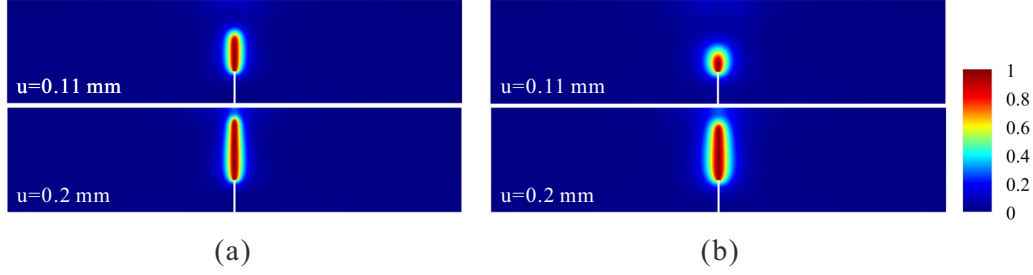


Fig. 2.7 Elastic brittle crack fields for (a) $g_c = 0.029$ N/mm; (b) $g_c = 0.045$ N/mm.

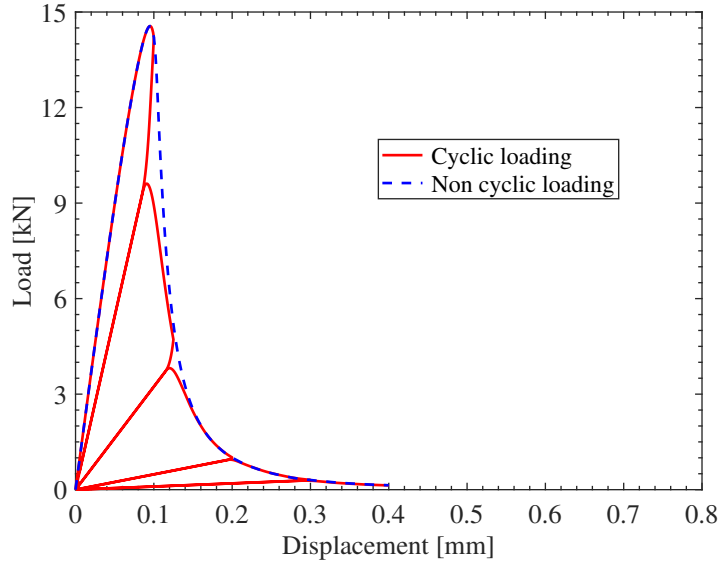


Fig. 2.8 Load-displacement curves of elastic brittle fracture with cyclic loading and non cyclic loading.

Elastoplastic brittle fracture

In this test, we try simulating the available experimental results with the elastoplastic brittle fracture model. The material parameters are: $\sigma_Y = 2.5$ MPa, $H = 2$ MPa and $g_c = 0.045$ N/mm. The length scale parameter is chosen as $\ell_d = 20$ mm. External loading increment value is $\Delta u = 1 \times 10^{-4}$ mm. Fig. 2.9 shows the comparison of simulated curves and the experimental data. It is observed that, after several unloading processes, there are obvious plastic deformations in the simulated curve with elastoplastic brittle fracture model. Compared to the simulated curve with elastic brittle fracture model,

with elastoplastic brittle fracture model can reproduce satisfactorily the experimental curve, especially the cyclic loading/unloading response. Fig. 2.10 shows the evolution of the crack phase field and the equivalent plastic strain field. As can be observed from this figure, the equivalent plastic strain mainly occurs at the tip of the initial crack.

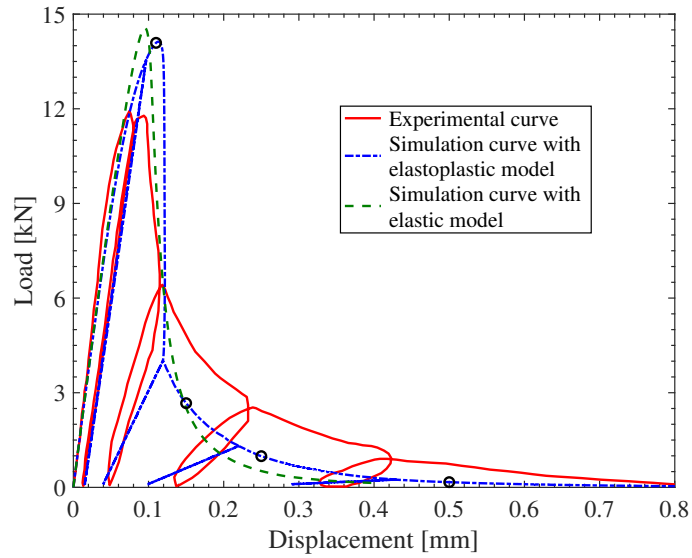


Fig. 2.9 Load-displacement curve of elastoplastic brittle fracture with cyclic loading.

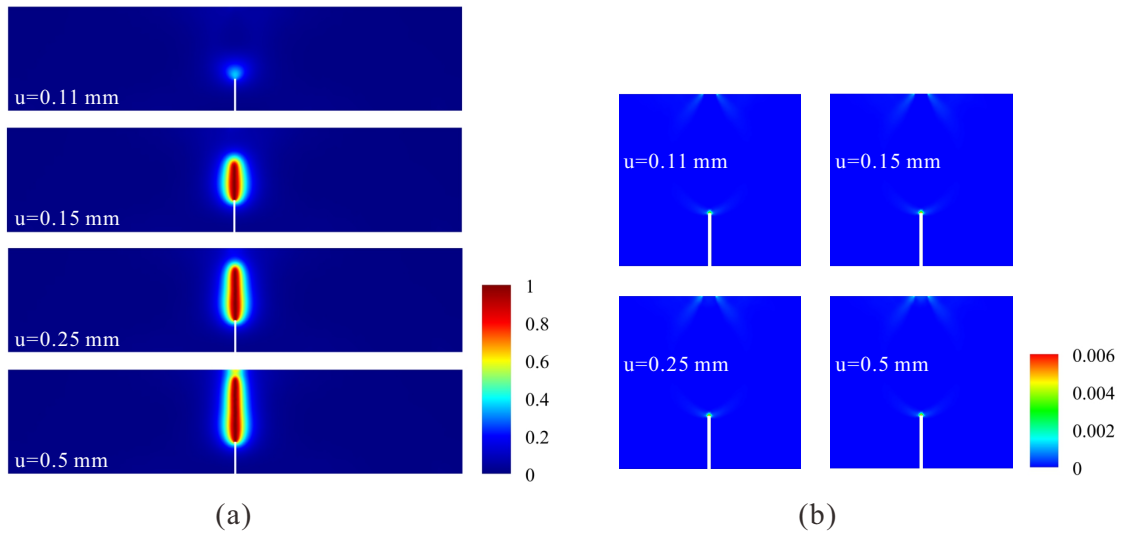


Fig. 2.10 Three-point bending test with cyclic loading: (a) elastoplastic brittle crack fields; (b) equivalent plastic strains. (see Fig. 2.9 for corresponding displacement points)

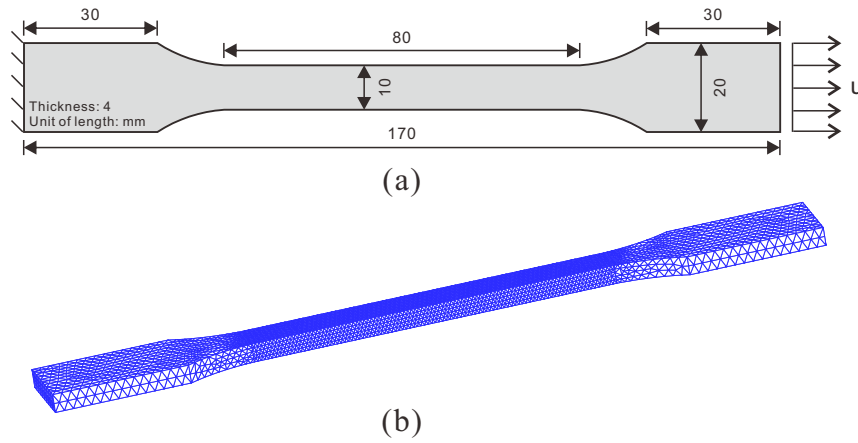


Fig. 2.11 I-shaped specimen: (a) geometry and boundary conditions; (b) finite element model.

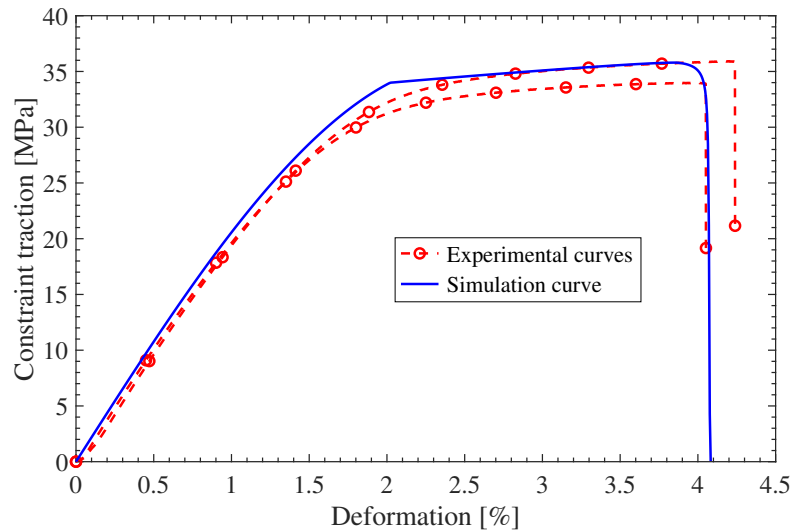


Fig. 2.12 I-shaped specimen: simulation curve and experimental curves.

2.2.4.3 I-shaped specimen

In this last example, we identify this elastoplastic brittle phase field model on a 3D printed I-shaped specimen, which is made from Polyamide 12 (PA12). The specimen and experimental data were kindly provided by Prof. Mohammed Nouari and Hamid Makich in LEM3 Laboratory, University of Lorraine, through a collaboration founded by the MMELED ANR project. The geometry and boundary conditions are illustrated in Fig. 2.11(a). The finite element model with a refinement in the central region is shown in Fig. 2.11(b), where 39594 4-node tetrahedron elements are used. External loading increment value in this simulation

is $\Delta u = 0.01$ mm. The material parameters are: $E = 3.45$ GPa, $\nu = 0.25$, $\sigma_Y = 68$ MPa, $H = 125$ MPa and $g_c = 14$ N/mm. The length scale parameter is chosen as $\ell_d = 1$ mm.

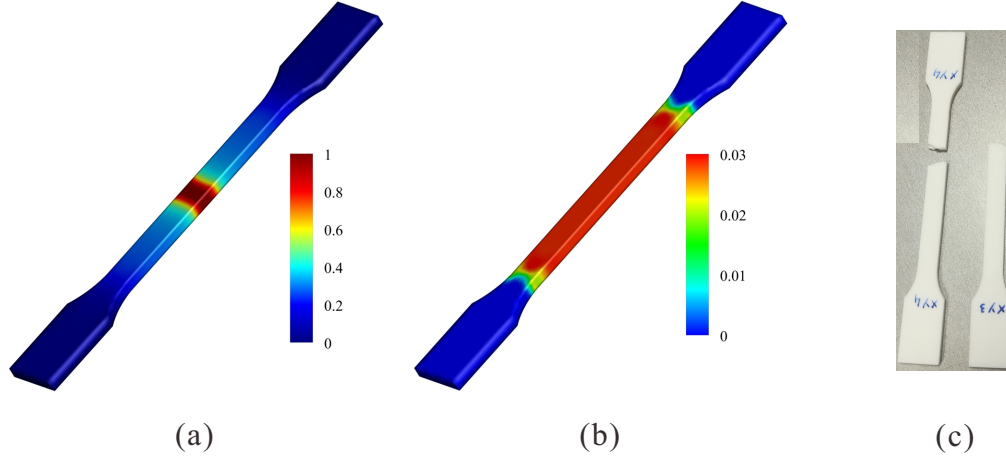


Fig. 2.13 I-shaped specimen: (a) final crack field; (b) final equivalent plastic strain; (c) experimental results.

The experimental curves and final failure patterns are shown in Fig. 2.12 and Fig. 2.13(c), respectively. It is observed that the specimen exhibits an obvious plastic deformation stage before the final failure. Meanwhile, the final failure shows a brittle crack pattern. Note that 2 specimens were experimentally tested, this is why 2 curves are presented in Fig. 2.12. The simulated curve in Fig. 2.12 exhibits a good agreement with the experimental curves. Fig. 2.13(a) and (b) show the final crack field and final equivalent plastic strain field. As can be observed from Fig. 2.13, the final equivalent plastic strain field is distributed in a large range of the center of the specimen, and the final crack occurs in the center of specimen, whereas the experimental crack is not strictly in the center of the specimen. However, it should be noted that due to defects (microvoids) in the experimental samples, the crack does not occur at the center (see Fig. 2.13(c)).

2.3 Phase field modeling elastoplastic brittle fracture in heterogeneous materials with interfaces

In this section, we present an original contribution developed in this PhD work, where we introduce a framework for modeling interfacial damage interacting with elastoplastic fracture within the phase field method.

2.3.1 Diffuse approximation of discontinuous fields

Let $\Omega \subset \mathbb{R}^D$ be an open domain with $D = 2, 3$, describing a heterogeneous medium which contains internal interfaces between two elasto-plastic phases. The external boundary of Ω is denoted by $\partial\Omega \in \mathbb{R}^{D-1}$. During the loading, cracks may propagate in the medium phases and can pass through the interfaces as depicted in Fig. 2.14(a), where the crack surfaces and the interfaces are collectively denoted by Γ and Γ^I , respectively. In this work, we adopt the framework proposed in [12, 108] for a regularized representation of discontinuities extended to interfaces as in [130, 179]. In this regularized framework, the cracks are approximately represented by a scalar phase field $d(\mathbf{x}, t)$ (see Fig. 2.14(b)) and the interfaces by a fixed scalar function $\beta(\mathbf{x})$ (see Fig. 2.14(c)).

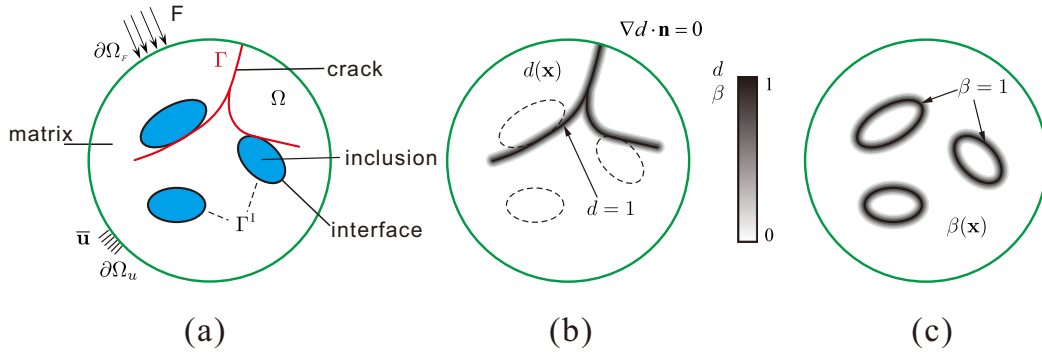


Fig. 2.14 Diffused approximation of cracks and interfaces: (a) a medium containing sharp cracks and interface; (b) diffused approximation of cracks; (c) diffuse approximation of interfaces.

2.3.1.1 Phase field approximation of bulk cracks and interfaces

For a known fixed crack surface Γ (see Fig. 2.14(a)), the scalar crack phase field $d(\mathbf{x}, t)$ can be determined through solving (2.1). With the same manner, The scalar interface function $\beta(\mathbf{x})$ can also be determined through solving the following boundary value problem subjected to Dirichlet boundary conditions $\beta = 1$ on the interfaces Γ^I :

$$\begin{cases} \beta(\mathbf{x}) - \ell_\beta^2 \Delta \beta(\mathbf{x}) = 0 & \text{in } \Omega, \\ \beta(\mathbf{x}) = 1 & \text{on } \Gamma^I, \\ \nabla \beta(\mathbf{x}) \cdot \mathbf{n} = 0 & \text{on } \partial\Omega, \end{cases} \quad (2.57)$$

where ℓ_β is a length scale parameter which governs the width of the regularization zone of the interface and gives for $\ell_\beta \rightarrow 0$ the exact sharp interfaces in Fig.2.14(a). Similarly, (2.57)

corresponds to the Euler-Lagrange equation of the variational problem:

$$\beta = \text{Arg} \left\{ \inf_{\beta \in S_\beta} \Gamma^\beta(\beta) \right\}, \quad \Gamma^\beta(\beta) = \int_{\Omega} \gamma_\beta(\beta) d\Omega, \quad S_\beta = \{\beta \mid \beta(\mathbf{x}) = 1, \forall \mathbf{x} \in \Gamma^I\}, \quad (2.58)$$

where $\gamma_\beta(\beta)$ is defined by:

$$\gamma_\beta(\beta) = \frac{\beta^2}{2\ell_\beta} + \frac{\ell_\beta}{2} \nabla \beta \cdot \nabla \beta. \quad (2.59)$$

In the present work, the length scale parameter ℓ_d and ℓ_β are interpreted as material parameters. Then, one possibility to select these parameters is to perform an inverse identification from experimental data. Such identification procedure has been described in [126] in the context of quasi-brittle heterogeneous materials and could be extended to the present elastoplastic framework in future studies using similar ideas. Then, in the present paper, the numerical values of ℓ_d and ℓ_β have been chosen arbitrarily as small values in the numerical examples of section 2.3.4.

2.3.1.2 Regularized representation of the displacement jumps within interfaces

In this section, an approximation for the displacement jump $[[\mathbf{u}]]$ is introduced to consider the interface debonding (see [130]). Let Γ^I be the interface. We define Γ^I as the zero level-set of a function $\phi(\mathbf{x})$, such that (see [130] for its construction):

$$\begin{cases} \phi(\mathbf{x}) > 0 \text{ for } \mathbf{x} \in \Omega^i, \\ \phi(\mathbf{x}) < 0 \text{ for } \mathbf{x} \in \Omega^m, \\ \phi(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \Gamma^I, \end{cases} \quad (2.60)$$

where Ω^i and Ω^m denote the set of inclusions and matrix, respectively. Using a Taylor expansion of the displacement field around a point $\mathbf{x}$ located on the interface (see Fig. 2.15):

$$[[\mathbf{u}]] \simeq \mathbf{w}(\mathbf{x}) = \mathbf{u}\left(\mathbf{x} + \frac{h}{2}\mathbf{n}^I\right) - \mathbf{u}\left(\mathbf{x} - \frac{h}{2}\mathbf{n}^I\right) = h \nabla(\mathbf{u}(\mathbf{x})) \mathbf{n}^I, \quad (2.61)$$

where $\mathbf{n}^I$ is the normal vector to Γ^I at the point $\mathbf{x}$ defined by:

$$\mathbf{n}^I = \frac{\nabla \phi(\mathbf{x})}{\|\nabla \phi(\mathbf{x})\|} \quad (2.62)$$

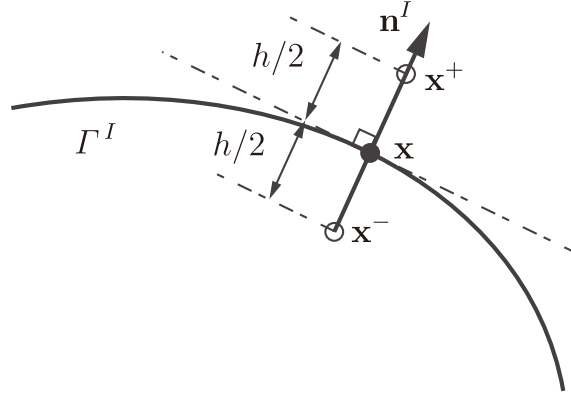


Fig. 2.15 Approximation of the displacement jump across an interface Γ^I at a point $\mathbf{x}$, with $\mathbf{n}^I$ the normal unit vector to Γ^I .

and $\mathbf{w}(\mathbf{x})$ denotes the smooth displacement jump approximation. Above, h is a small scalar parameter, chosen as $h = h^e$ to minimize the estimation error (see [130]), with h^e the typical element size of the finite element mesh around the interface. A detailed description for the numerical computation of $\phi(\mathbf{x})$ is introduced in [130].

It should be noted that $\phi(\mathbf{x})$ and $\mathbf{n}^I$ do not change throughout the simulation because the interfaces do not evolve. For a sharp interface, the singular part of the strain along the interface can be defined by:

$$\boldsymbol{\varepsilon}^I(\mathbf{x}) = \mathbf{n}^I(\mathbf{x}) \otimes^s \llbracket \mathbf{u}(\mathbf{x}) \rrbracket \delta(\mathbf{x}) \quad \forall \mathbf{x} \in \Gamma. \quad (2.63)$$

Then using the above regularization framework, this expression can be approximated as [130]:

$$\boldsymbol{\varepsilon}^I(\mathbf{x}) \simeq \mathbf{n}^I(\mathbf{x}) \otimes^s \mathbf{w}(\mathbf{x}) \gamma_\beta(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega. \quad (2.64)$$

2.3.2 Phase field modeling of elastoplastic damage interacting with interfacial damage

In this section, we propose a phase field model for modeling interactions between interfacial damage and bulk cracking in elasto-plastic composites. The framework is developed using the variational framework for fracture as introduced in [6, 145].

Here, the total strain is introduced as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}^I, \quad (2.65)$$

where ε^I has been defined in (2.64).

2.3.2.1 Total energy

Let us consider a two-phase medium whose phases are elasto-plastic with possible bulk damage and interfacial damage. Small strains are assumed. The total energy of the medium is defined by

$$W(\mathbf{u}, p, d, \beta) = \int_{\Omega} \psi^e(\varepsilon(\mathbf{u}), p, d) d\Omega + \int_{\Omega} \left[\psi^p(p) + \psi^d(\beta, d) + \psi^I(\mathbf{w}(\mathbf{u}), \beta) \right] d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\Omega, \quad (2.66)$$

where ψ^I denotes a strain density function depending on the approximated displacement jump across the interfaces. β plays the role of a parameter, as this field does not change during the evolution of the system.

2.3.2.2 Variational framework

We follow the same framework presented in section 2.2 to construct the variational principle, which involves: irreversibility condition, stability condition and energy balance.

Irreversibility condition

See section 2.2.2.2.

First-order stability condition

The first order stability condition (see [113, 114, 143]) is expressed by:

$$D_{\delta\mathbf{u}}W(\mathbf{u}, p, d) + D_{\delta p}W(\mathbf{u}, p, d) + D_{\delta d}W(\mathbf{u}, p, d) \geq 0. \quad (2.67)$$

Applied to (2.66), it yields:

$$\begin{aligned} & \int_{\Omega} \left[\boldsymbol{\sigma} : \varepsilon^e(\delta\mathbf{u}) + \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\delta\mathbf{u}) \right] d\Omega + \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} + \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega \\ & + \int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta\mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta\mathbf{u} d\Omega \geq 0 \end{aligned} \quad (2.68)$$

From (2.65):

$$\varepsilon^e = \varepsilon - \varepsilon^p - \varepsilon^I \quad (2.69)$$

and then:

$$D_{\delta \mathbf{u}} \varepsilon^e = \varepsilon^e(\delta \mathbf{u}) = \varepsilon(\delta \mathbf{u}) - \varepsilon^I(\delta \mathbf{u}). \quad (2.70)$$

From (2.63),

$$\varepsilon^I(\delta \mathbf{u}) = \mathbf{n}^I \otimes^s \mathbf{w}(\delta \mathbf{u}) \gamma_\beta, \quad \mathbf{w}(\delta \mathbf{u}) = h \nabla(\delta \mathbf{u}) \mathbf{n}^I. \quad (2.71)$$

From this expression, the following results stem out:

- For $\delta p = \delta d = 0$ we obtain:

$$\int_{\Omega} \boldsymbol{\sigma} : \varepsilon^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (2.72)$$

which is the weak form of the equilibrium equation.

- For $\delta d = 0$ and $\delta \mathbf{u} = \mathbf{0}$, we obtain (2.15), (2.16) and (2.17).
- For $\delta p = 0$ and $\delta \mathbf{u} = \mathbf{0}$ we obtain (2.18) and (2.19).

Energy balance

The energy balance represents the need for the total energy to remain constant as the state variables evolve. Following a procedure analogous to the treatment of the stability condition, this condition leads to

$$\begin{aligned} \int_{\Omega} \left[-\boldsymbol{\sigma} : \varepsilon^e(\dot{\mathbf{u}}) - \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\dot{\mathbf{u}}) + \left(\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} - \frac{\partial \psi^p}{\partial p} \right) \dot{p} - \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \dot{d} \right] d\Omega \\ + \int_{\partial \Omega_F} \mathbf{F} \cdot \dot{\mathbf{u}} dS + \int_{\Omega} \mathbf{f} \cdot \dot{\mathbf{u}} d\Omega = 0. \end{aligned} \quad (2.73)$$

The following cases are analyzed.

- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{d} = 0$, the plasticity consistency condition in (2.21) is obtained.
- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{p} = 0$, the damage consistency condition in (2.22) is obtained.

Alternate minimization

In this section, a staggered alternate minimization algorithm is applied. With the total energy (2.66) at hand, the alternate minimization follows.

- Minimization with respect to the displacement field:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d) = 0 \quad (2.74)$$

leads to

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (2.75)$$

which corresponds to the weak form of the mechanical problem to be solved for $\mathbf{u}$, given d .

- Minimization with respect to the equivalent plastic strain, we obtain (2.25).
- Minimization with respect to the damage field, we obtain (2.26).

2.3.2.3 Specialization

We now specialize the energy components introduced in (2.66). The new damage dissipative potential with interfacial damage penalization is defined as:

$$\psi^d(\beta, d) = (1 - \beta)^2 g_c \left(\frac{d^2}{2\ell_d} + \frac{\ell_d}{2} \nabla d \cdot \nabla d \right), \quad (2.76)$$

Note that the elastoplastic brittle fracture case model can be recovered by simply setting $\beta = 0$ in (2.76).

Following our recent work [130], we specialize the energy of interfacial jump component as:

$$\psi^I(\mathbf{u}, \beta) = \bar{\psi}^I(\mathbf{w}(\mathbf{u})) \gamma_{\beta}(\beta), \quad (2.77)$$

where the traction acting on the interface oriented by $\mathbf{n}^I$ (see Fig. 2.15) is defined by:

$$\mathbf{t}(\mathbf{w}) = \frac{\partial \bar{\psi}^I(\mathbf{w})}{\partial \mathbf{w}}. \quad (2.78)$$

Above, $\bar{\psi}^I$ is the interface strain density depending on the regularized displacement jump $\mathbf{w}$. Note that as discussed in [130], it is not required in this formulation to include history variables for the interfaces, the diffuse damage field being used to describe the irreversibility of the interfacial damage.

For 2D problems, the traction $\mathbf{t}(\mathbf{w})$ is in the form

$$\mathbf{t}(\mathbf{w}) = [t^n, t^t]^T, \quad (2.79)$$

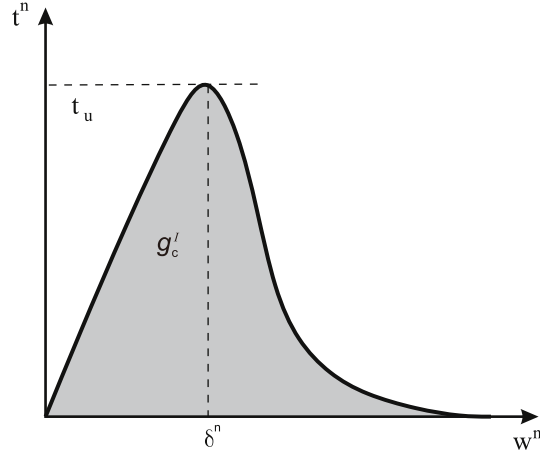


Fig. 2.16 Cohesive model for the interfaces: evolution of the normal traction component t^n with respect to the approximated jump normal displacement component w^n .

where t^n and t^t denote normal and tangential parts of the traction vector $\mathbf{t}$. In this paper, we neglect the effects of the tangential component in the interface model ($t^t = 0$), and use [169]:

$$t^n = g_c^I \frac{w^n}{(\delta^n)^2} \exp\left(-\frac{w^n}{\delta^n}\right), \quad (2.80)$$

where δ^n is related to the interface fracture toughness g_c^I and the interface fracture strength t_u by:

$$\delta^n = \frac{g_c^I}{t_u \exp(1)}, \quad (2.81)$$

w^n is the normal displacement jump defined by:

$$w^n = \mathbf{w} \cdot \mathbf{n}^I, \quad (2.82)$$

and $\mathbf{w}$ and $\mathbf{n}^I$ are given in (2.61) and (2.62), respectively. This relationship is illustrated in Fig. 2.16, where the fracture toughness g_c^I denotes the value of the interface energy function ψ^I at full crack opening. Relation (2.81) can be easily obtained by expressing the extremum of the function (2.80) ($\partial t^n(w^n)/\partial w^n = 0$), which is found at $w^n = \delta^n$, and then simply replacing this solution in (2.80).

The associated Euler-Lagrange equations to (2.75) are given by:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} - \gamma_\beta(\beta) \mathbf{f}^I + \mathbf{f} = \mathbf{0} & \text{in } \Omega, \\ \mathbf{u} = \bar{\mathbf{u}} & \text{on } \partial\Omega_u, \\ \boldsymbol{\sigma} \mathbf{n} = \mathbf{F} & \text{on } \partial\Omega_F. \end{cases} \quad (2.83)$$

where the body force term $\mathbf{f}^I$ is expressed by $\mathbf{f}^I = -h\nabla \mathbf{t}(\mathbf{w}) \cdot \mathbf{n}^I$, and is obtained from (2.75) by applying the divergence theorem to the term $\int_{\Omega} \gamma_{\beta}(\beta) \mathbf{t}(\mathbf{w}) h \nabla(\delta \mathbf{u}) d\Omega$, and assuming $\mathbf{t} \cdot \mathbf{n} = 0$ over the external boundary of the domain.

Using (2.26) and the property:

$$(\Delta d) \delta d = \nabla \cdot (\nabla d \delta d) - \nabla d \cdot \nabla(\delta d) \quad (2.84)$$

as well as the divergence theorem and $\nabla d \cdot \mathbf{n} = 0$, we obtain the weak form of the phase field problem as:

$$\int_{\Omega} \left(\left\{ -2(1-d)\psi_0^{e+} + (1-\beta)^2 \frac{g_c d}{\ell_d} \right\} \delta d + g_c (1-\beta)^2 \ell_d \nabla d \cdot \nabla(\delta d) \right) d\Omega = 0. \quad (2.85)$$

To prescribe irreversibility, we employ the technique introduced in [111] which consists in substituting the above weak form with:

$$\int_{\Omega} (\{ -2(1-d)\mathcal{H}(\varepsilon^e) + 2(1-\beta)^2 \psi_c d \} \delta d + 2(1-\beta)^2 \psi_c \ell_d^2 \nabla d \cdot \nabla(\delta d)) d\Omega = 0, \quad (2.86)$$

where

$$\mathcal{H}(\varepsilon^e) = \max_{s \in [0,1]} [\langle \psi_0^{e+}(\varepsilon^e, s) - \psi_c \rangle_+] \quad (2.87)$$

and ψ_c is a specific fracture energy density, which can be further related to a critical fracture stress σ_c by:

$$\psi_c = \frac{1}{2E} \sigma_c^2, \quad (2.88)$$

where E is the Young's modulus.

The corresponding Euler-Lagrange equations to (2.86) are given by:

$$\begin{cases} (1-\beta)^2 \psi_c (d - \ell_d^2 \Delta d) = (1-d) \mathcal{H}(\varepsilon^e) \\ \nabla d \cdot \mathbf{n} = 0 \text{ on } \partial\Omega, \\ d = 1 \text{ on } \Gamma. \end{cases} \quad (2.89)$$

The different equations of the model are summarized in Table 2.3. The weak forms of the problems to be solved alternatively are summarized in Table 2.4.

Remark: In the present work, we did not consider coupling between damage and plasticity. The reason is that currently, the available models from the literature which introduce such phenomena are not able to control the evolution of the plastic strain when damage occurs. In other words, the plastic strain continues to increase when the damage occurs within the crack. So far, it seems that the only model able to deal with this issue is the

Table 2.3 Governing equations of the elastoplastic phase field model with interfacial damage.

Irreversibility	$\dot{d} \geq 0, \quad 0 \leq d \leq 1$
Mechanical balance	$\nabla \cdot \boldsymbol{\sigma} - \gamma_\beta(\beta) \mathbf{f}' + \mathbf{f} = \mathbf{0} \text{ in } \Omega$ $\mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial\Omega_u, \quad \boldsymbol{\sigma} \mathbf{n} = \mathbf{F} \text{ on } \partial\Omega_F$
Constitutive law	$\boldsymbol{\sigma} = g(d) \boldsymbol{\sigma}_{\text{eff}}^+ + \boldsymbol{\sigma}_{\text{eff}}^-$ $\boldsymbol{\sigma}_{\text{eff}}^+ = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_+ \mathbf{1} + 2\mu \mathbf{e}^e, \quad \boldsymbol{\sigma}_{\text{eff}}^- = \kappa \langle \text{Tr}(\boldsymbol{\varepsilon}^e) \rangle_- \mathbf{1}$
Cohesive law	$\mathbf{t}(\mathbf{w}) = \left[g_c^I \frac{w^n}{(\delta^n)^2} \exp\left(-\frac{w^n}{\delta^n}\right), 0 \right]^T$
Damage criterion	$(1 - \beta)^2 \psi_c (d - \ell_d^2 \Delta d) - (1 - d) \mathcal{H}(\boldsymbol{\varepsilon}^e) \geq 0$ $\mathcal{H}(\boldsymbol{\varepsilon}^e) = \max_{s \in [0, t]} \left[\langle \psi_0^{e+}(\boldsymbol{\varepsilon}^e, s) - \psi_c \rangle_+ \right]$
Damage consistency	$\left((1 - \beta)^2 \psi_c (d - \ell_d^2 \Delta d) - (1 - d) \mathcal{H}(\boldsymbol{\varepsilon}^e) \right) \dot{d} = 0$
Plastic yield criterion	$F^p(p) = \sqrt{\frac{3}{2}} \ \mathbf{s}\ - (\sigma_Y + Hp) \leq 0,$
Plastic flow rule	$\dot{\boldsymbol{\varepsilon}}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\ \mathbf{s}\ } \text{ with } \dot{p} \geq 0$

the model proposed in [106], involving gradient plasticity and gradient damage and strong plasticity-damage coupling. Extension of the present interfacial damage framework with the gradient plasticity model could be found in Chapter 4.

2.3.3 Discretization and numerical implementation

In this section, we detail the weak forms and FEM discretizations for displacement and damage problems, and finally provide the different algorithms.

2.3.3.1 Weak forms the linearized mechanical problem

Using (2.77) and (2.78), we can re-write the associated weak form for the displacement problem (2.75) as:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_\beta \mathbf{t} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega = \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega + \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS, \quad (2.90)$$

where $\mathbf{t}$ and $\boldsymbol{\sigma}$ are given in (2.79) and (2.33), respectively. We can rewrite the balance equation (2.90) as

$$\mathbf{R} = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_\beta \mathbf{t} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS = 0. \quad (2.91)$$

Table 2.4 Problems to be solved in the staggered procedure

Mechanical problem: given d , solve for $\mathbf{u}$:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_{\beta}(\beta) \mathbf{t}(\mathbf{w}) \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0$$

$$F^p(p) = \sqrt{\frac{3}{2}} \|\mathbf{s}\| - (\sigma_Y + Hp) \leq 0$$

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\|\mathbf{s}\|} \text{ with } \dot{p} \geq 0$$

Phase Field problem: given $\mathbf{u}$, solve for d :

$$\int_{\Omega} \left([\mathcal{H}(\mathbf{u}) + (1 - \beta)^2 \psi_c] d \delta d + (1 - \beta)^2 \psi_c \ell_d^2 \nabla d \cdot \nabla (\delta d) \right) d\Omega = \int_{\Omega} \mathcal{H}(\mathbf{u}) \delta d d\Omega.$$

In a standard Newton method, the displacements are updated for each loading increment by solving the tangent problem:

$$D_{\Delta \mathbf{u}} \mathbf{R}(\mathbf{u}^{(k)}, d) = -\mathbf{R}(\mathbf{u}^{(k)}, d) = 0, \quad (2.92)$$

where $\mathbf{u}^{(k)}$ is the displacement solution known from the previous iteration. The displacement corrections are obtained as

$$\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta \mathbf{u}. \quad (2.93)$$

In (2.92),

$$D_{\Delta \mathbf{u}} \mathbf{R}(\mathbf{u}^{(k)}) = \int_{\Omega} \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}^e} : \boldsymbol{\varepsilon}^e(\Delta \boldsymbol{\varepsilon}) : \boldsymbol{\varepsilon}^e(\delta \boldsymbol{\varepsilon}) d\Omega + \int_{\Omega} \gamma_{\beta} \frac{\partial \mathbf{t}(\mathbf{w})}{\partial \mathbf{w}} : \Delta \mathbf{w} : \delta \mathbf{w} d\Omega, \quad (2.94)$$

with

$$\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}^e} = \mathbb{C}_s(\mathbf{u}, d). \quad (2.95)$$

Using (2.89), we can re-write the associated weak form for the damage problem as:

$$\int_{\Omega} \left\{ \left[\mathcal{H} + (1 - \beta)^2 \psi_c \right] d \delta d + (1 - \beta)^2 \psi_c \ell_d^2 \nabla d \cdot \nabla (\delta d) \right\} d\Omega = \int_{\Omega} \mathcal{H} \delta d d\Omega. \quad (2.96)$$

2.3.3.2 Discretization of the displacement problem

In this work, for the sake of clarity, only 2D FEM discretization is detailed. The vector form of second-order tensors are introduced as $[\boldsymbol{\varepsilon}] = [\varepsilon_{11}, \varepsilon_{22}, \sqrt{2}\varepsilon_{12}]^T$, $[\boldsymbol{\sigma}] = [\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12}]^T$, as well as the FEM approximations $\mathbf{u} = \mathbf{N}_{\mathbf{u}} \mathbf{u}^e$, $\delta \mathbf{u} = \mathbf{N}_{\mathbf{u}} \delta \mathbf{u}^e$, and $\Delta \mathbf{u} = \mathbf{N}_{\mathbf{u}} \Delta \mathbf{u}^e$ where $\mathbf{u}^e$, $\delta \mathbf{u}^e$, $\Delta \mathbf{u}^e$ and $\mathbf{N}_{\mathbf{u}}$ are nodal displacement components in one element, nodal trial function components, nodal incremental displacement components and a matrix of displacement

shape function, respectively. Then we obtain:

$$[\varepsilon](\mathbf{u}) = \mathbf{B}_\mathbf{u} \mathbf{u}^e, \quad [\varepsilon^e](\Delta \mathbf{u}) = \mathbf{B}_\mathbf{w} \Delta \mathbf{u}^e, \quad [\varepsilon^e](\delta \mathbf{u}) = \mathbf{B}_\mathbf{w} \delta \mathbf{u}^e, \quad (2.97)$$

and

$$\mathbf{w}(\mathbf{u}) = h \mathbf{N} \mathbf{B} \mathbf{u}^e, \quad \Delta \mathbf{w}(\mathbf{u}) = h \mathbf{N} \mathbf{B} \Delta \mathbf{u}^e, \quad \delta \mathbf{w} = h \mathbf{N} \mathbf{B} \delta \mathbf{u}^e, \quad (2.98)$$

where $\mathbf{B}_\mathbf{u}$ is a matrix of displacement shape function derivatives, and

$$\mathbf{N} = \begin{bmatrix} n_1 & n_2 & 0 & 0 \\ 0 & 0 & n_1 & n_2 \end{bmatrix}, \quad (2.99)$$

$$\mathbf{B} = \begin{bmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} \end{bmatrix}^T = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & 0 & 0 \\ 0 & 0 & \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} \end{bmatrix}^T \mathbf{N}_\mathbf{u}, \quad (2.100)$$

where n_1 and n_2 are the x - and y - components of the normal vector $\mathbf{n}^I$ in (2.62) and $\mathbf{B}_\mathbf{w}$ is a modified spatial strain-displacement matrix defined by:

$$\mathbf{B}_\mathbf{w} = \mathbf{B}_\mathbf{u} - h \gamma_\beta \mathbf{M} \mathbf{B} \quad (2.101)$$

in which $\mathbf{M}$ is a matrix expressed by [130]:

$$\mathbf{M} = \begin{bmatrix} n_1 & 0 \\ 0 & n_2 \\ \frac{1}{\sqrt{2}} n_2 & \frac{1}{\sqrt{2}} n_1 \end{bmatrix} \mathbf{N} = \begin{bmatrix} n_1^2 & n_1 n_2 & 0 & 0 \\ 0 & 0 & n_1 n_2 & n_2^2 \\ \frac{1}{\sqrt{2}} n_1 n_2 & \frac{1}{\sqrt{2}} n_2^2 & \frac{1}{\sqrt{2}} n_1^2 & \frac{1}{\sqrt{2}} n_1 n_2 \end{bmatrix}. \quad (2.102)$$

After discretization, the linear system (2.92) with the displacement corrections (2.93) reduces to a standard Newton-type iteration:

$$\mathbf{K}_{\tan} \Delta \mathbf{u} = -\mathbf{R}(\mathbf{u}^{(k)}), \quad \mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \Delta \mathbf{u}, \quad (2.103)$$

where $\mathbf{u}^{(k)}$ is the displacement field known from the previous (k -th) Newton-Raphson iteration,

$$\mathbf{K}_{\tan} = \int_{\Omega} \mathbf{B}_\mathbf{w}^T \mathbf{C}_s \mathbf{B}_\mathbf{w} d\Omega + \int_{\Omega} \gamma_\beta (h \mathbf{N} \mathbf{B})^T \mathbf{C}_I (h \mathbf{N} \mathbf{B}) d\Omega, \quad (2.104)$$

and

$$\mathbf{R}(\mathbf{u}^{(k)}) = \int_{\Omega} \mathbf{B}_\mathbf{w}^T \boldsymbol{\sigma}^{(k)} d\Omega + \int_{\Omega} \gamma_\beta (h \mathbf{N} \mathbf{B})^T \mathbf{t}(\mathbf{w}^{(k)}) d\Omega - \int_{\Omega} \mathbf{N}_\mathbf{u}^T \mathbf{f} d\Omega - \int_{\partial \Omega_F} \mathbf{N}_\mathbf{u}^T \mathbf{F} dS, \quad (2.105)$$

where

$$\mathbf{C}_I = \frac{\partial \mathbf{t}(\mathbf{w})}{\partial \mathbf{w}} = \begin{bmatrix} \frac{\partial t^n}{\partial w^n} & 0 \\ 0 & 0 \end{bmatrix}, \quad (2.106)$$

and where $\mathbf{C}_s$ is the matrix form corresponding to the fourth-order elastoplastic consistent tangent operator $\mathbb{C}_s$ in (2.95). The iterative update (2.103) is performed until convergence is achieved in the sense $\|\Delta \mathbf{u}\| / \|\mathbf{u}^{(k+1)} - \mathbf{u}^{(0)}\| \leq \text{tol}$.

2.3.3.3 Discretization of the phase field problem

The damage and damage gradient are approximated in one element by

$$d = \mathbf{N}_d \mathbf{d}^e, \quad \nabla d = \mathbf{B}_d \mathbf{d}^e, \quad (2.107)$$

where $\mathbf{N}_d$ and $\mathbf{B}_d$ are matrices of damage shape function and of damage shape function derivatives, respectively, and $\mathbf{d}^e$ denote nodal damage in one element.

The discretization of damage problem (2.96) results into the following discrete system of equations:

$$\mathbf{K}_d \mathbf{d} = \mathbf{F}_d \quad (2.108)$$

in which

$$\mathbf{K}_d = \int_{\Omega} \left\{ \left[\mathcal{H} + (1 - \beta)^2 \psi_c \right] \mathbf{N}_d^T \mathbf{N}_d + (1 - \beta)^2 \psi_c \ell_d^2 \mathbf{B}_d^T \mathbf{B}_d \right\} d\Omega \quad (2.109)$$

and

$$\mathbf{F}_d = \int_{\Omega} \mathbf{N}_d^T \mathcal{H} d\Omega, \quad (2.110)$$

where $\mathcal{H}$ is given in (2.87).

Table 2.5 Material parameters used in the numerical simulations, from [104]

Name	Symbol	Material I	Material II
Shear modulus	κ	27.28 GPa	70.3 GPa
Bulk modulus	μ	71.66 GPa	136.5 GPa
Yield stress	σ_Y	0.345 GPa	0.443 GPa
Hardening modulus	H	0.25 GPa	0.3 GPa
Critical fracture stress	σ_c	1 GPa	2 GPa

2.3.3.4 Numerical implementation

In the present work, a staggered scheme is employed following [108], where at each load increment the displacement problem is solved for fixed damage field which is known from the previous time step. The damage problem is then solved with the new displacement field. The overall algorithm is illustrated in Algorithm 3.

Algorithm 3: Overall algorithm for elastoplastic brittle fracture model with inter-faces

Initialize $\mathbf{u}_0$, d_0 , $\boldsymbol{\varepsilon}_0^p$, and p_0 with assumption of not plasticised and undamaged state.

Compute the level-set function ϕ and interface damage β .

Loop over load increments n

for $i = 1, \dots, n$ **do**

Displacement problem

 Newton-Raphson iterative solution scheme

$k = 1, err = 1, tol = 10^{-5}, \mathbf{u}_i^{(0)} = \mathbf{u}_{i-1}$

while $err > tol$ **do**

$\boldsymbol{\varepsilon}^{ep} = \mathbf{B}_w \mathbf{u}_i^{(k-1)}, \mathbf{w} = h \mathbf{N} \mathbf{B} \mathbf{u}_i^{(k-1)}$

 Compute $\mathbf{t}(\mathbf{w})$ and $\mathbf{C}_I$ from (2.79) and (2.106)

 Return-mapping algorithm

 Given $(\boldsymbol{\varepsilon}^{ep}, \boldsymbol{\varepsilon}_{i-1}^p, p_{i-1}, d_{i-1})$, Compute $(\mathbf{C}_s, \boldsymbol{\varepsilon}_i^{p,(k)}, p_i^{(k)})$ from Algorithm 2

 Compute $\mathbf{K}_{tan}$ and $\mathbf{R}(\mathbf{u}_i^{(k-1)})$ from (2.104) and (2.105)

 Compute $\Delta \mathbf{u}$ from (2.103)

 Update $\mathbf{u}_i^{(k)} = \mathbf{u}_i^{(k-1)} + \Delta \mathbf{u}$

$\mathbf{u}_i = \mathbf{u}_i^{(k)}, \boldsymbol{\varepsilon}_i^p = \boldsymbol{\varepsilon}_i^{p,(k)}, p_i = p_i^{(k)}$

$err = \|\Delta \mathbf{u}\| / \|\mathbf{u}_i - \mathbf{u}_{i-1}\|, k = k + 1$

end

Damage problem

 Compute $\mathcal{H}$ with $\mathbf{u}_i$ and $\boldsymbol{\varepsilon}_i^p$ from (2.87)

 Compute $\mathbf{K}_d$ and $\mathbf{F}_d$ from (2.109) and (2.110)

 Compute the damage field d_i from (2.108)

$i = i + 1$

end

2.3.4 Numerical examples

In this section, all numerical computations are performed within the finite element framework and assuming plain strain conditions. Both damage and displacement fields are discretized

with 4-node bilinear elements. The material properties are shown in Table 2.5. Displacement controlled conditions are always assumed. We adopt the staggered solution strategy presented in 2.3.3.4. For the sake of simplicity, we recall that both length scale parameters ℓ_d and ℓ_β are assumed to be equal, i.e $\ell_d = \ell_\beta = \ell$.

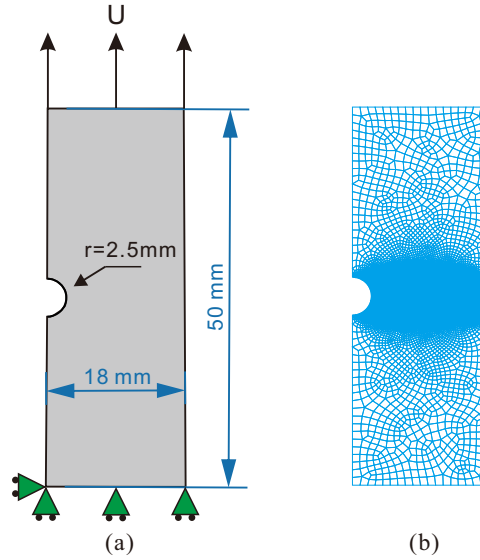


Fig. 2.17 Semicircular notched specimen: (a) geometry and boundary conditions; (b) finite element model.

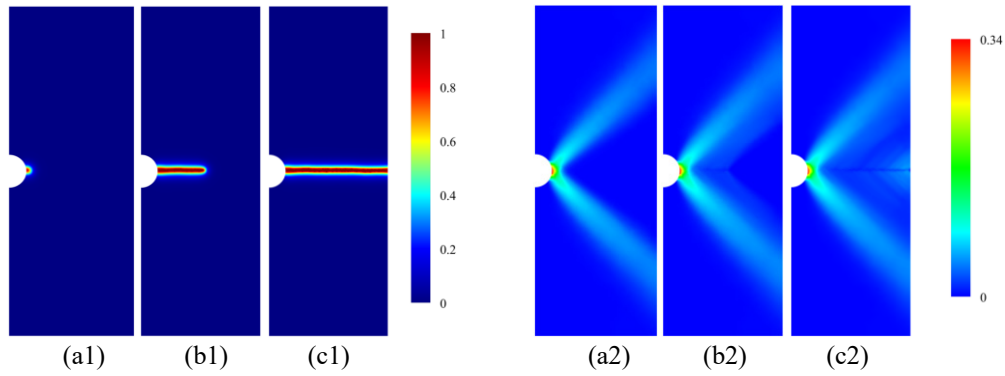


Fig. 2.18 Semicircular notched specimen: a1-c1 crack phase field and a2-c2 equivalent plastic strain field at three different prescribed displacements (see Fig. 2.20).

2.3.4.1 Semicircular notched specimen

In this example, we first validate the convergence of the elastoplastic phase field with respect to mesh refinement, in absence of interfaces. Then, we analyze the influence of the critical

fracture stress σ_c . For this purpose, a specimen with a semicircular notch, as described in Fig. 2.17(a), is considered. The boundary conditions are as follows: on the lower end ($y = 0$), the y -displacement are fixed, while the x -displacement are free and the node ($x = 0, y = 0$) is fixed. On the upper end, the x -displacement are free, while the y -displacement are prescribed to an increasing value of U with $\Delta U = 0.001$ mm during the simulation. The material parameters are those of Material I in Table 2.5 and $\ell = 0.5$ mm. The spatial discretization of the model comprises 8953 4-node quadrilateral elements, with refinement in the central region where the crack is expected to propagate (see Fig. 2.17(b)). Fig. 2.18 shows the evolution of the crack phase field and the equivalent plastic strain field at three different prescribed displacements. As can be observed from Fig. 2.18 (a1)-(c1), the crack propagates horizontally towards the right-end boundary. The equivalent plastic strain as shown in Fig. 2.18 (a2)-(c2) is maximum at the notch root and localization branches form near the notch at an angle of about 45° . The same simulation has been repeated on two other finite element meshes of 6834 and 11,325 elements (coarse and fine mesh) to study the convergence with respect to the mesh size. Results are provided in Fig. 2.19, demonstrating the convergence of the method as the mesh is refined. In the following, the medium mesh has been used to limit the computational costs.

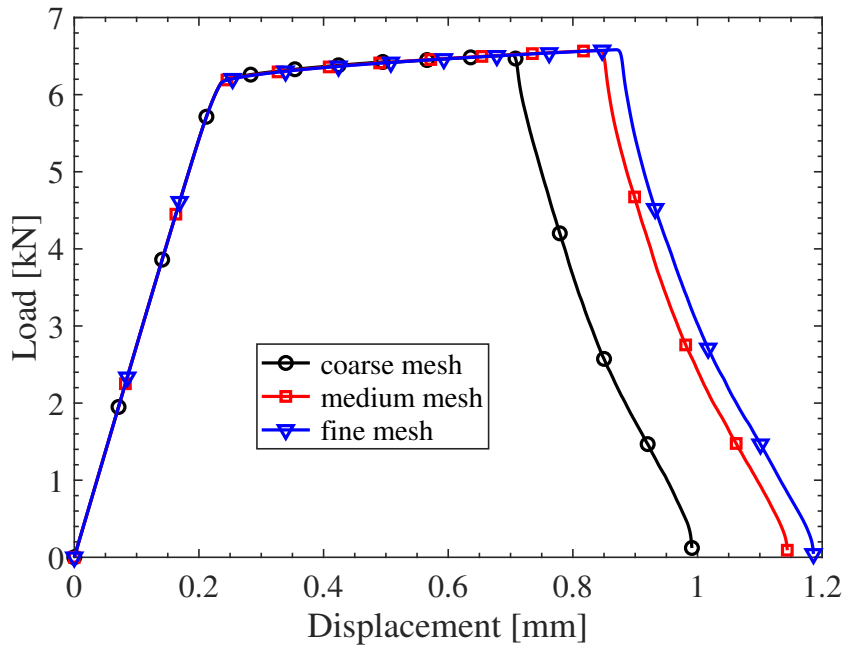


Fig. 2.19 Load-displacement curve of a semicircular notched specimen showing convergence with respect to the finite element mesh size (6834, 8953 and 11,325 elements).

Fig. 2.20 and Fig. 2.21 show the effect of the critical fracture stress σ_c on results in terms of load-displacement curve, crack path and the equivalent plastic strain field. As can be observed, with the increase of the critical fracture stress σ_c , the prescribed displacement corresponding to the point (maximum load) of initiation of the fracture rises, thus leading to an increase of the equivalent plastic strain field. This observation has been reported in many other works [107, 30, 20]. Here we define the critical fracture stress σ_c as a material parameter which controls the initiation of the fracture.

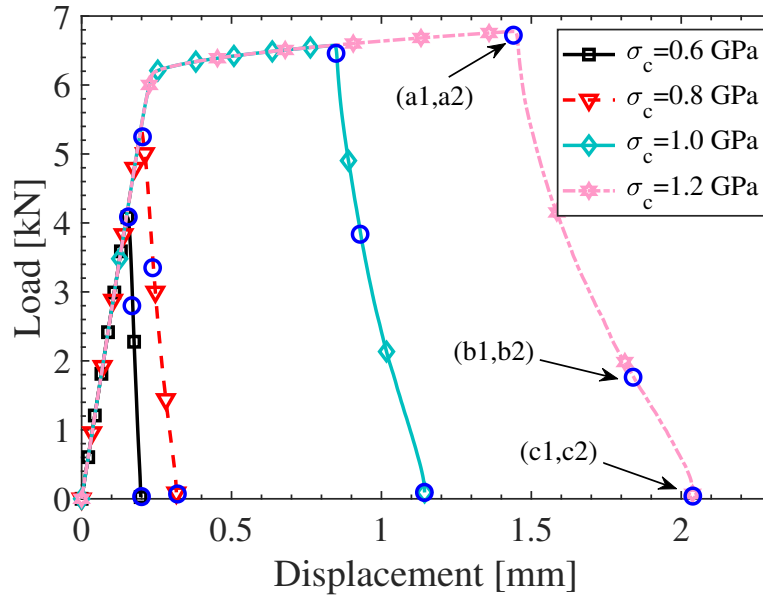


Fig. 2.20 Load-displacement curve of a semicircular notched specimen: sensitivity with respect to the critical fracture stress σ_c .

2.3.4.2 Fatigue cracking

In this next example, we include a cohesive interface and validate the convergence of the model with respect to the mesh size. Additionally we investigate the capability of the framework to handle fatigue cracking under cyclic loading. A square domain is considered. The domain contains a cohesive interface, whose geometry is depicted in Fig. 2.22(a). In order to provide a good balance between simulation accuracy and computational costs, a finely refined mesh is used in the region close to the cohesive interface, with finite element size: $h^e = 0.05$ mm (see Fig. 2.22(b)). The material parameters are those of Material I in Table 2.4, in addition to $\ell = 0.1$ mm, $h = h^e = 0.05$ mm in (2.61), fracture strength and toughness $t_u = 10$ MPa and $g_c^I = 0.1$ N/mm, respectively.

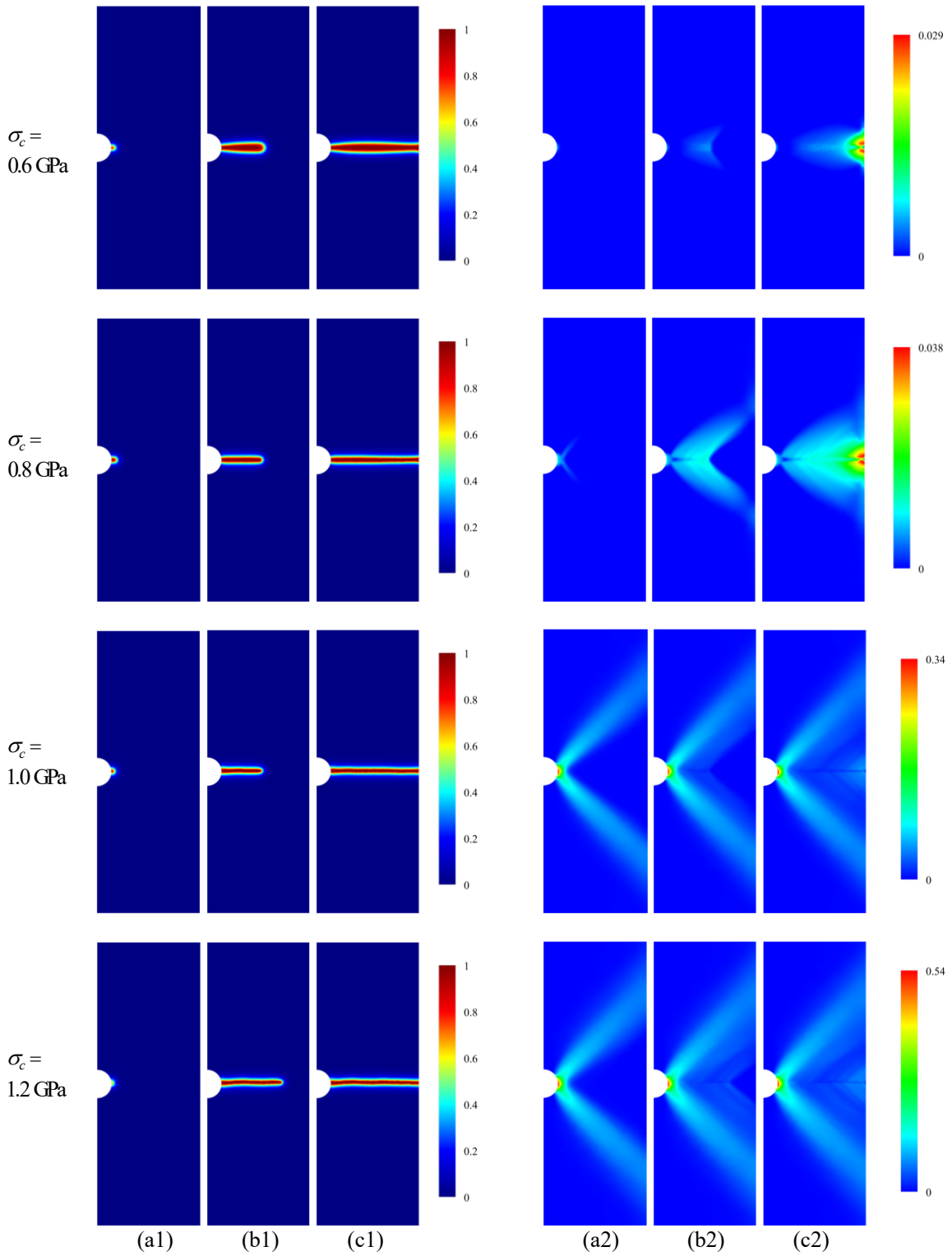


Fig. 2.21 Semicircular notched specimen: effect of the critical fracture stress σ_c on the fracture process; a1-c1: crack phase field; a2-c2: equivalent plastic strain field at three different prescribed displacements (see Fig. 2.20).

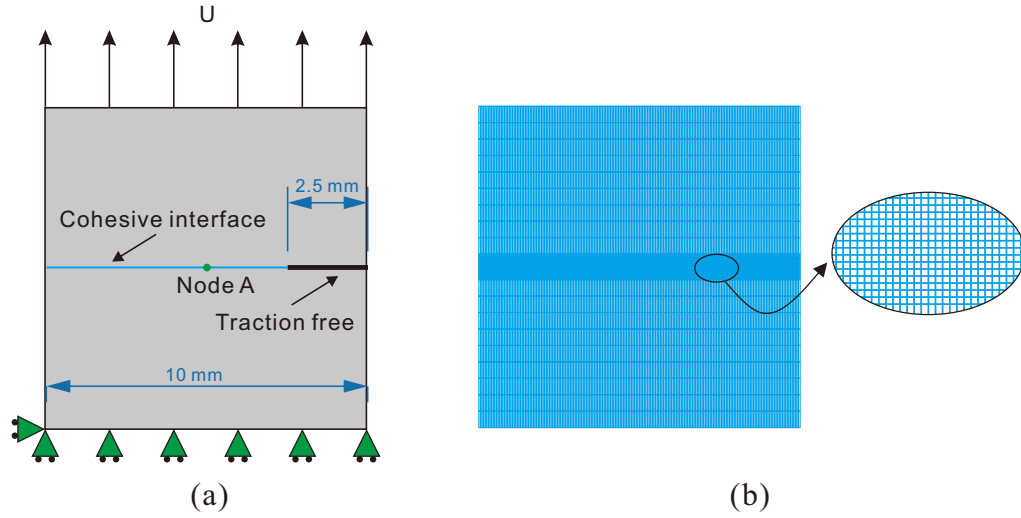


Fig. 2.22 Definition of the fatigue crack test: (a) geometry and boundary conditions; (b) finite element model (medium mesh).

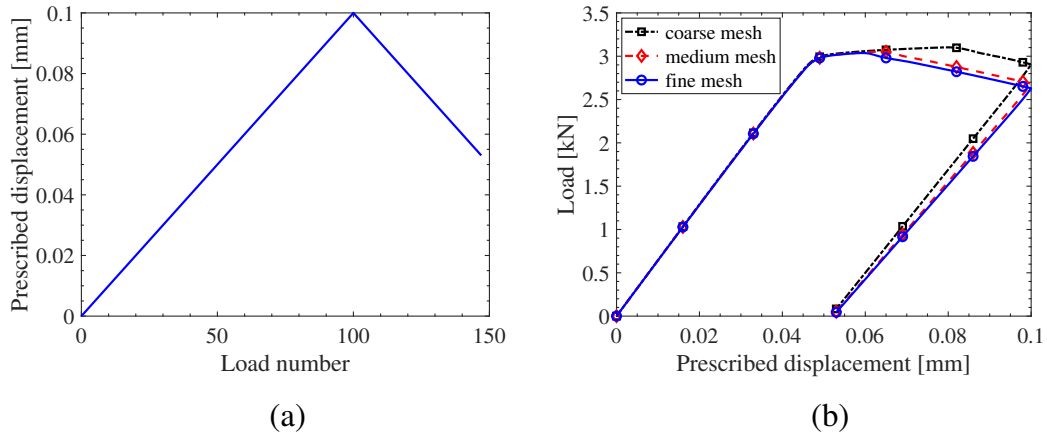


Fig. 2.23 Fatigue crack test: (a) evolution of the load; (b) effect of the mesh size (3500, 6800 and 10,028 elements) on the load-displacement curve.

In a first case, we validate the convergence with respect to the mesh refinement. For this purpose, two other finite element meshes have been used: a coarse mesh with 3500 elements and a fine mesh with 10,028 elements. A displacement U ($\Delta U = 0.001$ mm) whose evolution is described in Fig. 2.23(a) is prescribed on the upper end, as depicted in Fig. 2.22(a). Results for 3 meshes are provided in Fig. 2.23(b), which show the convergence of the method with mesh refinement. In the following case, the medium mesh has been used to limit the computational costs.

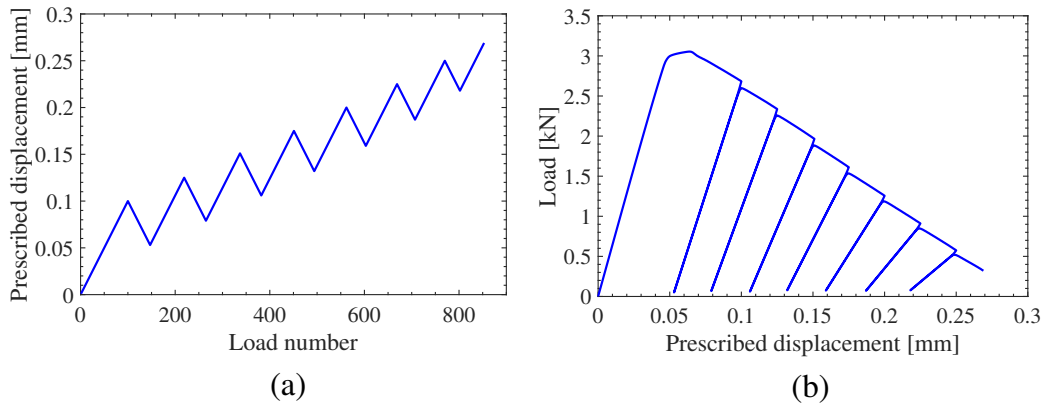


Fig. 2.24 Fatigue crack test: (a) evolution of the load; (b) corresponding load-displacement curve.

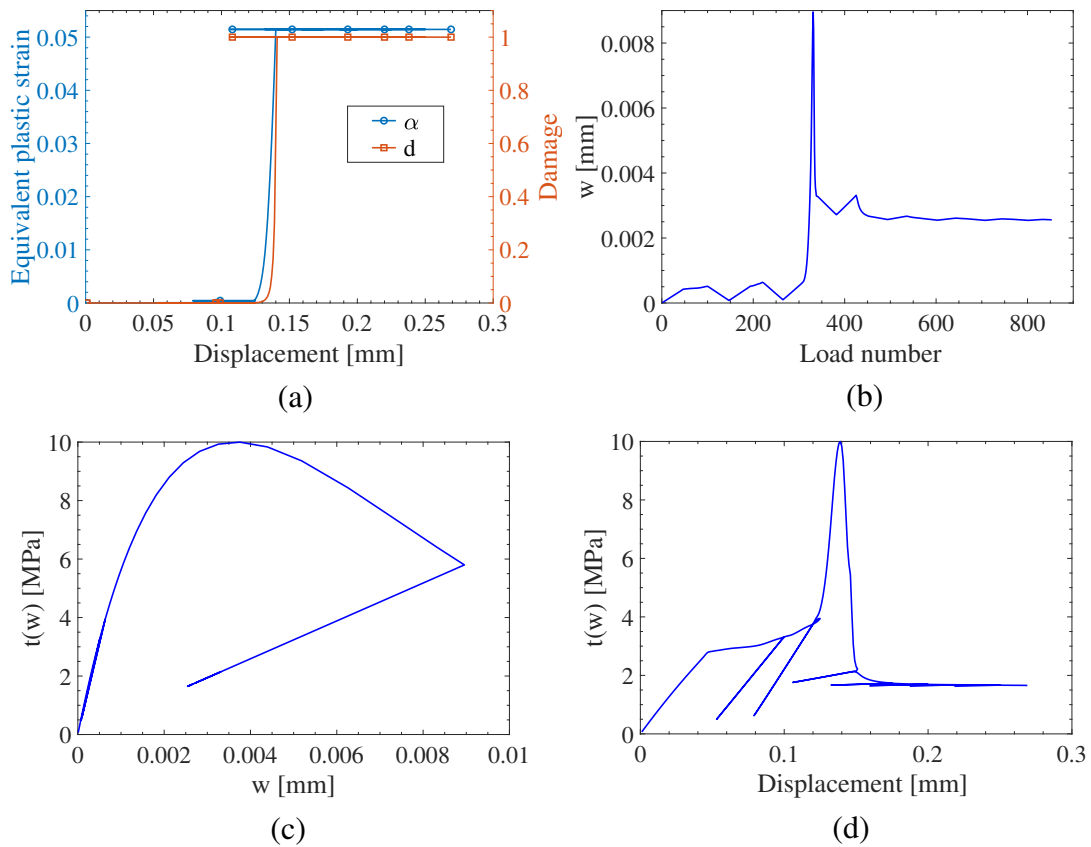


Fig. 2.25 Fatigue crack test: (a) equivalent plastic strain and damage with respect to the prescribed displacement; (b) displacement jump along y with respect to the load number; (c) cohesive traction with respect to the displacement jump; (d) cohesive traction with respect to the prescribed displacement.

In this next case, the evolution of U ($\Delta U = 0.001$ mm) is described in Fig. 2.24(a), involving multiple cycles. The corresponding load-displacement curve is depicted in Fig. 2.24(b). As shown in this figure, the irreversible strains upon unloading are well produced by this model. The evolution of the equivalent plastic strain in the element near node A (which is located in the center of the domain) and damage on node A are depicted in Fig. 2.25(a). The computed displacement jump along y in the element near node A is shown in Fig. 2.25(b). The normal traction force in the element near node A, with respect to the computed displacement jump and the prescribed displacement, are depicted in Fig. 2.25(c) and (d), respectively.

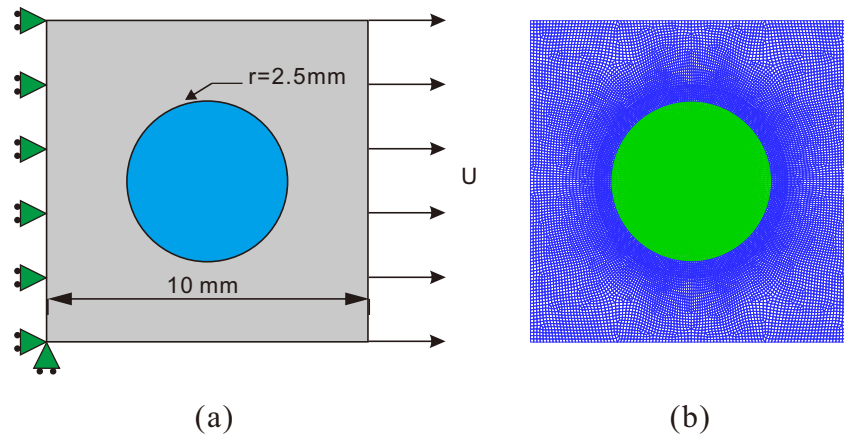


Fig. 2.26 Traction test of a microstructure with a single fiber: (a) geometry and boundary conditions; (b) finite element model.

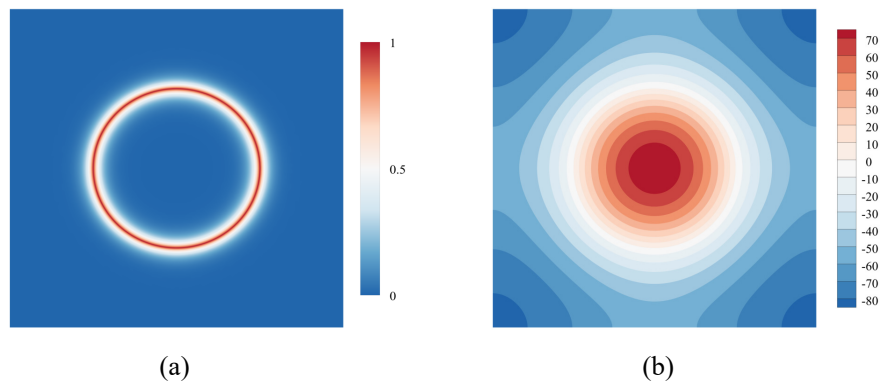


Fig. 2.27 Traction test of a microstructure with a single fiber: (a) smeared interface represented by the interface phase field $\beta(\mathbf{x})$; (b) corresponding level-set function $\phi(\mathbf{x})$.

2.3.4.3 Traction test of a microstructure with a single fiber

In this example, we investigate a microstructure involving one fiber in an elastoplastic matrix with damageable interface. The importance of interfacial damage and the influence of its parameters on the results will be studied. The geometry and boundary conditions are depicted in Fig. 2.26(a). The finite element model (medium mesh with 24,688 elements) is shown in Fig. 2.26(b). External loading is applied by displacement control through a series of load increments with a fixed step value $\Delta U = 5 \times 10^{-4}$ mm. The material parameters for the matrix and fiber are those of Material I and Material II in Table 2.4, in addition to $\ell = 0.2$ mm, $h = 0.1$ mm, $g_c^I = 0.1$ N/mm and $t_u = 0.3$ MPa (model I). An illustration of the interface indicator $\beta(\mathbf{x})$ and associated level-set $\phi(\mathbf{x})$ for the present microstructure is depicted in Fig. 2.27. In this composite example, we also validate the mesh convergence with two other finite element meshes: a coarse mesh with 13,268 elements and a fine mesh with 34,802 elements. The load-displacement curves are shown in Fig. 2.28(a). The evolution of the crack phase field is presented in Fig. 2.29. From these results it is observed that the crack nucleates from the interface and then kinks into the matrix when reaching a certain point. This leads to the final predicted semi-debonding angle of 65.10° which is similar to the quasi brittle cases [131, 188]. The difference compared with similar cases but involving a quasi brittle matrix [130, 188] is that the initial interface debonding position in this model is about 45° direction in the fiber surface (see Fig. 2.29(a)).

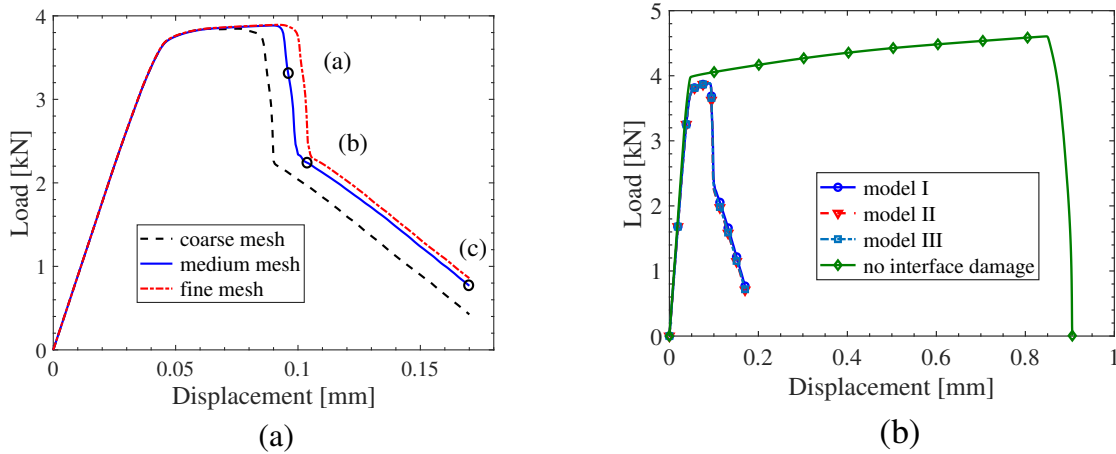


Fig. 2.28 Traction test of a microstructure with a single fiber: (a) load-displacement curves for three finite element meshes (13,268, 24,688 and 34,802 elements); (b) comparison of load-displacement curves for different interfacial damage models.

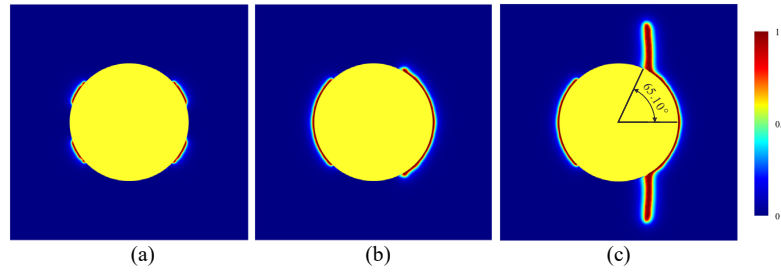


Fig. 2.29 Traction test of a microstructure with a single fiber. Evolution of the crack phase field for an applied traction displacement U : (a) $U = 0.095$ mm, (b) $U = 0.105$ mm and (c) $U = 0.17$ mm.

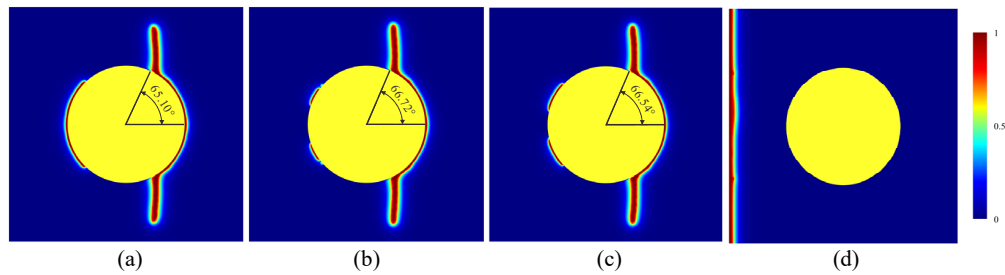


Fig. 2.30 Traction test of a microstructure with a single fiber. Crack phase field for for an applied traction displacement U and different interfacial models: (a) model I ($U = 0.17$ mm), (b) model II ($U = 0.17$ mm), (c) model III ($U = 0.17$ mm) and (d) no interface damage ($U = 0.906$ mm)

To evaluate the capability of the method to describe interfacial damage and investigate the effect of the interfacial cohesive model, another three simulations are performed: in the first one, called “model II”: $g_c^I = 0.1$ N/mm and $t_u = 1$ MPa, in the second one, called “model III”: $g_c^I = 0.2$ N/mm and $t_u = 1$ MPa and in the third one, called “no interface damage” model, only takes into account damage of the bulk (basic phase field method). The comparison of load-displacement curves for all four simulations is depicted in Fig. 2.28(b). The crack phase fields are shown in Fig. 2.30. For the three cohesive models, it can be observed that the cracks are similar which nucleate from the interface and then propagate into the matrix, while for the no interface damage model, the cracks nucleate and propagate within the matrix around the boundary after a very long plastic hardening process. We can then observe that the different interfacial damage models do not have a significant influence on the response, but when removed, the response of the sample is drastically changed. This shows the crucial importance of incorporating such interfacial damage model to properly describe the overall behavior of damaged microstructures.

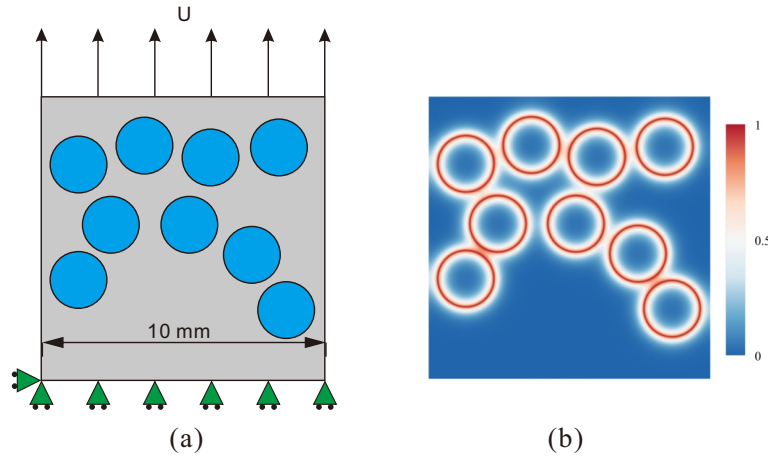


Fig. 2.31 Traction test of a microstructure with randomly distributed fibers: (a) geometry of the domain and boundary conditions; (b) smeared interfaces represented by the interface phase field $\beta(\mathbf{x})$.

2.3.4.4 Traction test of a microstructure with randomly distributed fibers

A microstructure with elastoplastic matrix and damageable interfaces, containing 9 randomly distributed circular fibers (radius $r = 1$ mm) is considered, whose geometry and boundary conditions are illustrated in Fig. 2.31(a). External loading is applied by displacement control through a series of load increments with a fixed step value $\Delta U = 2 \times 10^{-4}$ mm. The material parameters for the matrix and fiber are those of Material I and Material II in Table 2.4, in addition to $\ell = 0.2$ mm and $h = 0.1$ mm. The cohesive model parameters are $g_c^I = 0.1$ N/mm and $t_u = 0.3$ MPa. The distribution of interface phase field is shown in Fig. 2.31(b). It is observed that the diffusive interface concentrates in the nearby area of the interface, and quickly attenuates. The microcracking initiation and final distribution for 9 realizations of microstructures is depicted in Fig. 2.32. The corresponding load-displacement curves are depicted in Fig. 2.33. In the different figures of Fig. 2.32, we can note that in each case, the cracks nucleate at the interface between the matrix and the fibers, and then kink into the matrix. For most cases, a crack path is created between the fibers passing through the interfaces and then leading to the rupture of the specimen. This example illustrates well the capability and robustness of the technique to handle brittle crack propagation from interfaces to the bulk in elasto-plastic composites. In Fig. 2.33, it can be observed that all curves match with each others in the elastic and plastic stages. However, a large dispersion of the individual results in the damaged stage is observed. This shows a strong sensitivity of the overall brittle response to the local distribution of fibers in microstructure as well as the capability of the proposed method to capture these effect.

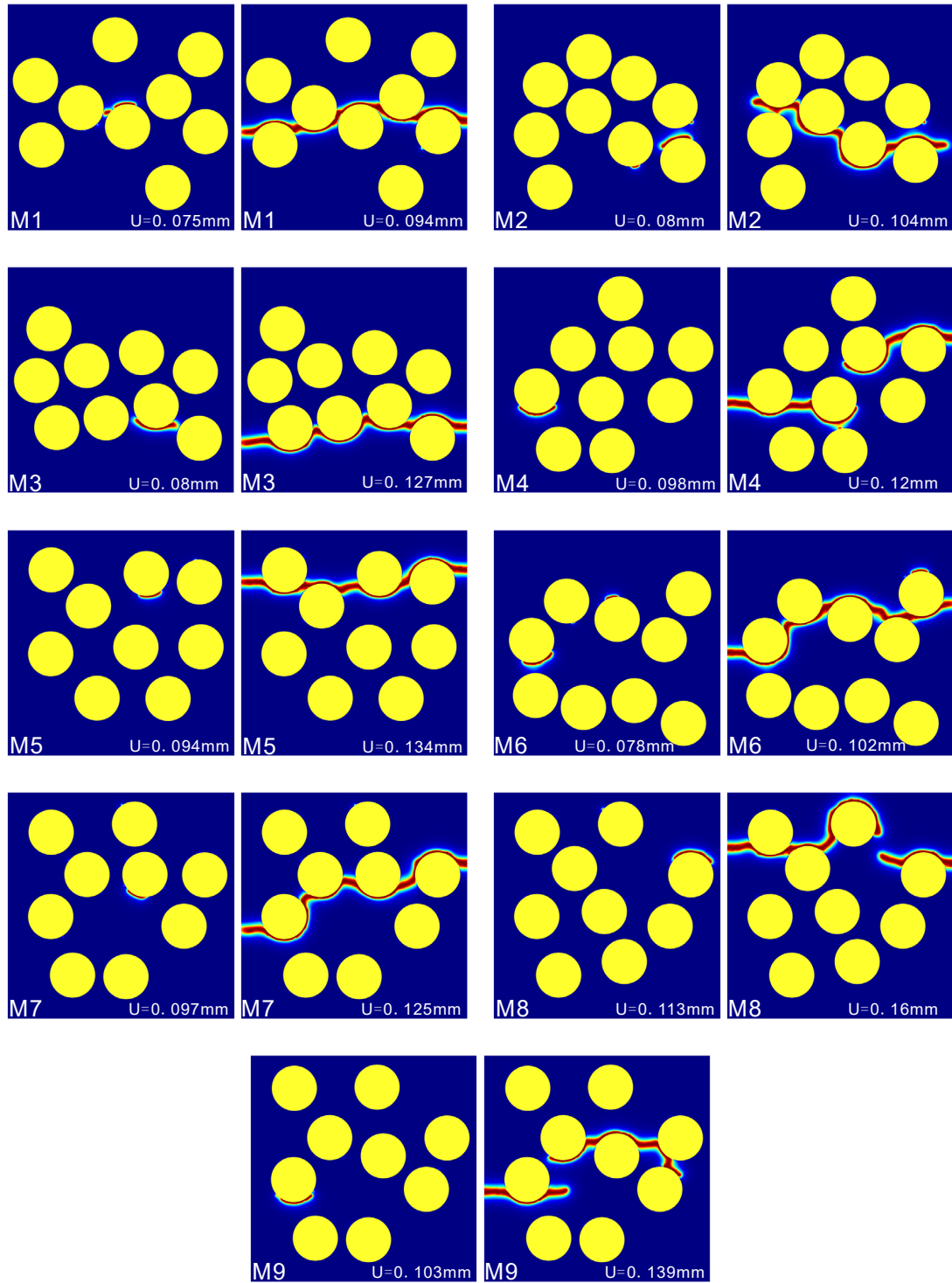


Fig. 2.32 Evolution of crack networks in random elastoplastic microstructures subjected to traction. For each realization, the crack phase field is depicted at early and final stages of propagation. The microstructures are subjected to displacement traction U .

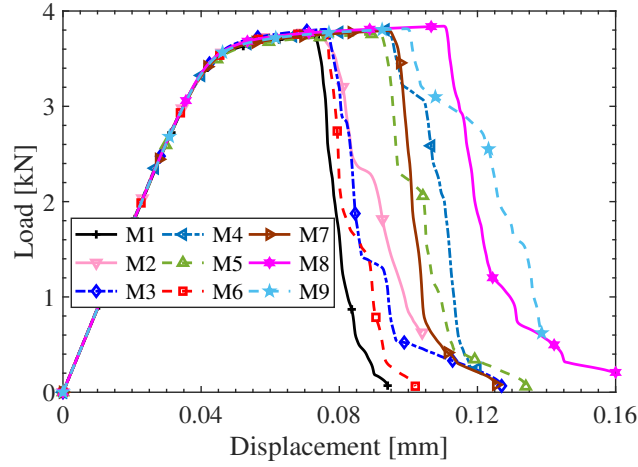


Fig. 2.33 Load-displacement curves corresponding to 9 realizations of random microstructures with interfacial damage subjected to traction.

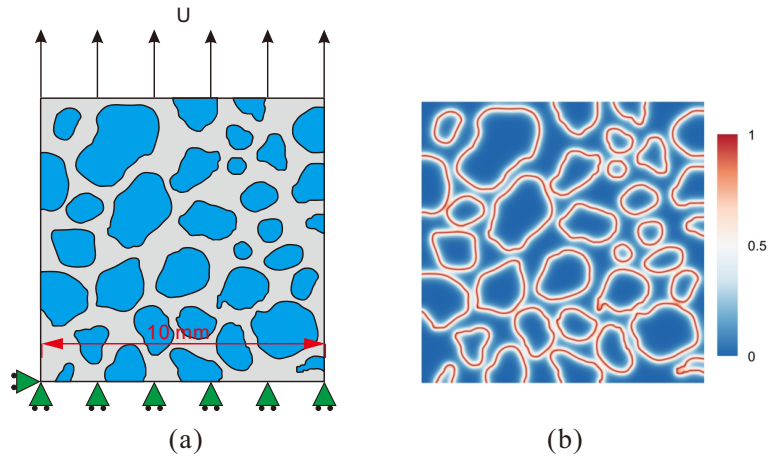


Fig. 2.34 Traction test of a sample whose geometry is obtained from microtomography: (a) geometry of the microstructure and boundary conditions; (b) smeared interface represented by the interface phase field $\beta(\mathbf{x})$.

2.3.4.5 Traction test of a sample whose complex microstructure is obtained from microtomography

In this example, we investigate the capabilities of the method to simulate microcrack propagation in complex microstructures such as obtained by experimental imaging techniques, like X-ray microtomography. The geometry and mechanical boundary conditions are illustrated in Fig. 2.34(a). The material parameters for the matrix and inclusion are those of Material

I and Material II in Table 2.4, in addition to $\ell = 0.1$ mm and $h = 0.1$ mm. The cohesive model parameters are $g_c^I = 0.1$ N/mm and $t_u = 0.3$ MPa. External loading is applied by displacement control through 1800 load increments with a fixed step value $\Delta U = 1 \times 10^{-4}$ mm. The distribution of interface phase field is shown in Fig. 2.34(b). Comparing with the single fiber system and the randomly distributed fibers system, it is much more complicated due to material heterogeneities.

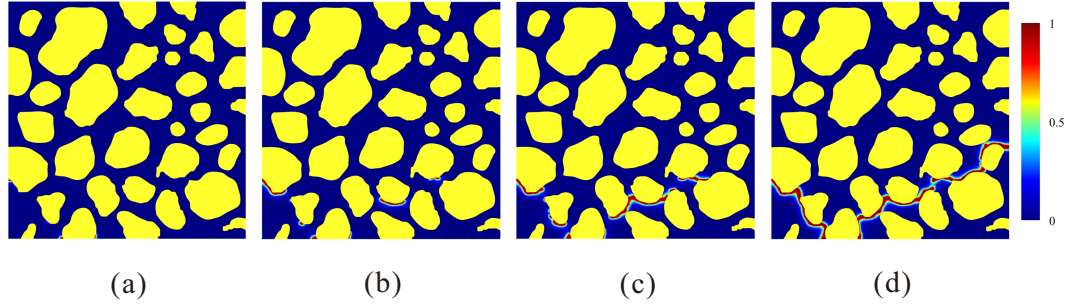


Fig. 2.35 Traction test of an elastoplastic sample whose microstructure is obtained from microtomography. Evolution of the crack phase field for traction displacements $U = 0.09$ mm, $U = 0.11$ mm, $U = 0.13$ mm and $U = 0.18$ mm.

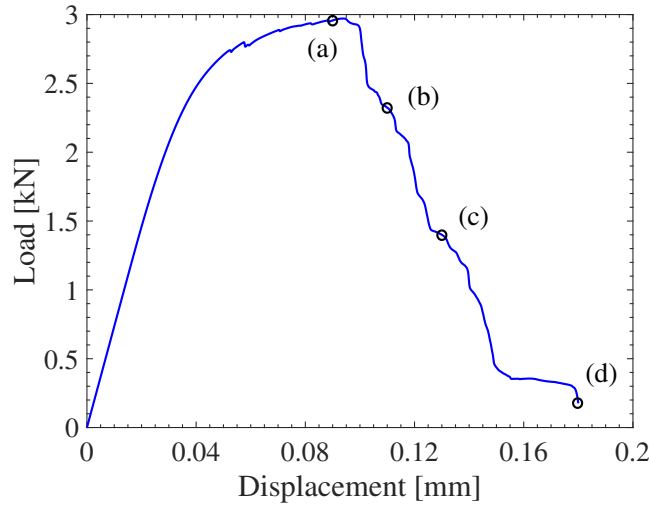


Fig. 2.36 Traction test of an elastoplastic sample whose microstructure is obtained from microtomography: load-displacement curve.

The microcracking evolution in the domain is presented in Fig. 2.35. We can observe that with the increase of the external loading, cracks are initiated in the form of interface debonding and then migrate into the matrix in the form of matrix cracks. Subsequently,

these interface cracks and matrix cracks are interconnected and then lead to the final failure of the microstructure. The crack paths are very complex and show the potential of the method to describe microcracking with interfacial damage in very complex, heterogeneous microstructures. The corresponding load-displacement curve is depicted in Fig. 2.36. It can be seen that the load-displacement curve shows several abrupt stress drops. These stress drops result mainly from the initiation of the microcracking in the complex, heterogeneous microstructure.

2.4 Conclusion

In this chapter, we have firstly presented a numerical implementation framework to simulate brittle fracture in elastoplastic solids as proposed in [53, 9]. Application of the variational principle provides the different equations to be solved in a straightforward manner. A staggered scheme for solving the different equations is implemented to simulate crack initiation and propagation in elastoplastic solids. The modeling of fracture response can be achieved efficiently and robustly by decoupling the fracturing phase field and displacement field. Both 2D and 3D comparisons with available experimental results have validated the present numerical implementation framework.

Then, we have extended the elastoplastic brittle phase field method to consider interfacial damage. To introduce interfacial damage, the energetic formulation has been modified by adding: (i) a strain density depending of the displacement jump related to matrix/inclusions decohesion; (ii) a modified description of the total energy involving a regularized approximation of the singular strain part along the interfaces and (iii) the use of a regularized description of interfaces through diffuse weighting functions which are introduced in the energetic formulation to differentiate the bulk and interfacial damage mechanisms. In that manner, different damage mechanisms can be associated with interfaces as compared to the matrix cracking mechanisms. As a result, the technique allows simulating initiation, propagation and interactions between both fracture and interfacial cracks in elastoplastic composites without special treatment and using standard finite elements. Several numerical examples involving complex microstructures (composites, concrete micro tomography images) have shown the capability of the method to handle complex micro cracks interactions for arbitrary complexity of the microstructures, and convergent solutions with respect to the mesh size.

In Chapter 4, we extend this chapter to gradient plasticity models such as in [106] to involve full damage and plasticity coupling, then a topology optimization framework with this extension is provided to improve elastoplastic fracture resistance of composite solids.

Chapter 3

A SIMP-Phase field topology optimization framework to maximize quasi-brittle fracture resistance of 2D and 3D composites

The main content of this chapter is adapted from our submitted paper in [93].

3.1 Introduction

In this chapter, we extend our previous BESO framework [176] to a combined SIMP and phase field for maximizing the fracture resistance of two-phase materials. It is worth noting that the present framework shares many similarities with the recent framework of [149]: phase field and SIMP are combined for maximizing fracture resistance and the objective function used in both of these works include the external work computed incrementally during a full crack propagation simulation. The main contribution here is the application of the SIMP-phase field to two-material structures, where the objective here is not to minimize the total weight as in [149] but to modify the topology of a second phase material under the constraint of a volume fraction. Another contribution is that we compare our results with BESO formulations with respect to convergence and performance (value of objective function). Finally, the last contribution is applications of this framework to 3D 2-material structures which show the full potential of the approach.

This chapter is organized as follows. In Section 3.2, we review the phase field method for brittle fracture based on the variational framework and provide the details of the finite element

discretization. In Section 3.3, we propose the SIMP topology optimization approach for the design of brittle composites to maximize the fracture resistance in two-phase composites. Section 3.4 provides the overall algorithms to practically implement the present framework. Finally, a series of 2D and 3D numerical examples are presented in Section 3.5 to show the efficiency and potential of the approach.

3.2 Phase field fracture formulation

In this section, we briefly review the phase field method for fracture which will serve as one main ingredient in the present topology optimization framework.

3.2.1 Variational framework

We follow the framework presented in [6] to construct the variational principle, which involves: irreversibility condition, stability condition and energy balance. In this framework, stability condition provides mechanical balance equation and damage criteria. The energy balance provides damage consistency. The total energy for a cracked body is defined as

$$W(\mathbf{u}, d) = \int_{\Omega} \psi_e(\boldsymbol{\varepsilon}(\mathbf{u}), d) d\Omega + \int_{\Omega} \psi_d(d) d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\Omega, \quad (3.1)$$

in which $\mathbf{u}$ is displacement field, $\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$, $\mathbf{f}$ and $\mathbf{F}$ are body forces and prescribed traction over the boundary $\partial\Omega_F$, respectively. Above, ψ_d is the damage dissipative potential defined as

$$\psi_d = g_c \gamma_d(d), \quad (3.2)$$

where $\gamma_d(d)$ is defined in (2.3). ψ_e is the stored elastic energy density function defined as [108]

$$\psi_e(\boldsymbol{\varepsilon}, d) = \left((1-d)^2 + k \right) \psi_e^+(\boldsymbol{\varepsilon}) + \psi_e^-(\boldsymbol{\varepsilon}) \quad (3.3)$$

in which k is a small numerical parameter to prevent loss of definite posedness of the elastic tensor in case of full damage, ψ_e^+ and ψ_e^- are the tensile and compressive energies,

$$\psi_e^{\pm} = \frac{1}{2} \lambda \langle \text{tr}[\boldsymbol{\varepsilon}] \rangle_{\pm}^2 + \mu \text{tr}[\boldsymbol{\varepsilon}^{\pm}]^2, \quad (3.4)$$

with λ and μ the standard lame parameters. Note that only tensile damage degradation is taken into account in the elastic energy density (3.3) through a decomposition of the elastic

strain ε into tensile/positive and compressive/negative parts:

$$\varepsilon = \varepsilon^+ + \varepsilon^- \quad \text{with} \quad \varepsilon^\pm = \sum_{i=1}^3 \langle \varepsilon^i \rangle_\pm \mathbf{n}^i \otimes \mathbf{n}^i, \quad (3.5)$$

where $\langle x \rangle_\pm = \frac{1}{2} (x \pm |x|)$, ε^i and $\mathbf{n}^i$ are the eigenvalues and eigenvectors of ε .

3.2.1.1 Irreversibility condition

See section 2.2.2.2.

3.2.1.2 First-order stability condition

The first order stability condition (see [113, 114, 143]) is expressed by:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, d) + D_{\delta d} W(\mathbf{u}, d) \geq 0, \quad (3.6)$$

Applied to (3.1), it yields:

$$\int_{\Omega} \sigma : \varepsilon(\delta \mathbf{u}) d\Omega + \int_{\Omega} \left(\frac{\partial \psi_e}{\partial d} + \frac{\partial \psi_d}{\partial d} \right) \delta d d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega \geq 0 \quad (3.7)$$

where

$$\sigma = \frac{\partial \psi_e}{\partial \varepsilon} = \left((1-d)^2 + k \right) \left(\lambda \langle \text{tr}[\varepsilon] \rangle_+ \mathbf{1} + 2\mu \varepsilon^+ \right) + \lambda \langle \text{tr}[\varepsilon] \rangle_- \mathbf{1} + 2\mu \varepsilon^- \quad (3.8)$$

in which $\mathbf{1}$ is the second-order identity tensor and σ^+/σ^- are the undamaged tensile/compressive stress tensors.

From (3.7), the following results stem out:

- For $\delta d = 0$, find $\mathbf{u} \in \mathcal{S}_u$, $\mathcal{S}_u = \{ \mathbf{u} | \mathbf{u}(\mathbf{x}) = \bar{\mathbf{u}} \text{ on } \partial \Omega_u, \mathbf{u} \in H^1(\Omega) \}$ such that:

$$\int_{\Omega} \sigma : \varepsilon(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0, \quad (3.9)$$

which is the weak form of the mechanical equilibrium equation, with $\delta \mathbf{u} \in \mathcal{S}_u^0$, $\mathcal{S}_u^0 = \{ \delta \mathbf{u} | \delta \mathbf{u}(\mathbf{x}) = 0 \text{ on } \partial \Omega_u, \mathbf{u} \in H^1(\Omega) \}$.

- For $\delta \mathbf{u} = \mathbf{0}$ we obtain:

$$\int_{\Omega} \left(\frac{\partial \psi_e}{\partial d} + \frac{\partial \psi_d}{\partial d} \right) \delta d d\Omega \geq 0 \quad (3.10)$$

which is the weak form of the damage criterion. In local form, it can be expressed as:

$$f^d(d) = - \left(\frac{\partial \psi_e}{\partial d} + \frac{\partial \psi_d}{\partial d} \right) \leq 0 \text{ in } \Omega. \quad (3.11)$$

3.2.1.3 Energy balance

The energy balance represents the need for the total energy to remain constant as the state variables evolve. Following a procedure analogous to the treatment of the stability condition, this condition leads to

$$\int_{\Omega} \left[-\boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\dot{\mathbf{u}}) - \left(\frac{\partial \psi_e}{\partial d} + \frac{\partial \psi_d}{\partial d} \right) \dot{d} \right] d\Omega + \int_{\partial\Omega_F} \mathbf{F} \cdot \dot{\mathbf{u}} dS + \int_{\Omega} \mathbf{f} \cdot \dot{\mathbf{u}} d\Omega = 0. \quad (3.12)$$

For $\dot{\mathbf{u}} = \mathbf{0}$, and using (3.11), the damage consistency condition is obtained:

$$f^d(d) \dot{d} = 0. \quad (3.13)$$

3.2.1.4 Alternate minimization

In this section, a staggered alternate minimization algorithm is applied, which naturally stems out from the energetic principles. With the total energy (3.1) at hand, the alternate minimization follows.

- Minimization with respect to the displacement field:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, d) = 0 \quad (3.14)$$

which leads to

$$R_1 = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\delta \mathbf{u}) d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (3.15)$$

which corresponds to the weak form of the mechanical problem to be solved for $\mathbf{u}$, given d .

- Minimization with respect to the damage field:

$$D_{\delta d} W(\mathbf{u}, d) = \int_{\Omega} \left(\frac{\partial \psi_e}{\partial d} + \frac{\partial \psi_d}{\partial d} \right) \delta d d\Omega = 0. \quad (3.16)$$

which corresponds to the global problem to be solved to find the field $d(\mathbf{x})$ (phase field problem), given $\mathbf{u}$.

3.2.1.5 Governing equations

The associated Euler-Lagrange equations to (3.15) are given by:

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} & \text{in } \Omega, \\ \mathbf{u} = \bar{\mathbf{u}} & \text{on } \partial\Omega_u, \\ \boldsymbol{\sigma} \mathbf{n} = \mathbf{F} & \text{on } \partial\Omega_F. \end{cases} \quad (3.17)$$

Using (3.16) and the property:

$$(\Delta d) \delta d = \nabla \cdot (\nabla d \delta d) - \nabla d \cdot \nabla (\delta d) \quad (3.18)$$

as well as the divergence theorem and $\nabla d \cdot \mathbf{n} = 0$, we obtain the weak form of the phase field problem as:

$$\int_{\Omega} \left(\left\{ -2(1-d)\psi_e^+ + \frac{g_c d}{\ell_d} \right\} \delta d + g_c \ell_d \nabla d \cdot \nabla (\delta d) \right) d\Omega = 0. \quad (3.19)$$

To prescribe irreversibility, we employ the technique introduced in [111] which consists in substituting the above weak form with:

$$\int_{\Omega} (\{-2(1-d)\mathcal{H}(\varepsilon) + 2\psi_c d\} \delta d + 2\psi_c \ell_d^2 \nabla d \cdot \nabla (\delta d)) d\Omega = 0, \quad (3.20)$$

in which

$$\mathcal{H}(\varepsilon) = \max_{s \in [0,1]} [\langle \psi_e^+(\varepsilon, s) - \psi_c \rangle_+] \quad (3.21)$$

and ψ_c is a specific fracture energy density, which can be further related to a critical fracture stress σ_c by:

$$\psi_c = \frac{1}{2E} \sigma_c^2, \quad (3.22)$$

where E is the Young's modulus.

The corresponding Euler-Lagrange equations to (3.20) are given by:

$$\begin{cases} \psi_c (d - \ell_d^2 \Delta d) = (1-d) \mathcal{H}(\varepsilon) \\ \nabla d \cdot \mathbf{n} = 0 & \text{on } \partial\Omega, \\ d = 1 & \text{on } \Gamma. \end{cases} \quad (3.23)$$

The different equations of the model are summarized in Table 3.1.

Table 3.1 Governing equations of the phase field model.

Irreversibility	$\dot{d} \geq 0, \quad 0 \leq d \leq 1$
Mechanical balance	$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \text{ in } \Omega$ $\mathbf{u} = \bar{\mathbf{u}} \text{ on } \partial\Omega_u, \quad \boldsymbol{\sigma}\mathbf{n} = \mathbf{F} \text{ on } \partial\Omega_F$
Constitutive law	$\boldsymbol{\sigma} = \left((1-d)^2 + k \right) (\lambda \langle \text{tr}[\boldsymbol{\varepsilon}] \rangle_+ \mathbf{1} + 2\mu \boldsymbol{\varepsilon}^+) + \lambda \langle \text{tr}[\boldsymbol{\varepsilon}] \rangle_- \mathbf{1} + 2\mu \boldsymbol{\varepsilon}^-$
Damage criterion	$\psi_c (d - \ell_d^2 \Delta d) - (1-d) \mathcal{H}(\boldsymbol{\varepsilon}) \geq 0$ $\mathcal{H}(\boldsymbol{\varepsilon}) = \max_{s \in [0, t]} [\langle \psi_e^+(\boldsymbol{\varepsilon}, s) - \psi_c \rangle_+]$
Damage consistency	$(\psi_c (d - \ell_d^2 \Delta d) - (1-d) \mathcal{H}(\boldsymbol{\varepsilon})) \dot{d} = 0$

3.2.2 Finite element discretization

The weak form of the mechanical problem can be found in (3.15). Using (3.23), we can re-write the associated weak form for the damage problem (3.16) as: find $d(\mathbf{x}) \in \mathcal{S}_d$, $\mathcal{S}_d = \{d | d(\mathbf{x}) = 1 \text{ on } \Gamma, \quad d \in H^1(\Omega)\}$:

$$R_2 = \int_{\Omega} \{(\mathcal{H} + \psi_c) d \delta d + \psi_c \ell_d^2 \nabla d \cdot \nabla (\delta d)\} d\Omega - \int_{\Omega} \mathcal{H} \delta d d\Omega = 0. \quad (3.24)$$

and $\delta d(\mathbf{x}) \in \mathcal{S}_d^0$, $\mathcal{S}_d^0 = \{\delta d | \delta d(\mathbf{x}) = 0 \text{ on } \partial\Omega, \quad d \in H^1(\Omega)\}$. In this work, we adopt the same finite element discretization for the approximation of the crack phase field d and the displacement field $\mathbf{u}$. We can express the discretization of the phase field problem as:

$$d = \mathbf{N}_d \mathbf{d}_e, \quad \nabla d = \mathbf{B}_d \mathbf{d}_e, \quad (3.25)$$

where $\mathbf{N}_d$ and $\mathbf{B}_d$ are matrices of damage shape function and of damage shape function derivatives, respectively, and $\mathbf{d}_e$ denote nodal damage in one element. The discretization of damage problem (3.24) results into the following discrete system of equations:

$$\mathbf{K}_d \mathbf{d} = \mathbf{F}_d \quad (3.26)$$

in which

$$\mathbf{K}_d = \int_{\Omega} \{[\mathcal{H} + \psi_c] \mathbf{N}_d^T \mathbf{N}_d + \psi_c \ell_d^2 \mathbf{B}_d^T \mathbf{B}_d\} d\Omega \quad (3.27)$$

and

$$\mathbf{F}_d = \int_{\Omega} \mathbf{N}_d^T \mathcal{H} d\Omega, \quad (3.28)$$

where $\mathcal{H}$ is given in (3.21). The displacement problem can be discretized as:

$$\mathbf{u} = \mathbf{N}_u \mathbf{u}_e, \quad \delta \mathbf{u} = \mathbf{N}_u \delta \mathbf{u}_e, \quad [\boldsymbol{\varepsilon}](\mathbf{u}) = \mathbf{B}_u \mathbf{u}_e, \quad [\boldsymbol{\varepsilon}](\delta \mathbf{u}) = \mathbf{B}_u \delta \mathbf{u}_e \quad (3.29)$$

where $\mathbf{u}_e$, $\mathbf{N}_u$ and $\mathbf{B}_u$ are nodal displacement components in one element, a matrix of displacement shape function and a matrix of displacement shape function derivatives, respectively. Using the weak form (3.15), we obtain the following discrete system of equations:

$$\mathbf{K}_u \mathbf{u} = \mathbf{F}_u \quad (3.30)$$

with the force vector

$$\mathbf{F}_u = \int_{\Omega} \mathbf{N}_u^T \mathbf{f} d\Omega + \int_{\partial\Omega_F} \mathbf{N}_u^T \mathbf{F} dS \quad (3.31)$$

and the stiffness matrix

$$\mathbf{K}_u = \int_{\Omega} \mathbf{B}_u^T \underbrace{\left[(1-d)^2 \left(\lambda R^+ [\mathbf{1}] [\mathbf{1}]^T + 2\mu \mathbf{P}^+ \right) + \left(\lambda R^- [\mathbf{1}] [\mathbf{1}]^T + 2\mu \mathbf{P}^- \right) \right]}_{\frac{\partial[\boldsymbol{\sigma}]}{\partial[\boldsymbol{\varepsilon}]}} \mathbf{B}_u d\Omega \quad (3.32)$$

where $[\boldsymbol{\sigma}]$ and $[\boldsymbol{\varepsilon}]$ are the vector forms corresponding to the second order tensors of stress $\boldsymbol{\sigma}$ and strain $\boldsymbol{\varepsilon}$. $R^\pm$ and $\mathbf{P}^\pm$ are two operators for the decomposition of strain into the tensile and compressive parts (see [129] for more details) and $\mathbf{P}^\pm$ are the matrix forms corresponding to the fourth order projection tensor $\mathbb{P}^\pm = \frac{\partial \boldsymbol{\varepsilon}^\pm}{\partial \boldsymbol{\varepsilon}}$, which can be found in [109, 7].

3.3 SIMP Topology optimization formulation

In this section, we present a SIMP topology optimization framework for maximizing the fracture resistance of a two-phase (composite) structure.

3.3.1 Optimization problem statement

The topology optimization problem is conducted with respect to a density variable $\rho(\mathbf{x})$ which is associated with the inclusion phase. In other words, $\rho(\mathbf{x}) = 1$ corresponds to inclusion phase and $\rho(\mathbf{x}) = 0$ corresponds to the matrix phase.

For stability considerations, here displacement-controlled loading is adopted. For a prescribed displacement load, the fracture resistance maximization is equivalent to the maximization of the mechanical work. Recalling that the fracture problem is quasi-static, we introduce a pseudo time t associated with the external load evolution, with $t \in [0, t^{max}]$,

where t^{max} denotes the maximum loading time corresponding to the maximum prescribed displacement $\bar{u}^{max}$ at the failure step.

The optimization problem is then defined as follows:

$$\text{Maximize : } J(\rho, \mathbf{u}, d) \quad (3.33)$$

$$\text{subject : } R_1(\rho, \mathbf{u}(t), d(t)) = 0, \quad \forall t \in [0, t^{max}] \quad (3.34)$$

$$R_2(\rho, \mathbf{u}(t), d(t)) = 0, \quad \forall t \in [0, t^{max}] \quad (3.35)$$

$$f^{inc} = \frac{V(\Omega^{inc})}{V(\Omega)} = \frac{\int_{\Omega} \rho(\mathbf{x}) d\Omega}{V(\Omega)} \quad (3.36)$$

$$0 \leq \rho(\mathbf{x}) \leq 1 \quad (3.37)$$

$$\mathbf{u}(t) \in \mathcal{S}_u \quad (3.38)$$

$$d(t) \in \mathcal{S}_d, \quad (3.39)$$

where $V(\Omega^{inc})$ is the inclusion volume, $V(\Omega)$ is the total volume of the domain, and

$$J = \int_0^{t^{max}} \mathbf{F}_{ext}(t) \cdot \bar{\mathbf{u}}(t) dt, \quad (3.40)$$

where R_1 and R_2 are given by (3.15) and (3.24), $\mathbf{F}_{ext}$ is the external force response at the load point and f^{inc} is the prescribed volume fraction of the inclusion phase.

Following [26], the material interpolations for the two-phase material are defined as

$$\begin{cases} E(\mathbf{x}) = (\rho(\mathbf{x}))^p E_{inc} + (1 - (\rho(\mathbf{x}))^p) E_{mat}, \\ \psi_c(\mathbf{x}) = (\rho(\mathbf{x}))^p \psi_{c,inc} + (1 - (\rho(\mathbf{x}))^p) \psi_{c,mat}, \end{cases} \quad (3.41)$$

where E and ψ_c are the Young's modulus and the fracture energy density. $(\cdot)_{inc}$ and $(\cdot)_{mat}$ are the parameters corresponding to the inclusion and the matrix phase, respectively. The Poisson's ratios of the two material phases are assumed identical. Above, p is the penalty coefficient to enforce solutions close to $\rho = 0$ or 1. Following [156], we choose $p = 3$. Fig. 3.1 shows the difference of Young's modulus interpolation for SIMP and BESO [176]. The continuous material interpolations for SIMP ensures that the optimization problem is smooth and that the objective function is differentiable.

3.3.2 Discrete topology optimization problem

The design domain Ω is discretized into N_e finite elements and each element e is assigned with a topology design variable, or element density ρ_e , which is allowed to vary continuously in the range $[0, 1]$. Here, a density of $\rho_e = 1$ corresponds to an element completely filled with

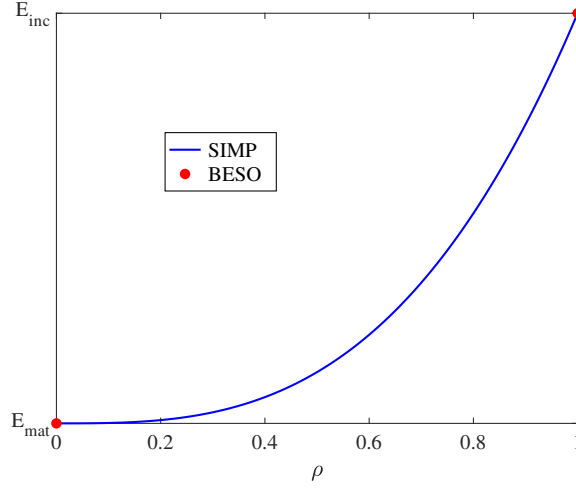


Fig. 3.1 Young's modulus interpolations for SIMP and BESO.

the inclusion phase, whereas $\rho_e = 0$ corresponds to an element completely filled with the matrix phase. We define the vector $\{\rho\} = \{\rho_1, \rho_2, \dots, \rho_{N_e}\}$ containing the discrete values of densities in elements of the mesh.

The discrete form of (3.33)-(3.39) is then defined as:

$$\text{Maximize : } J^{\Delta u}(\rho, \mathbf{u}, \mathbf{d}) \quad (3.42)$$

$$\text{subject : } \mathbf{K}_u^n \mathbf{u}^n - \mathbf{F}_u^n = \mathbf{0}, \quad n = 1, 2, \dots, n_{load} \quad (3.43)$$

$$\sum_{e=1}^{N_e} \rho_e v_e / \left(\sum_{e=1}^{N_e} v_e \right) = f^{inc} \quad (3.44)$$

$$0 \leq \rho_e \leq 1, \quad e = 1, 2, \dots, N_e \quad (3.45)$$

$$\mathbf{u}^n \in \mathcal{S}_u, \quad n = 1, 2, \dots, n_{load} \quad (3.46)$$

$$\mathbf{d}^n \in \mathcal{S}_d, \quad n = 1, 2, \dots, n_{load}, \quad (3.47)$$

and $J^{\Delta u}$ in (3.42) is approximated by:

$$J^{\Delta u} = \sum_{n=1}^{n_{load}} \Delta J^n \approx \frac{1}{2} \sum_{n=1}^{n_{load}} (\mathbf{F}_{ext}^n + \mathbf{F}_{ext}^{n-1})^T \Delta \mathbf{u}^n, \quad (3.48)$$

where $\Delta \mathbf{u}^n$ denotes the prescribed load increment at load n . Above, v_e is the volume (area in 2D) of the e -th element and f^{inc} is the target inclusion volume which is prescribed during the optimization process. The stiffness matrix $\mathbf{K}_u^n$ at the n -th load increment is constructed following (3.32).

It should be noted that in this work the continuous topology design variable $\rho_e \in [0, 1]$ allows using well-proven gradient-based optimization update approaches (e.g., Optimality Criteria methods (OC) [156, 17], the Method of Moving Asymptotes (MMA) [166] and so on), in turn ensuring algorithmic convergence within a reasonable number of topological iterations (from 10 to 1000 iterations) [157].

Another important remark is that in the present paper, we do not explicitly use the second constraint (3.35) in the discrete problem (3.42)-(3.47) and in the following sensitivity analysis. In fact, this constraint is taken into account implicitly as the regularized fracture problem is solved in a staggered solving procedure. When the mechanical problem (3.15) is solved, the damage variable $d(\mathbf{x})$ is assumed to be known from previous iteration and then the phase field problem equation R_2 in (3.24) is supposed to be verified. This assumption considerably simplifies the sensitivity analysis presented next.

3.3.3 Sensitivity analysis

In order to solve the optimization problem (3.42)-(3.47), the sensitivity of the objective function J corresponding to change in the design variable must be determined. The derivation of the sensitivity requires using the adjoint method (e.g., [40, 176]). Assuming that the mechanical problem (3.30) has been solved, we introduce the Lagrangian:

$$J^{\Delta u} \approx \bar{J} = \frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\mathbf{F}_u^n + \mathbf{F}_u^{n-1})^T \Delta \mathbf{u}^n + (\lambda_1^n)^T \mathbf{R}^n + (\lambda_2^n)^T \mathbf{R}^{n-1} \right\} \quad (3.49)$$

in which $\mathbf{R}^n$ and $\mathbf{R}^{n-1}$ are the residuals of (3.30) at n -th and $(n-1)$ -th load increments, respectively. λ_1^n and λ_2^n are Lagrange multipliers which have the same dimension with the displacement vector $\mathbf{u}$.

Notice that for displacement-controlled loading problem, displacement components at the boundary nodes and force components at the free nodes are fixed, hence, they are independent of the current value of ρ . Here we introduce a division of all degrees of freedom into essential (index E; associated with Dirichlet boundary conditions) and free (index F) nodal values. For a vector $\mathbf{v}$ and a matrix $\mathbf{M}$ we have

$$\mathbf{v} \sim \begin{bmatrix} \mathbf{v}_E \\ \mathbf{v}_F \end{bmatrix} \quad \text{and} \quad \mathbf{M} \sim \begin{bmatrix} \mathbf{M}_{EE} & \mathbf{M}_{EF} \\ \mathbf{M}_{FE} & \mathbf{M}_{FF} \end{bmatrix}. \quad (3.50)$$

We then have these unknowns at the n -th load increment

$$\frac{\partial \mathbf{u}^n}{\partial \rho_e} = \begin{bmatrix} \mathbf{0} \\ \frac{\partial \mathbf{u}_E^n}{\partial \rho_e} \end{bmatrix}, \quad \frac{\partial \Delta \mathbf{u}^n}{\partial \rho_e} = \begin{bmatrix} \mathbf{0} \\ \frac{\partial \Delta \mathbf{u}_E^n}{\partial \rho_e} \end{bmatrix}, \quad \mathbf{F}_u^n = \begin{bmatrix} \mathbf{F}_{u,E}^n \\ \mathbf{0} \end{bmatrix}, \quad \frac{\partial \mathbf{F}_u^n}{\partial \rho_e} = \begin{bmatrix} \frac{\partial \mathbf{F}_{u,E}^n}{\partial \rho_e} \\ \mathbf{0} \end{bmatrix} \quad (3.51)$$

Here for arbitrary load increment indices $n = 1, \dots, n_{\text{load}}$, $m = 1, \dots, n_{\text{load}}$, we have

$$\frac{\partial}{\partial \rho_e} \left((\mathbf{F}_u^m)^T \Delta \mathbf{u}^n \right) = \left(\frac{\partial \mathbf{F}_u^m}{\partial \rho_e} \right)^T \Delta \mathbf{u}^n + (\mathbf{F}_u^m)^T \frac{\partial \Delta \mathbf{u}^n}{\partial \rho_e} = \left(\frac{\partial \mathbf{F}_u^m}{\partial \rho_e} \right)^T \Delta \mathbf{u}^n. \quad (3.52)$$

With the above property at hand, the derivative of the objective function J in (3.49) is given by

$$\frac{\partial \bar{J}}{\partial \rho_e} = \frac{1}{2} \sum_{n=1}^{n_{\text{load}}} \left\{ \frac{\partial (\mathbf{F}_u^n + \mathbf{F}_u^{n-1})^T}{\partial \rho_e} \Delta \mathbf{u}^n + (\lambda_1^n)^T \frac{\partial \mathbf{R}^n}{\partial \rho_e} + (\lambda_2^n)^T \frac{\partial \mathbf{R}^{n-1}}{\partial \rho_e} \right\}. \quad (3.53)$$

The derivatives of $\mathbf{R}^m$ at the equilibrium of the m -th load increment with respect to ρ_e can be expanded as

$$\frac{\partial \mathbf{R}^m}{\partial \rho_e} = \frac{\partial \mathbf{F}_u^m}{\partial \rho_e} - \frac{\partial \mathbf{K}_u^m}{\partial \rho_e} \mathbf{u}^m - \mathbf{K}_u^m \frac{\partial \mathbf{u}^m}{\partial \rho_e}. \quad (3.54)$$

Using (3.51) and (3.54), (3.53) can be reformulated as

$$\begin{aligned} \frac{\partial \bar{J}}{\partial \rho_e} = \frac{1}{2} \sum_{n=1}^{n_{\text{load}}} \left\{ \left(\frac{\partial \mathbf{F}_{u,E}^n}{\partial \rho_e} \right)^T (\Delta \mathbf{u}_E^n + \lambda_{1,E}^n) + \left(\frac{\partial \mathbf{F}_{u,E}^{n-1}}{\partial \rho_e} \right)^T (\Delta \mathbf{u}_E^n + \lambda_{2,E}^n) \right. \\ \left. - (\lambda_1^n)^T \left(\frac{\partial \mathbf{K}_u^n}{\partial \rho_e} \mathbf{u}^n + \mathbf{K}_u^n \frac{\partial \mathbf{u}^n}{\partial \rho_e} \right) - (\lambda_2^n)^T \left(\frac{\partial \mathbf{K}_u^{n-1}}{\partial \rho_e} \mathbf{u}^{n-1} + \mathbf{K}_u^{n-1} \frac{\partial \mathbf{u}^{n-1}}{\partial \rho_e} \right) \right\}. \end{aligned} \quad (3.55)$$

In order to eliminate the unknowns $\frac{\partial \mathbf{F}_{u,E}^n}{\partial \rho_e}$ and $\frac{\partial \mathbf{F}_{u,E}^{n-1}}{\partial \rho_e}$ in (3.55), we choose

$$\lambda_{1,E}^n = -\Delta \mathbf{u}_E^n \quad \text{and} \quad \lambda_{2,E}^n = -\Delta \mathbf{u}_E^n. \quad (3.56)$$

Then we can re-write (3.55) as

$$\begin{aligned} \frac{\partial \bar{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{\text{load}}} \left\{ (\lambda_1^n)^T \frac{\partial \mathbf{K}_u^n}{\partial \rho_e} \mathbf{u}^n + (\mathbf{K}_{u,FE}^n \lambda_{1,E}^n + \mathbf{K}_{u,FF}^n \lambda_{1,F}^n)^T \frac{\partial \mathbf{u}_F^n}{\partial \rho_e} \right. \\ \left. + (\lambda_2^n)^T \frac{\partial \mathbf{K}_u^{n-1}}{\partial \rho_e} \mathbf{u}^{n-1} + (\mathbf{K}_{u,FE}^{n-1} \lambda_{2,E}^n + \mathbf{K}_{u,FF}^{n-1} \lambda_{2,F}^n)^T \frac{\partial \mathbf{u}_F^{n-1}}{\partial \rho_e} \right\}. \end{aligned} \quad (3.57)$$

To eliminate the unknowns $\frac{\partial \mathbf{u}_E^n}{\partial \rho_e}$ and $\frac{\partial \mathbf{u}_F^{n-1}}{\partial \rho_e}$ in (3.57), we choose

$$\lambda_{1,F}^n = (\mathbf{K}_{u,FF}^n)^{-1} \mathbf{K}_{u,FE}^n \Delta \mathbf{u}_E^n \quad \text{and} \quad \lambda_{2,F}^n = \left(\mathbf{K}_{u,FF}^{n-1} \right)^{-1} \mathbf{K}_{u,FE}^{n-1} \Delta \mathbf{u}_E^n. \quad (3.58)$$

Using (3.56) and (3.58), we can obtain the final objective derivative

$$\frac{\partial \bar{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_1^n)^T \frac{\partial \mathbf{K}_u^n}{\partial \rho_e} \mathbf{u}^n + (\lambda_2^n)^T \frac{\partial \mathbf{K}_u^{n-1}}{\partial \rho_e} \mathbf{u}^{n-1} \right\}. \quad (3.59)$$

For each element e , (3.59) can be re-written as

$$\begin{aligned} \alpha_e &= \sum_{n=1}^{n_{load}} (\Delta \alpha_e)^n \\ &= -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_{1,e}^n)^T \frac{\partial \mathbf{k}_{u,e}^n}{\partial \rho_e} \mathbf{u}_e^n + (\lambda_{2,e}^n)^T \frac{\partial \mathbf{k}_{u,e}^{n-1}}{\partial \rho_e} \mathbf{u}_e^{n-1} \right\}, e = 1, \dots, N_e, \end{aligned} \quad (3.60)$$

in which $(\cdot)_e$ is the element component of $(\cdot)$ and $\mathbf{k}_{u,e}^n$ is the element stiffness matrix for element e at the n -th load step. For the sake of simplicity, we use α_e and α to represent element sensitivity and vector of all element sensitivities. It should be noted that in this work we need to evaluate the sensitivities of all elements, unlike our previous works [176, 49] which only compute the sensitivities of the inclusion elements and set directly the sensitivities of the matrix elements to zeros.

3.4 Overall algorithm

This section present the overall algorithms of the proposed method. We first introduce the algorithm used to simulate one crack simulation from the initial nucleation to complete failure, which will be used within one step of the topology optimization. During this simulation, the sensitivities are computed at the same time than the fracture evolution. Then, the overall topology optimization is presented.

In the fracture evolution problem, a staggered scheme is employed following [108], where at each load increment the crack phase field problem is solved for fixed displacement field which is known from the previous time step. The displacement problem is then solved for the obtained crack phase field. Finally the sensitivity analysis is implemented after the staggered scheme.

The flowchart for fracture evolution problem and sensitivity calculations is provided in Algorithm 4.

Algorithm 4: Fracture evolution problem and sensitivity calculations.

Input: Densities $\{\rho^k\}$

Output: the total mechanical work J^k and sensitivity vector α^k

Initialize $\mathbf{u}^0 = \mathbf{0}$, $\mathcal{H}^0 = \mathbf{0}$, $J^0 = 0$ and $\alpha^0 = \mathbf{0}$.

Loop over load increments n_{load}

for $n = 1, \dots, n_{\text{load}}$ **do**

%% Crack phase field problem %%

 Given $\mathbf{u}^{n-1}$ and $\mathcal{H}^{n-1}$,

 Compute $\mathcal{H}^n$ by (3.21)

 Compute $\mathbf{K}_d^n$ and $\mathbf{F}_d^n$ from (3.27) and (3.28)

 Compute the crack phase field $\mathbf{d}^n$ from (3.26)

%% Displacement problem %%

 Given $\bar{\mathbf{u}}^n$ and $\mathbf{d}^n$

 Compute $\mathbf{K}_u^n$ and $\mathbf{F}_u^n$ from (3.32) and (3.31)

 Compute the displacement field $\mathbf{u}^n$ from (3.30)

%% Sensitivity calculations %%

 Compute Lagrange multipliers λ_1^n and λ_2^n from (3.56) and (3.58)

 Compute increment of sensitivity vector $\Delta\alpha^n$ with λ_1^n and λ_2^n from (3.60)

 Compute increment of mechanical work ΔJ^n from (3.48)

 Update $\alpha^n = \alpha^{n-1} + \Delta\alpha^n$ and $J^n = J^{n-1} + \Delta J^n$

$n = n + 1$

end

$\alpha^k = \alpha^{n_{\text{load}}}$ and $J^k = J^{n_{\text{load}}}$

In order to remove instabilities such as checkerboard patterns and to avoid mesh-dependency in topology optimization process, element sensitivities are smoothed by means of a filtering scheme [156]

$$\alpha_e = \frac{\sum_{j=1}^{N_e} w_{ej} \alpha_j}{\sum_{j=1}^{N_e} w_{ej}}, \quad (3.61)$$

in which w_{ej} is a linear weight factor

$$w_{ej} = \max(0, r_{\min} - \Delta(e, j)) \quad (3.62)$$

which is determined by the prescribed filter radius $r_{\min}$ and the element center-to-center distance $\Delta(e, j)$ between element e and j .

The optimization problem (3.33)-(3.39) could be solved using several different approaches such as OC method [156, 17] and the MMA [166] as illustrated in section 3.3.2. In this work, the OC method is employed to update the design variables. The overall algorithm is illustrated in Algorithm 5.

Algorithm 5: Overall topology optimization algorithm

```

Initialize inclusion densities  $\{\rho^1\}$ .
%% Topology optimization iteration %%
Set  $k = 1, Err = 1$  and iterative tolerance  $tol$ 
while  $Err > tol$  do
    %% Regularized fracture problem and sensitivity calculations %%
    Compute regularized fracture problem, obtain sensitivity vector  $\alpha^k$  and total
    mechanical work  $J^k$  with  $\rho^k(\mathbf{x})$  from Algorithm 4
    %% Filtering scheme %%
    Obtain the smoothed  $\alpha^k$  with (3.61)
    %% OC method %%
    Update the design variable  $\rho^{k+1}$  with smoothed  $\alpha^k$ 
    %% Compute convergence %%
    if  $k \geq 10$  then
        |  $Err = \frac{|\sum_{m=k-4}^k J^m - \sum_{n=k-9}^{k-5} J^n|}{\sum_{n=k-9}^{k-5} J^n}$ 
    else
        |  $Err = 1$ 
    end
     $k = k + 1$ 
end

```

3.5 Numerical examples

In this section we present several examples in both 2D and 3D to show the capability and convergence of the method, and compare the results with our previous work done by BESO method [176]. In all 2D examples uniform meshes of quadrilateral bilinear elements with the plane strain assumption have been employed. Uniform meshes of eight-node cubic elements have been used for the 3D examples. Both damage and displacement fields are discretized with the same finite element meshes. The characteristic length scale parameter ℓ_d for the phase field problem in (2.3) and the filter radius r_{min} in (3.62) are both set to be twice the typical finite element size $\ell_d = r_{min} = 2h_e$. For the sake of clear visualization, only the crack phase field with values higher than 0.4 in 2D examples and values higher than 0.95 in 3D

examples are plotted. The material properties are shown in Table 3.2. The inclusion volume fraction f^{inc} is defined by (3.36). In the different simulations, the following features are noted.

- For SIMP topology optimization simulations, there is no initialization of the inclusion geometry. The initial density ρ_e^1 is set to be uniform and equal to f^{inc} .
- For BESO topology optimization simulations, an initial geometry of inclusion is required to match f^{inc} at the first iteration. If a homogeneous design is used, the volume fraction has to be reduced at each iteration by setting $\rho_e = 0$ in more elements, as ρ_e can only be zero or one in each element. We refer to this initial geometry to "initial BESO design".
- To evaluate the improvement of the fracture resistance in the present SIMP context which does not require an initial geometry, a "guess" design is defined in some examples to evaluate the improvement of the fracture resistance between optimized and guess designs.
- The volume fraction f^{inc} is fixed during the whole optimization process.
- To avoid interfering with the topology optimization process, a region around the initial crack is defined where the design variable are enforced to $\rho_e = 0$ (remain matrix material). This region is defined as embedding all nodes at a distance $2\ell_d$ from the initial crack surface.
- The incremental loading process goes on until the reaction force is below a prescribed value, indicating that the structure is fully broken.

3.5.1 2D reinforced plate with one pre-existing crack notch

In the following example, a 2D plate with one pre-existing crack notch, as described in Fig. 3.2, is considered. The structure is composed of a matrix material, and we seek the shape of an inclusion which provides the maximal fracture resistance for the whole composite structure. The dimensions of the plate are $100 \times 50 \text{ mm}^2$, and the domain is uniformly discretized into 120×60 square bilinear elements. The boundary conditions are as follows: on the upper and lower ends, the y -displacement are fixed, while the x -displacement are free. On the left and right ends, the horizontal displacements are prescribed with incremental displacement loads with $\Delta\bar{U} = 0.004 \text{ mm}$ for the first five load increments and $\Delta\bar{U} = 0.001 \text{ mm}$ for the following load increments. The pre-existing crack is simulated by prescribing

Dirichlet conditions on the crack phase field with $d = 1$ along the crack. Additionally, the optimality convergence tolerance is set at 10^{-5} ($tol = 10^{-5}$).

Table 3.2 Material parameters used in the numerical simulations [176]

Name	Notations	Inclusion	Matrix
Young's modulus	E^{inc}, E^{mat}	52 GPa	10.4 GPa
Poisson's ratio	ν	0.3	0.3
Critical fracture stress	$\sigma_c^{inc}, \sigma_c^{mat}$	0.03 GPa	0.01 GPa

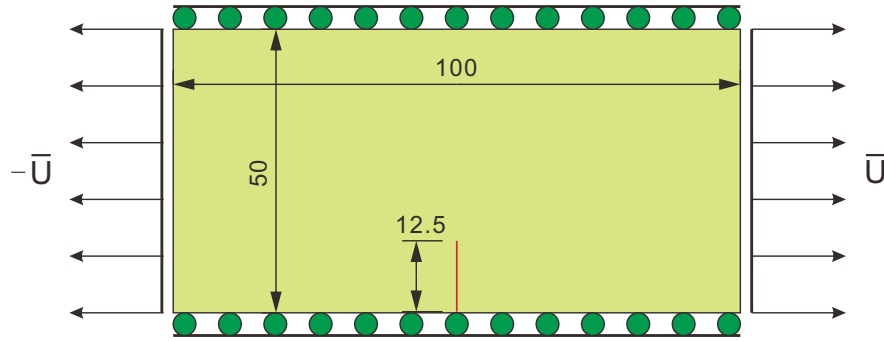


Fig. 3.2 Plate with one pre-existing crack notch subjected to incremental traction load: geometry and boundary conditions.

Fig. 3.3 shows the evolution histories of inclusion topologies and their final crack patterns. Here, the inclusion volume fraction is set to $f^{inc} = 5\%$. As can be observed from Fig. 3.3, the fracture resistance of the composite structure increases with accumulation of the inclusion material around the crack paths obtained from previous design iteration and reduction of intermediate densities (sometimes called "grey zones" in the topology optimization studies), and then converges to an almost constant value of 18.8 mJ. Detailed propagation of the crack phase field corresponding to its load-displacement curve for the optimized design is shown in Fig. 3.4. The crack propagates vertically into the inclusion material and two other cracks initiate around the left and right corners of the inclusion pattern, and then continue to propagate until the structure is fully broken.

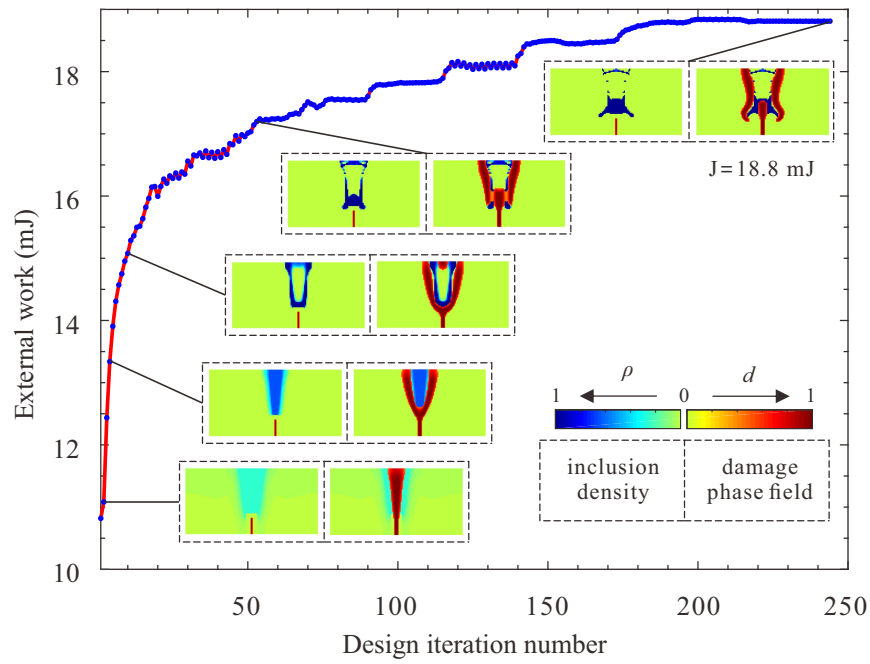


Fig. 3.3 Evolution of inclusion topologies and associated final crack patterns ($f^{inc} = 5\%$).

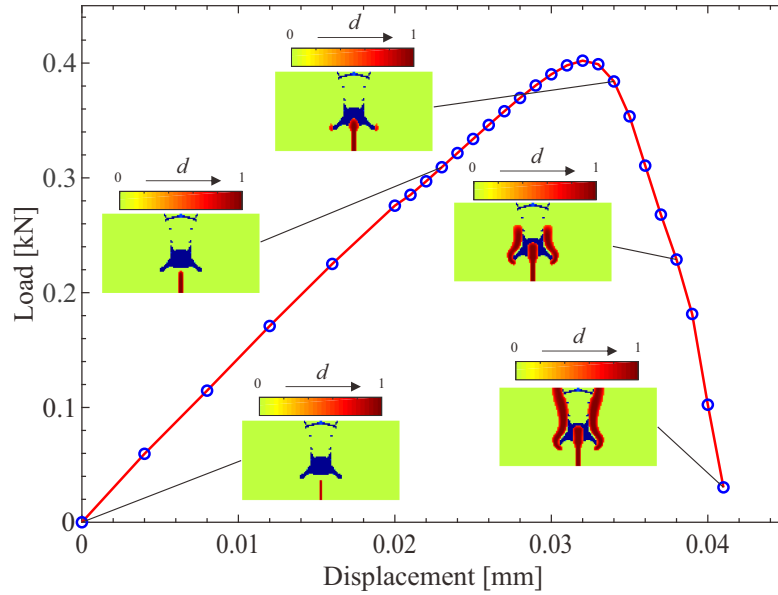


Fig. 3.4 Load-displacement curve and crack propagation for the optimized design: (a) $\bar{U} = 0$ mm; (b) $\bar{U} = 0.023$ mm; (c) $\bar{U} = 0.034$ mm; (d) $\bar{U} = 0.038$ mm; (e) $\bar{U} = 0.041$ mm.

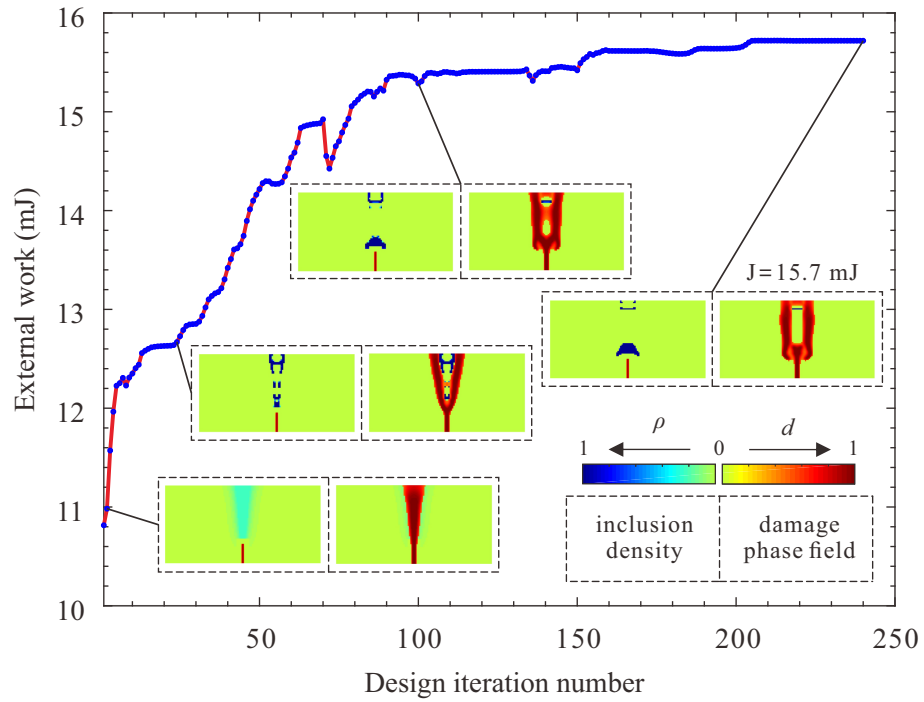


Fig. 3.5 Evolution of inclusion topologies and associated final crack patterns ($f^{inc} = 2\%$).

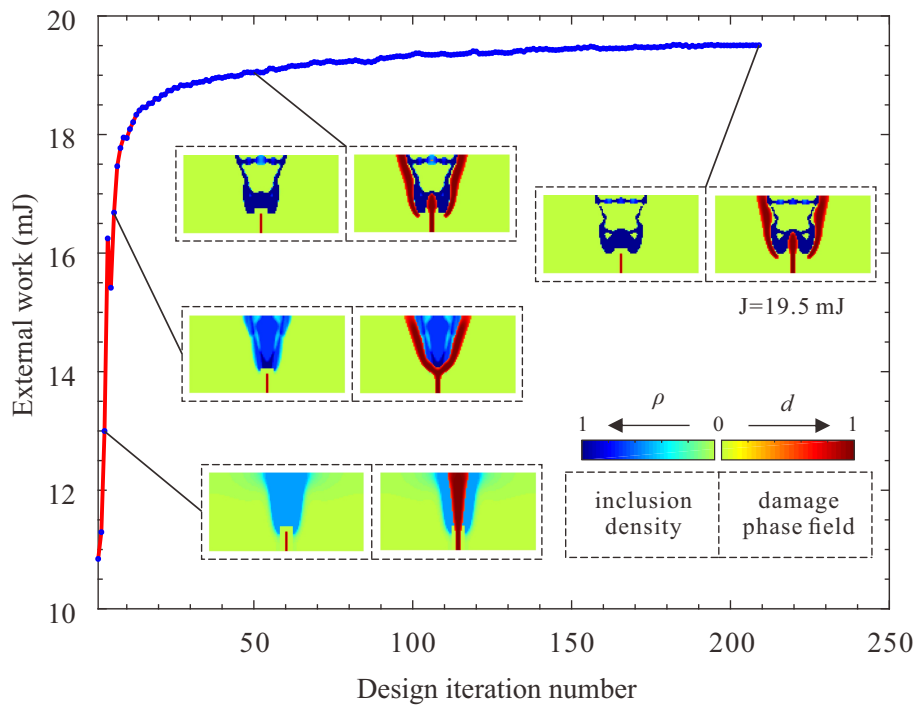


Fig. 3.6 Evolution of inclusion topologies and associated final crack patterns ($f^{inc} = 10\%$).

In order to illustrate the robustness of the method for other inclusion volume fractions and investigate the influence of f^{inc} on the numerical results, two additional simulations are conducted: $f^{inc} = 2\%$ and $f^{inc} = 10\%$. Fig. 3.5 and Fig. 3.6 show the evolution histories of inclusion topologies and their final crack patterns for cases $f^{inc} = 2\%$ and $f^{inc} = 10\%$, respectively. Fig. 3.7 shows comparison of the optimized designs and corresponding final crack patterns for cases $f^{inc} = 2\%$, $f^{inc} = 5\%$ and $f^{inc} = 10\%$. As can be observed, with the increase of the volume fraction, significant changes and more complex shapes of inclusions are obtained, in tandem with an increase of the fracture resistance.

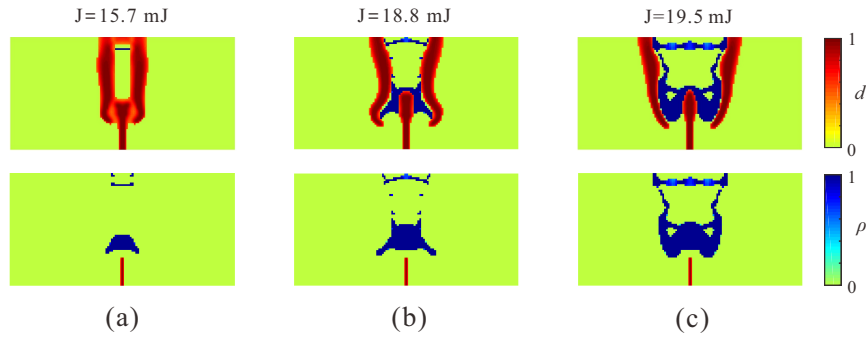


Fig. 3.7 Comparison of optimized inclusion designs and corresponding final crack pattern at the failure load: (a) $f^{inc} = 2\%$, (b) $f^{inc} = 5\%$ and (c) $f^{inc} = 10\%$.

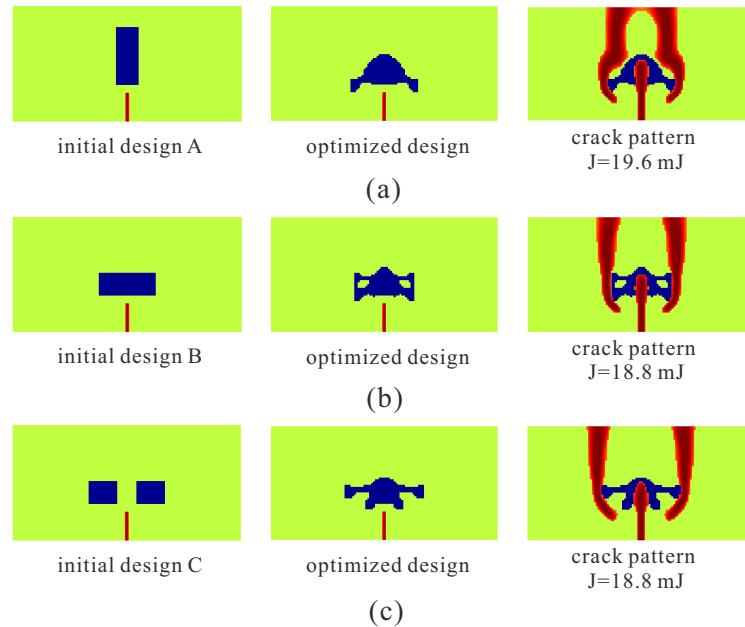


Fig. 3.8 Influence of initial design on the optimized inclusion topologies using BESO method ($f^{inc} = 5\%$). Crack and inclusions are denoted by red and blue color, respectively.

In the following, we compare the proposed SIMP approach with BESO topology optimization solution [176]. Three additional simulations using the BESO method with the same volume fraction $f^{inc} = 5\%$ but different initial designs (see Fig. 3.8) are performed. To fully display the convergence histories of BESO method, we do not prescribe a convergence criterion for these three BESO simulations and let the algorithm run until a maximum number of iterations equal to 500 is reached. Fig. 3.9 shows the comparison of convergence histories for BESO and SIMP solutions. We can note that in the case of BESO, the initial designs have a strong influence on the optimized objective function and on the convergence rate: (i) using BESO with design B, C or SIMP, the same convergence value 18.8 mJ is reached, while for initial design A with BESO the convergence value is about 19.6 mJ; (ii) solutions by BESO with initial designs B, C and SIMP solution require a similar number of convergence steps of about 200, while for initial design A with BESO the convergence number is about 400. From Fig. 3.9, we can also observe spurious oscillations for initial design A and C with BESO after a stable convergence value, while this does not seem to occur with SIMP. Fig. 3.8 shows the influence of initial design on the optimized design with BESO method. Fig. 3.10 shows the comparison of load-displacement curves for the 7 optimization processes.

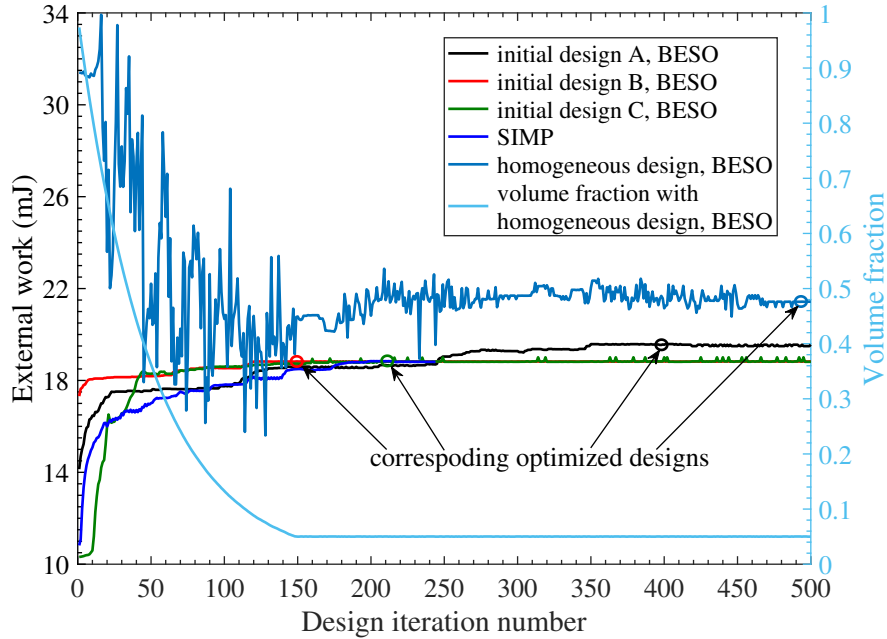


Fig. 3.9 Convergence of the topology optimization scheme for BESO and SIMP schemes ($f^{inc} = 5\%$).

From Fig. 3.9 and Fig. 3.10, we can conclude that even though SIMP has slightly better convergence properties with less oscillations, the convergence of both methods is comparable

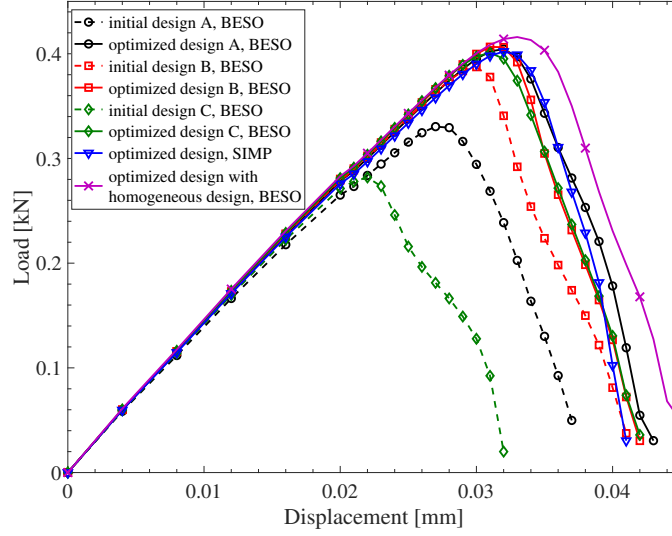


Fig. 3.10 Load-displacement curves for initial and optimized designs ($f^{inc} = 5\%$).

when an initial design is set such as the target volume fraction f^{inc} is met at the first iteration. The final results are also very close. The only difference is that starting from the target volume fraction f^{inc} is simpler with SIMP, as a value can be set in each element between 0 and 1, while in BESO an initial guess design matching the target volume fraction is required, which may be not trivial to define for more complex geometries. However, an initial homogeneous design is also possible using BESO, but the actual volume fraction will be changed at each iteration to reach f^{inc} as ρ_e in each element can only be 0 or 1. We investigate this case in Figs 3.9 and 3.10 (solution referred to as "homogeneous design, BESO": we can see that the convergence curve (Fig. 3.9) shows much more oscillations for BESO than SIMP for a homogeneous design, even though we can note in Fig. 3.10 that the optimized fracture energy is higher for BESO).

3.5.2 3D reinforced sample with one pre-existing crack notch surface

In this example, the aim is to illustrate the applicability and convergence of the present method for 3D problems. For this purpose, a 3D sample with one pre-existing crack notch surface, as described in Fig. 3.11(a), is considered. The dimensions of the 3D sample are $20 \times 20 \times 60 \text{ mm}^3$. The domain is discretized into $40 \times 40 \times 120$ eight-node cubic elements. The dimensions of the pre-existing crack notch surface are $10 \times 10 \text{ mm}^2$. As in the 2D case of section 3.5.1, the pre-existing crack is modeled by prescribing Dirichlet conditions on the crack phase field with $d = 1$ along the crack surface. On the upper and lower ends of the sample, vertical incremental displacement loads with $\Delta \bar{U} = 0.005 \text{ mm}$ are prescribed

for the first four load increments and $\Delta \bar{U} = 0.002$ mm for the following load increments. Additionally, the optimality convergence tolerance is set at 10^{-5} ($tol = 10^{-5}$).

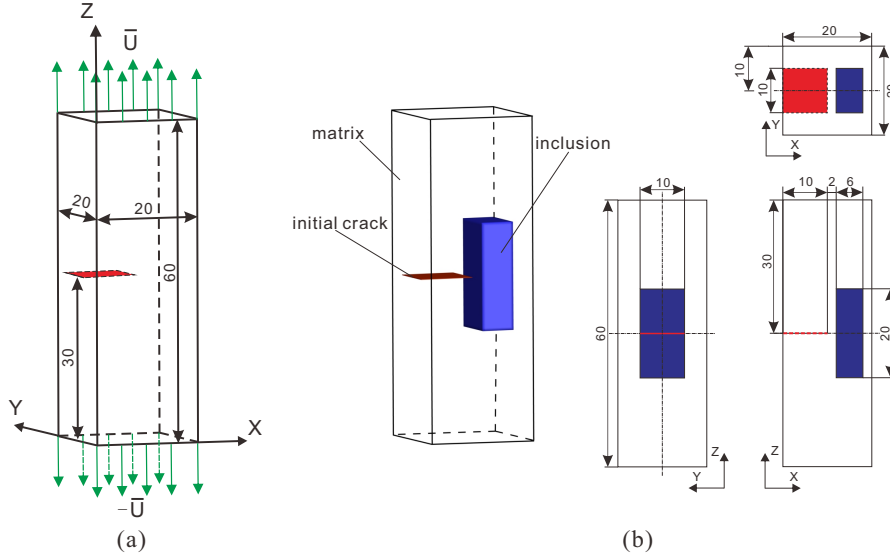


Fig. 3.11 3D sample with one pre-existing crack subjected to uniaxial tension: (a) geometry and boundary conditions; (b) guess design ($f^{inc} = 5\%$). Crack and inclusions are denoted by red and blue color, respectively.

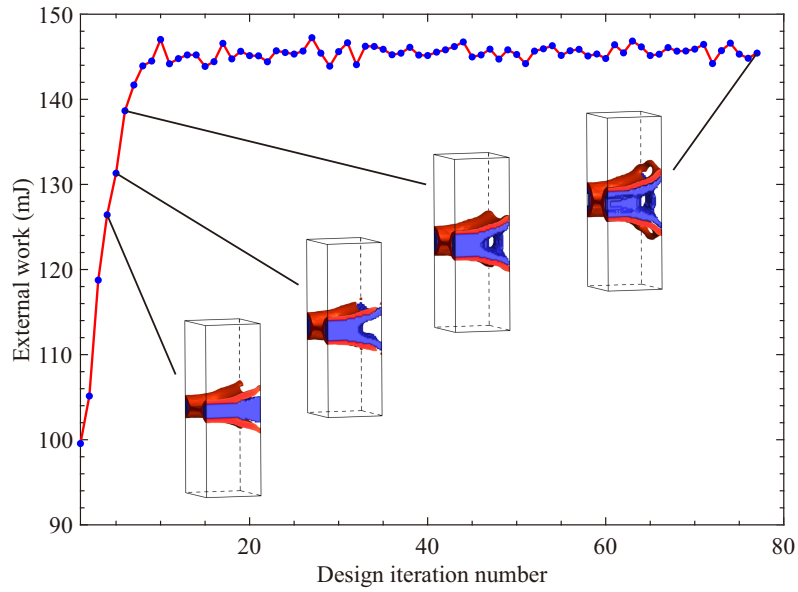


Fig. 3.12 3D sample with one pre-existing crack: evolution of inclusion topologies and associated final crack patterns ($f^{inc} = 5\%$). Crack and inclusions are denoted by red and blue color, respectively.

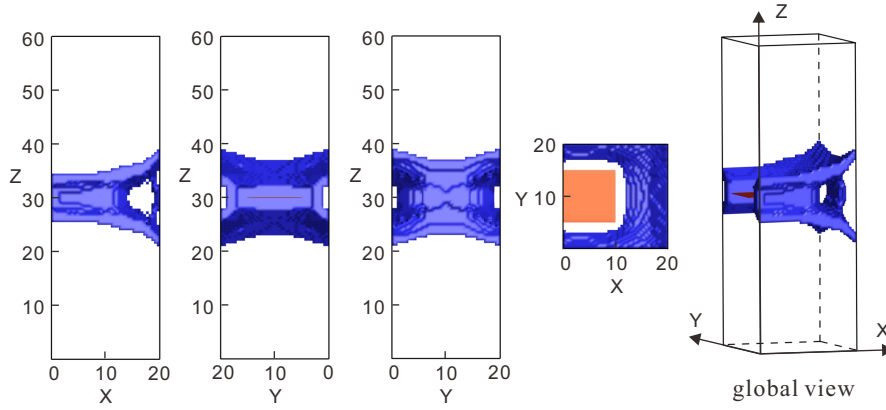


Fig. 3.13 Different views of the optimized design of inclusion for the 3D sample with one pre-existing crack.

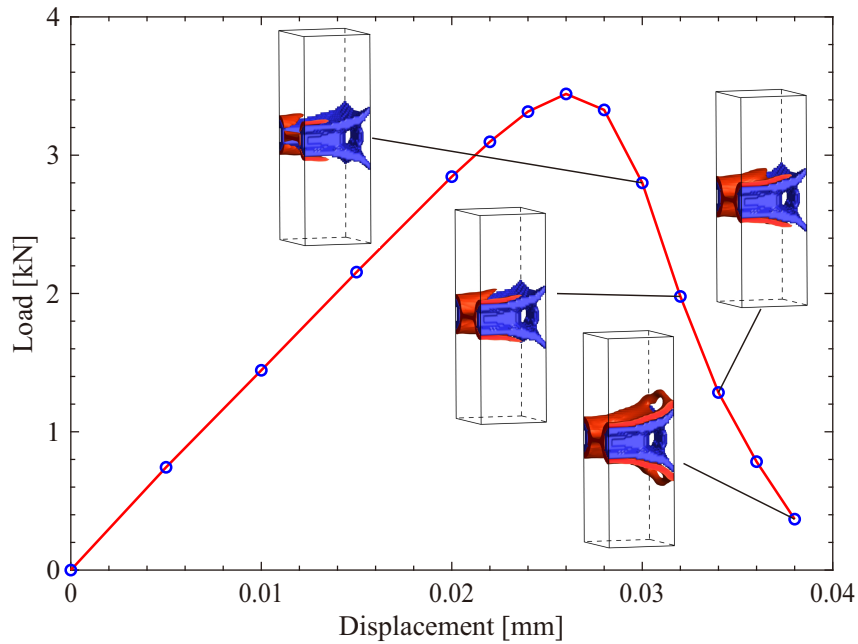


Fig. 3.14 Load-displacement curve and crack evolution for the optimized design in the 3D sample with one pre-existing crack: (a) $\bar{U} = 0.03$ mm; (b) $\bar{U} = 0.032$ mm; (c) $\bar{U} = 0.034$ mm; (d) $\bar{U} = 0.038$ mm. Crack and inclusions are denoted by red and blue color, respectively.

In Fig. 3.11(b) we provide a guess design for the inclusion, with $f^{inc} = 5\%$, corresponding to a simple parallelepipedic domain which will serve as a comparison with the SIMP optimized topology solution. Fig. 3.12 shows the evolution histories of inclusion topologies and their final crack patterns. For 3D visualization purpose, only values of $\rho_e \geq \rho_{thr}$ are

plotted in constant blue color (ρ_{thr} is a threshold value, defined to make sure elements with volume fraction around f^{inc} appear). Here the SIMP solution converges in roughly 10 iterations and strictly in 77 iterations. As a comparison, BESO with initial homogeneous design takes 150 iterations to reach $f^{inc} = 0.05$, showing the lower computational cost and better convergence of SIMP in this case. Different views of the optimized design are shown in Fig. 3.13. Detailed propagation of the crack phase field corresponding to its load-displacement curve for the optimized design is shown in Fig. 3.14. It can be observed that the crack first initiates from the surface of the inclusion phase and then interacts with the pre-existing crack. Next, it propagates along the surface of the inclusion phase until crossing the whole domain and leading to the failure of the structure. Fig. 3.15 shows comparison of load-displacement curves and final crack patterns for guess and optimized design. Here, the fracture resistance of the optimized design is 20% higher as compared with the guess design.

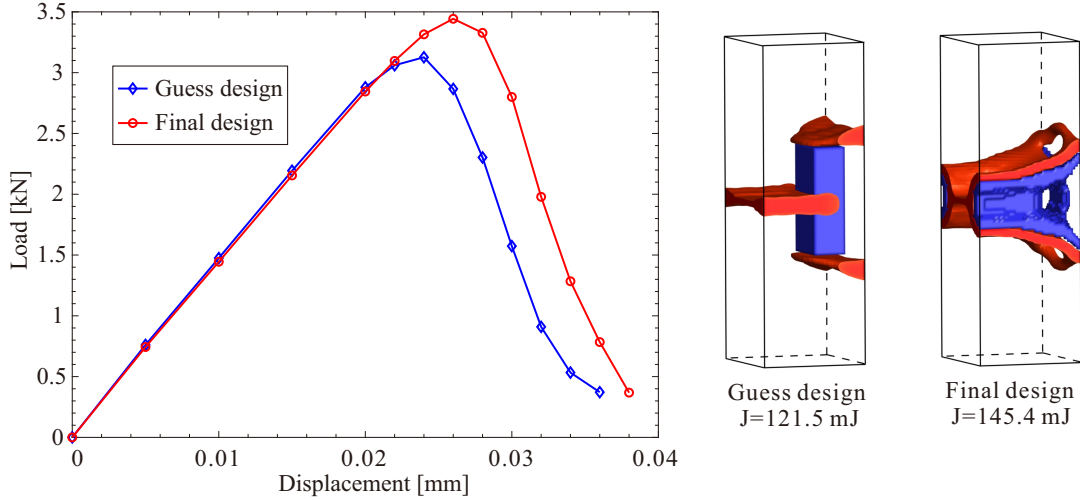


Fig. 3.15 Load-displacement curves and final crack pattern for guess and optimized design in the 3D structure with one pre-existing crack. On the right figure, crack and inclusions are denoted by red and blue color, respectively.

3.5.3 3D reinforced sample with two pre-existing crack surfaces and a parallelepipedic cavity

This final example demonstrates the potential of the method in complex 3D structural problems. The geometry and boundary conditions for this example are shown in Fig. 3.16. The dimensions of the 3D sample are $50 \times 50 \times 60 \text{ mm}^3$. The domain is discretized into $100 \times 100 \times 120$ eight-node cubic elements. As can be observed from Fig. 3.16, there are two pre-existing crack notch surfaces and a parallelepipedic cavity. The first pre-existing crack

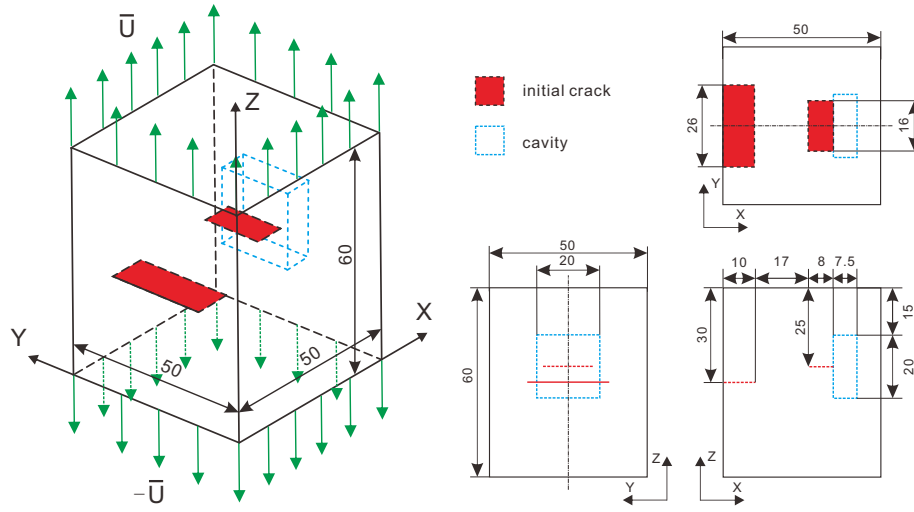


Fig. 3.16 3D sample with two pre-existing cracks and including parallelepipedic cavity: (a) geometry and boundary conditions.

notch whose geometry is $26 \times 10 \text{ mm}^2$ is embedded in the left surface of the whole sample, the second pre-existing crack notch whose geometry is $16 \times 8 \text{ mm}^2$ is embedded in the left surface of the parallelepipedic cavity, and the parallelepipedic cavity whose geometry is $20 \times 20 \times 7.5 \text{ mm}^3$ is created by removing the elements at the position of the parallelepipedic cavity. Similar to the 3D case in section 3.5.2, the pre-existing cracks are simulated by prescribing Dirichlet conditions on the crack phase field with $d = 1$ along the crack surfaces. On the upper and lower ends of the sample, vertical incremental displacement loads with $\Delta \bar{U} = 0.005 \text{ mm}$ are prescribed with for the first four load increments and $\Delta \bar{U} = 0.002 \text{ mm}$ for the following load increments. Additionally, the optimality convergence tolerance is set at 10^{-3} ($tol = 10^{-3}$).

Fig. 3.17 shows the evolution histories of inclusion topologies and their final crack patterns. Here f^{inc} is set to 5%. As can be observed from Fig. 3.17, the inclusion material tends to accumulate around the pre-existing crack notch surfaces and the parallelepipedic cavity to prevent crack propagation and interaction in the sample. From Fig. 3.17, we can note that the SIMP solution is converged in roughly 12 iterations and strictly in 23 iterations. As a comparison, BESO with initial homogeneous design takes about 150 iterations to reach $f^{inc} = 0.05$, showing again much less computational costs and better convergence of SIMP in this case. For better visualization, different views of the optimized design are shown in Fig. 3.18. Detailed propagation of the crack phase field corresponding to its load-displacement curve for the optimal design is shown in Fig. 3.19. It can be observed that the cracks nucleate firstly at the two pre-existing crack notch surfaces and the corners of the cuboidal cavity, and

then propagate and interact following the surface of the inclusion phase until reaching the fully broken state of the sample.

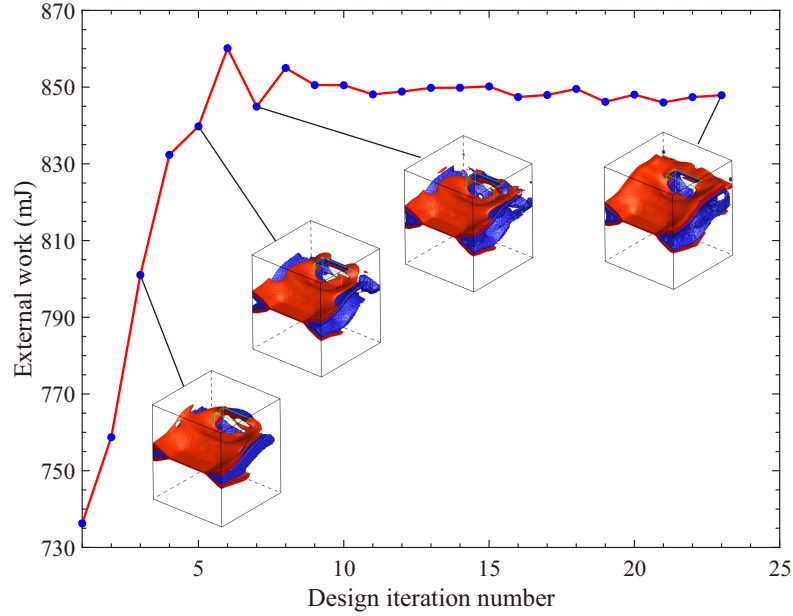


Fig. 3.17 3D sample with two pre-existing cracks: convergence of the topology optimization process, evolution of inclusion topologies and associated final crack patterns ($f^{inc} = 5\%$). Crack and inclusions are denoted by red and blue color, respectively.

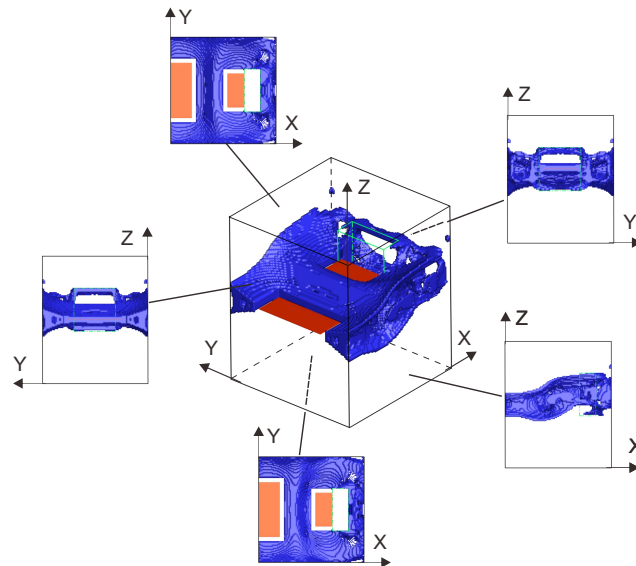


Fig. 3.18 Different views of the optimized design for the 3D sample with two pre-existing crack. Crack and inclusions are denoted by red and blue color, respectively.

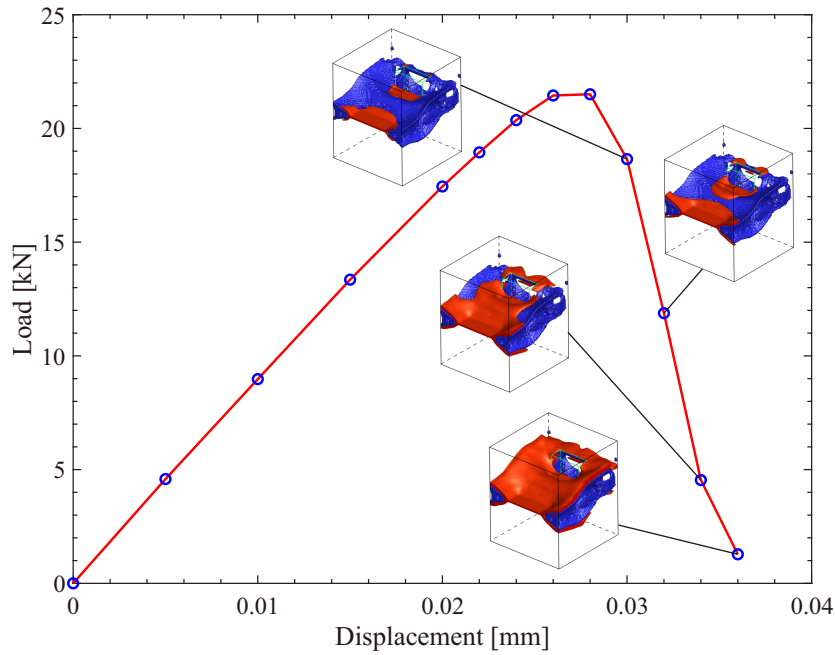


Fig. 3.19 Load-displacement curves and crack pattern evolution for optimized design in the 3D structure with two pre-existing crack: (a) $\bar{U} = 0.03$ mm; (b) $\bar{U} = 0.032$ mm; (c) $\bar{U} = 0.034$ mm; (d) $\bar{U} = 0.036$ mm. Crack and inclusions are denoted by red and blue color, respectively.

Table 3.3 Computational times for the different examples

Problem	No. elements	No. design iterations	Average CPU time (s)	Total simulation time (h)
2D reinforced plate ($f^{inc} = 5\%$)	7200	244	33.6	2.28
3D reinforced sample in 3.5.2	192,000	77	924	19.77
3D reinforced sample in 3.5.3	1,176,000	23	5055	32.3

3.5.4 Computational times

Finally, a summary of the computational times for the different examples is reported in Table 3.3. In this work, a workstation with 4 cores, 16 Go Ram and 3.00 GHz processor was used for all 2D cases. For all 3D cases, a workstation with 24 cores, 768 Go Ram and 2.70 GHz processor was used. The present code has been implemented in Matlab[®].

3.6 Conclusion

In this chapter, another contribution has been introduced, by proposing a framework employing SIMP topology optimization and phase field method to fracture to maximize the fracture resistance of composites (two-phase materials) structures. The method allows taking into account the whole fracture process, from initiation to complete failure of the specimen. The continuous density representation of density obtained by the SIMP method allows a good convergence of the scheme and to improve the fracture resistance of a structure embedding a reinforcement phase (inclusion) for a fixed volume fraction.

We have observed that even though SIMP has slightly better convergence properties with less oscillations than BESO, the convergence of both SIMP and BESO is comparable when the initial volume fraction is set by an appropriate initial design in BESO. The final results are also very close. However, it is not always easy to define such initial design, especially in 3D. When using a homogeneous design with BESO, the convergence can be much slower (up to 6 times in some examples) than SIMP, as the actual volume fraction will be changed at each iteration by removing/adding material in each element. Then, starting with an initial homogeneous design is straightforward and leads to faster convergence with the present SIMP framework than with BESO.

This has been illustrated by conducting 3D applications in complex configurations, where defining an initial design with a given volume fraction may be non-trivial. Then, the present SIMP-phase field framework is a good candidate for reducing the computational times in designing materials and structures with enhanced fracture energy.

Chapter 4

Phase field topology optimization maximizing the fracture resistance of elastoplastic composites

4.1 Introduction

This chapter introduces a topology optimization framework for maximizing the fracture resistance of elastoplastic composites. It constitutes an original contribution by extending the topology optimization framework [176, 93] for maximizing the fracture resistance where the ductile phase field model is employed for bi-materials, possibly including interfaces. As compared to Chapter 2, an elastoplastic phase field formulation with gradient plasticity is applied to simulate complex ductile fracture. This formulation includes an additional internal length scale to regularize the plastic response, and to ensure that the damage zones of ductile fracture are contained within plastic zones. Different examples are provided to illustrate the proposed methodology.

4.2 Phase field modeling ductile fracture with interfaces and plasticity gradient

In this section, we present the elastoplastic phase field formulation with plasticity gradient. For this purpose, we follow the framework developed in [130, 121] to interfacial damage and in [145] to bulk ductile cracking.

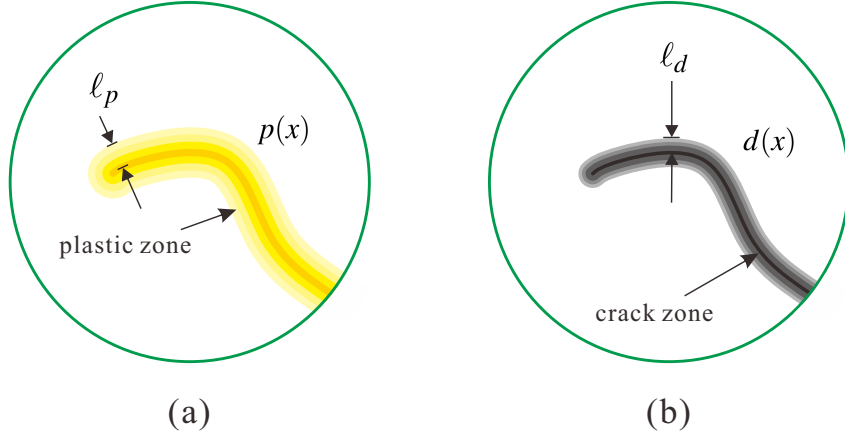


Fig. 4.1 Regularization of (a) the equivalent plastic strain $p(x)$ and (b) the crack phase field $d(x)$.

4.2.1 Variational framework

We follow the framework presented in [6] to construct the variational principle, which involves: irreversibility condition, stability condition and energy balance. In this framework, stability condition provides mechanical balance equation, damage and plastic criteria. The energy balance provides damage and plastic consistency. The total energy for an elastoplastic cracked body embedding interfaces is defined here as

$$W(\mathbf{u}, p, d, \beta) = \int_{\Omega} \psi^e(\boldsymbol{\varepsilon}(\mathbf{u}), p, d) d\Omega + \int_{\Omega} \left[\psi^p(p, d) + \psi^d(\beta, d) + \psi^I(\mathbf{w}(\mathbf{u}), \beta) \right] d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\Omega, \quad (4.1)$$

in which ψ^e , ψ^d and ψ^I have been defined in (2.27), (2.76) and (2.77) in Chapter 2. ψ^p is the stored plastic energy density function defined as

$$\psi^p(p, d) = (1 - d)^2 \left(\sigma_Y p + \frac{1}{2} H p^2 + \frac{1}{2} \ell_p^2 \nabla p \cdot \nabla p \right), \quad (4.2)$$

where we note a new term $\frac{1}{2} \ell_p^2 \nabla p \cdot \nabla p$ is introduced to regularize the plastic field. Above, ℓ_p is a plastic length scale related to a strain-gradient hardening effect and accounts for size effects to overcome the nonphysical mesh sensitivity of the localized plastic deformation in softening materials. For ductile fracture, we require additionally that $\ell_p \geq \ell_d$ such that the regularized crack zone lies inside of the plastic zone, as shown in Fig. 4.1 and outlined in [106, 1].

4.2.1.1 Irreversibility condition

The irreversibility condition is prescribed on the damage and plastic variable. For damage irreversibility condition, it can be found in (2.8). For plastic irreversibility condition, it can be expressed as

$$\dot{p} \geq 0, \quad (4.3)$$

which is applied numerically by simply considering the cumulated plastic strain value corresponding to the previous load step as the minimum admissible level of cumulated plastic strain for a given position in the body.

4.2.1.2 First-order stability condition

The first order stability condition is expressed by:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d) + D_{\delta p} W(\mathbf{u}, p, d) + D_{\delta d} W(\mathbf{u}, p, d) \geq 0. \quad (4.4)$$

Applied to (4.1), it yields:

$$\begin{aligned} & \int_{\Omega} \left[\boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) + \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\delta \mathbf{u}) \right] d\Omega + \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} \delta p + D_{\delta p} \psi^p \right) d\Omega \\ & + \int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^p}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega \geq 0, \end{aligned} \quad (4.5)$$

where $\boldsymbol{\sigma}$ has been obtained in (2.33) and $\boldsymbol{\varepsilon}^e$ has been expressed in (2.69).

From (4.5), the following results stem out:

- For $\delta p = \delta d = 0$, find $\mathbf{u} \in \mathcal{S}_u$, $\mathcal{S}_u = \{ \mathbf{u} | \mathbf{u}(\mathbf{x}) = \bar{\mathbf{u}} \text{ on } \partial \Omega_u, \mathbf{u} \in H^1(\Omega) \}$ such that:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_{\beta} \mathbf{t} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (4.6)$$

which is the weak form of the mechanical equilibrium equation, with $\delta \mathbf{u} \in \mathcal{S}_u^0$, $\mathcal{S}_u^0 = \{ \delta \mathbf{u} | \delta \mathbf{u}(\mathbf{x}) = 0 \text{ on } \partial \Omega_u, \mathbf{u} \in H^1(\Omega) \}$.

- For $\delta d = 0$ and $\delta \mathbf{u} = \mathbf{0}$, we first express the term:

$$D_{\delta p} \psi^p = (1 - d)^2 (\sigma_y \delta p + H p \delta p + \ell_p^2 \nabla p \cdot \nabla \delta p). \quad (4.7)$$

We then obtain:

$$\int_{\Omega} \left[\left(\sqrt{\frac{3}{2}} \|\mathbf{s}\| - (1-d)^2 (\sigma_Y + Hp) \right) \delta p - (1-d)^2 \ell_p^2 \nabla p \cdot \nabla \delta p \right] d\Omega \leq 0, \quad (4.8)$$

which is the weak form of the plasticity yield criterion. The local form of the plastic yield criterion can be expressed as

$$F^p(p) = \sqrt{\frac{3}{2}} \|\mathbf{s}\| - (1-d)^2 (\sigma_Y + Hp - \ell_p^2 \nabla \cdot \nabla p) \leq 0 \text{ in } \Omega. \quad (4.9)$$

- For $\delta p = 0$ and $\delta \mathbf{u} = \mathbf{0}$, it leads to

$$\begin{aligned} \int_{\Omega} \left\{ (1-d) (2\psi_0^{e+} + 2\sigma_Y p + Hp^2 + \ell_p^2 \nabla p \cdot \nabla p) \delta d \right. \\ \left. - (1-\beta)^2 \left(\frac{g_c}{\ell_d} d \delta d + g_c \ell_d \nabla d \cdot \nabla \delta d \right) \right\} d\Omega \leq 0, \end{aligned} \quad (4.10)$$

which is the weak form of the damage yield criterion. The local form of the damage yield criterion can be expressed as

$$\begin{aligned} F^d(d) = (1-d) (2\psi_0^{e+} + 2\sigma_Y p + Hp^2 + \ell_p^2 \nabla p \cdot \nabla p) \\ - (1-\beta)^2 \left(\frac{g_c}{\ell_d} d - g_c \ell_d \nabla \cdot \nabla d \right) \leq 0 \text{ in } \Omega. \end{aligned} \quad (4.11)$$

4.2.1.3 Energy balance

The energy balance represents the need for the total energy to remain constant as the state variables evolve. Following a procedure analogous to the treatment of the stability condition, this condition leads to

$$\begin{aligned} \int_{\Omega} \left[-\boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\dot{\mathbf{u}}) - \frac{\partial \psi^I}{\partial \mathbf{w}} \cdot \mathbf{w}(\dot{\mathbf{u}}) + \left(\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} - \frac{\partial \psi^p}{\partial p} \right) \dot{p} - \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^p}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \dot{d} \right] d\Omega \\ + \int_{\partial\Omega_F} \mathbf{F} \cdot \dot{\mathbf{u}} dS + \int_{\Omega} \mathbf{f} \cdot \dot{\mathbf{u}} d\Omega = 0. \end{aligned} \quad (4.12)$$

The following cases are analyzed.

- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{d} = 0$, and using (4.9), the plasticity consistency condition is obtained:

$$F^p(p)\dot{p} = 0. \quad (4.13)$$

- For $\dot{\mathbf{u}} = \mathbf{0}$ and $\dot{p} = 0$, and using (4.11), the damage consistency condition is obtained:

$$F^d(d)\dot{d} = 0. \quad (4.14)$$

4.2.1.4 Alternate minimization

In this section, a staggered alternate minimization algorithm for $\mathbf{u}$, p and d is applied. With the total energy (4.1) at hand, the alternate minimization follows.

- Minimization with respect to the displacement field:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d) = 0 \quad (4.15)$$

leads to

$$R_{\mathbf{u}} = \int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_{\beta} \mathbf{t} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0 \quad (4.16)$$

which corresponds to the weak form of the mechanical problem.

- Minimization with respect to the equivalent plastic strain:

$$R_p = D_{\delta p} W(\mathbf{u}, p, d) = \int_{\Omega} \left\{ \left[\sqrt{\frac{3}{2}} \|\mathbf{s}\| - (1-d)^2 (\sigma_Y + Hp) \right] \delta p - (1-d)^2 \ell_p^2 \nabla p \cdot \nabla \delta p \right\} d\Omega = 0, \quad (4.17)$$

which is the weak form of the plastic yield criterion to be solved for p with $\dot{p} \geq 0$. The increment of the plastic strain tensor can be obtained from the incremental equivalent plastic strain as

$$\dot{\boldsymbol{\varepsilon}}^p = \sqrt{\frac{3}{2}} \dot{p} \frac{\mathbf{s}}{\|\mathbf{s}\|} \quad (4.18)$$

- Minimization with respect to the damage field:

$$R_d = D_{\delta d} W(\mathbf{u}, p, d) = \int_{\Omega} \left\{ (1-d) (2\psi_0^{e+} + 2\sigma_Y p + H p^2 + \ell_p^2 \nabla p \cdot \nabla p) \delta d - (1-\beta)^2 \left(\frac{g_c}{\ell_d} d \delta d + g_c \ell_d \nabla d \cdot \nabla \delta d \right) \right\} d\Omega = 0. \quad (4.19)$$

To prescribe damage irreversibility, we employ the technique introduced in [111] which consists in substituting the above weak form with:

$$R_d = \int_{\Omega} \left[(1-d) \mathcal{H} \delta d - (1-\beta)^2 (\psi_c d \delta d + \psi_c \ell_d^2 \nabla d \cdot \nabla \delta d) \right] d\Omega = 0, \quad (4.20)$$

where

$$\mathcal{H}(\varepsilon^e, p) = \max_{s \in [0, t]} \left[\left\langle \psi_0^{e+}(\varepsilon^e, s) + \sigma_Y p(s) + \frac{1}{2} H p(s)^2 + \frac{1}{2} \ell_p^2 \nabla p(s) \cdot \nabla p(s) - \psi_c \right\rangle_+ \right] \quad (4.21)$$

and ψ_c is a specific fracture energy threshold.

The weak forms of the problems to be solved alternatively are summarized in Table 4.1

Table 4.1 Problems to be solved in the staggered procedure.

Displacement problem: given d and p , solve for $\mathbf{u}$:

$$R_{\mathbf{u}} = \int_{\Omega} \boldsymbol{\sigma} : \varepsilon^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \gamma_{\beta} \mathbf{t} \cdot \mathbf{w}(\delta \mathbf{u}) d\Omega - \int_{\partial \Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega = 0$$

$$\boldsymbol{\sigma} = (1-d)^2 (\kappa \langle \text{Tr}(\varepsilon^e) \rangle_+ \mathbf{1} + 2\mu \mathbf{e}^e) + \kappa \langle \text{Tr}(\varepsilon^e) \rangle_- \mathbf{1}$$

$$\mathbf{t}(\mathbf{w}) = \left[g_c^I \frac{w^n}{(\delta^n)^2} \exp\left(-\frac{w^n}{\delta^n}\right), 0 \right]^T$$

$$\dot{\varepsilon}^p = \sqrt{\frac{3}{2}} \dot{p} \frac{\mathbf{s}}{\|\mathbf{s}\|}$$

Plastic problem: given $\mathbf{u}$ and d , solve for p :

$$R_p = \int_{\Omega} \left[\left(\sqrt{\frac{3}{2}} \|\mathbf{s}\| - (1-d)^2 (\sigma_Y + H p) \right) \delta p - (1-d)^2 \ell_p^2 \nabla p \cdot \nabla \delta p \right] d\Omega = 0$$

Phase Field problem: given $\mathbf{u}$ and p , solve for d :

$$R_d = \int_{\Omega} \left[(1-d) \mathcal{H} \delta d - (1-\beta)^2 (\psi_c d \delta d + \psi_c \ell_d^2 \nabla d \cdot \nabla \delta d) \right] d\Omega = 0$$

4.2.2 Finite element discretization and numerical implementation

In this section, we detail the FEM discretizations for displacement, plastic and damage problems, and finally provide the overall algorithm.

4.2.2.1 Discretization of the displacement problem

In this work, we use an iterative approach to solve this nonlinear problem in (4.16). After rearranging, the discrete version of (4.16) can be expressed globally as

$$\mathbf{K}_u \mathbf{u} = \mathbf{F}_u \quad (4.22)$$

with the force vector

$$\mathbf{F}_u = \int_{\Omega} \mathbf{B}_w^T \mathbf{C} \varepsilon^{p,(k)} d\Omega + \int_{\Omega} \mathbf{N}_u^T \mathbf{f} d\Omega + \int_{\partial\Omega_F} \mathbf{N}_u^T \mathbf{F} dS - \int_{\Omega} \gamma_{\beta} (h \mathbf{N} \mathbf{B})^T \mathbf{t}(\mathbf{w}^{(k)}) d\Omega \quad (4.23)$$

and the stiffness matrix

$$\mathbf{K}_u = \int_{\Omega} \mathbf{B}_w^T \mathbf{C} \mathbf{B}_w d\Omega \quad (4.24)$$

with

$$\mathbf{C} = \begin{cases} (1-d)^2 (\kappa \mathbf{\Pi} + 2\mu \mathbf{\Pi}_d) & \text{Tr}(\varepsilon^e) \geq 0 \\ \kappa \mathbf{\Pi} + (1-d)^2 2\mu \mathbf{\Pi}_d & \text{Tr}(\varepsilon^e) < 0 \end{cases} \quad (4.25)$$

and

$$\mathbf{\Pi} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{\Pi}_d = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & 0 \\ -\frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (4.26)$$

Above, $\mathbf{B}_w$, $\mathbf{N}_u$, $\mathbf{N}$ and $\mathbf{B}$ can be found in Section 2.3.3.2, and $(\cdot)^{(k)}$ denotes the value of k -th iteration for each load step.

4.2.2.2 Discretization of the plastic problem

We first rewrite (4.18) with small pseudo-time step assumption as

$$\Delta \varepsilon^p = \sqrt{\frac{3}{2}} \Delta p \frac{\mathbf{s}}{\|\mathbf{s}\|} \quad (4.27)$$

where $\Delta p = p_{n+1} - p_n$ is the incremental equivalent plastic strain. Then we can rewrite (4.17) as

$$R_p = \int_{\Omega} (1-d)^2 \left[\left(\sqrt{\frac{3}{2}} \|\mathbf{s}_{\text{eff}}^{\text{tr}}\| - 3\mu p + 3\mu p_n - \sigma_Y - Hp \right) \delta p - \ell_p^2 \nabla p \cdot \nabla \delta p \right] d\Omega = 0. \quad (4.28)$$

Here, for the sake of simplicity, the subscript $n+1$ for p_{n+1} is omitted.

The equivalent plastic strain and equivalent plastic strain gradient are approximated in one element by

$$p = \mathbf{N}_p \mathbf{p}^e, \quad \nabla p = \mathbf{B}_p \mathbf{p}^e, \quad (4.29)$$

where $\mathbf{N}_p$ and $\mathbf{B}_p$ are matrices of equivalent plastic strain shape function and of equivalent plastic strain shape function derivatives, respectively, and $\mathbf{p}^e$ denote nodal equivalent plastic strain in one element.

The discretization of plastic problem (4.28) results into the following discrete system of equations:

$$\mathbf{K}_p \mathbf{p} = \mathbf{F}_p \quad (4.30)$$

in which

$$\mathbf{K}_p = \int_{\Omega} (1-d)^2 [(3\mu + H) \mathbf{N}_p^T \mathbf{N}_p + \ell_p^2 \mathbf{B}_p^T \mathbf{B}_p] d\Omega \quad (4.31)$$

and

$$\mathbf{F}_p = \int_{\Omega} (1-d)^2 \mathbf{N}_p^T \left(\sqrt{\frac{3}{2}} \|\mathbf{s}_{\text{eff}}^{\text{tr}}\| + 3\mu p_n - \sigma_Y \right) d\Omega. \quad (4.32)$$

4.2.2.3 Discretization of the damage problem

The damage and damage gradient are approximated in one element by

$$d = \mathbf{N}_d \mathbf{d}^e, \quad \nabla d = \mathbf{B}_d \mathbf{d}^e, \quad (4.33)$$

where $\mathbf{N}_d$ and $\mathbf{B}_d$ are matrices of damage shape function and of damage shape function derivatives, respectively, and $\mathbf{d}^e$ denote nodal damage in one element.

The discretization of damage problem (4.20) results into the following discrete system of equations:

$$\mathbf{K}_d \mathbf{d} = \mathbf{F}_d \quad (4.34)$$

in which

$$\mathbf{K}_d = \int_{\Omega} \left\{ \left[\mathcal{H} + (1-\beta)^2 \psi_c \right] \mathbf{N}_d^T \mathbf{N}_d + (1-\beta)^2 \psi_c \ell_d^2 \mathbf{B}_d^T \mathbf{B}_d \right\} d\Omega \quad (4.35)$$

and

$$\mathbf{F}_d = \int_{\Omega} \mathbf{N}_d^T \mathcal{H} d\Omega, \quad (4.36)$$

where $\mathcal{H}$ is given in (4.21).

4.2.2.4 Overall algorithm

In the present work, a staggered iterative scheme is employed following [145]. It consists of solving successively (4.22), (4.30) and (4.34). First, (4.22) is solved to obtain $\mathbf{u}_i^{(k+1)}$ with given $(\mathbf{u}_i^{(k)}, p_i^{(k)}, d_i^{(k)})$. Subindices i and supraindices k denoting the load step and subiteration, respectively. In a second step, (4.30) is solved to obtain $p_i^{(k+1)}$ with given $(\mathbf{u}_i^{(k+1)}, p_i^{(k)}, d_i^{(k)})$. In a third step, (4.34) is solved to obtain $d_i^{(k+1)}$ with given $(\mathbf{u}_i^{(k+1)}, p_i^{(k+1)}, d_i^{(k)})$. At each load step, the subiteration is performed until convergence is achieved by using three independent tolerances t_u , t_p and t_d . The detailed algorithm is illustrated in Algorithm 6.

Algorithm 6: Overall algorithm for elastoplastic ductile fracture model with interfaces

Initialize $\mathbf{u}_0$, p_0 and d_0 with assumption of elasticity and undamaged state.

Compute the level-set function ϕ and interface damage β .

Loop over load increments n

for $i = 1, \dots, n$ **do**

$k = 0, erru = errp = errd = 1$

$\mathbf{u}_i^{(0)} = \mathbf{u}_{i-1}, p_i^{(0)} = p_{i-1}, d_i^{(0)} = d_{i-1}$

while $erru > t_u$ **or** $errp > t_p$ **or** $errd > t_d$ **and** $k \leq k_{max}$ **do**

Given $\mathbf{u}_i^{(k)}$, $p_i^{(k)}$ and $d_i^{(k)}$, compute $\mathbf{u}_i^{(k+1)}$ from (4.22)

Given $\mathbf{u}_i^{(k+1)}$, $p_i^{(k)}$ and $d_i^{(k)}$, compute $p_i^{(k+1)}$ from (4.30)

Given $\mathbf{u}_i^{(k+1)}$, $p_i^{(k+1)}$ and $d_i^{(k)}$, compute $d_i^{(k+1)}$ from (4.34)

$erru = \|\mathbf{u}_i^{(k+1)} - \mathbf{u}_i^{(k)}\|$, $errp = \|p_i^{(k+1)} - p_i^{(k)}\|$, $errd = \|d_i^{(k+1)} - d_i^{(k)}\|$

$k = k + 1$

end

$\mathbf{u}_i = \mathbf{u}_i^{(k+1)}, p_i = p_i^{(k+1)}, d_i = d_i^{(k+1)}$

$i = i + 1$

end

4.3 Topology optimization without interfaces

In this section, we present a SIMP topology optimization framework for maximizing the ductile fracture resistance of a two-phase structure. The elastoplastic ductile fracture model introduced in Section 4.2 is used but without considering interface damage by simply setting $\beta = 0$.

4.3.1 Topology optimization formulation

4.3.1.1 Material interpolation and optimization problem statement

Similarly to Section 3.3.2, the design domain Ω is discretized into N_e finite elements and each element e is assigned with a topology design variable, or element density ρ_e , which is allowed to vary continuously in the range $[0, 1]$. Following [26], the material interpolations for the two-phase material are defined as

$$\begin{cases} \mu_e = \rho_e^p \mu_{inc} + (1 - \rho_e^p) \mu_{mat} \\ \kappa_e = \rho_e^p \kappa_{inc} + (1 - \rho_e^p) \kappa_{mat} \\ \sigma_{Y,e} = \rho_e \sigma_{Y,inc} + (1 - \rho_e) \sigma_{Y,mat} \\ h_e = \rho_e h_{inc} + (1 - \rho_e) h_{mat} \\ \psi_{c,e} = \rho_e \psi_{c,inc} + (1 - \rho_e) \psi_{c,mat} \end{cases} \quad (4.37)$$

Where $(\cdot)_e$ are the parameters of the e -th element. $(\cdot)_{inc}$ and $(\cdot)_{mat}$ are the parameters corresponding to the inclusion and the matrix phase, respectively. Following Section 3, we choose $p = 3$ in this work.

Similarly to Section 3, we optimize the total mechanical work to optimize the fracture resistance. The optimization problem is then defined as follows:

$$\begin{aligned} & \max_{\rho} : J(\rho, \mathbf{u}, \mathbf{p}, \mathbf{d}) \\ & \text{subject to : } \mathbf{R} = 0 \\ & : \sum_{e=1}^{N_e} \rho_e v_e / \left(\sum_{e=1}^{N_e} v_e \right) = f^{inc} \\ & : 0 \leq \rho_e \leq 1, e = 1, \dots, N_e. \end{aligned} \quad (4.38)$$

In the above, v_e is the volume (area in 2D) of the e -th element and f^{inc} is the target inclusion volume which is prescribed during the optimization process. The total mechanical

work is approximated by:

$$J \approx \frac{1}{2} \sum_{n=1}^{n_{load}} (\mathbf{F}_{ext}^n + \mathbf{F}_{ext}^{n-1})^T \Delta \mathbf{u}^n, \quad (4.39)$$

where $\mathbf{F}_{ext}^n$ is the external force response of the load point at the n -th load step. $\mathbf{R}$ denotes the nodal residual force:

$$\mathbf{R} = \mathbf{F}_{ext} - \int_{\Omega} \mathbf{B}_u^T \boldsymbol{\sigma} d\Omega. \quad (4.40)$$

As in Section 3, we do not explicitly use the plastic and damage constraint in (4.38) and in the following sensitivity analysis. In fact, these two constraints are taken into account implicitly as the regularized plasticity and fracture problem are solved in a staggered solving procedure.

4.3.1.2 Sensitivity analysis

In this section, in order to solve the optimization problem in (4.38), we first need to derive the sensitivity of the objective function J corresponding to change in the design variable. For this purpose, the adjoint method in [176] is employed. Assuming that the mechanical problem (4.40) has been solved, nothing is changed by rewriting the objective function J in (4.39) as

$$J \approx \bar{J} = \frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\mathbf{F}_{ext}^n + \mathbf{F}_{ext}^{n-1})^T \Delta \mathbf{u}^n + (\lambda_1^n)^T \mathbf{R}^n + (\lambda_2^n)^T \mathbf{R}^{n-1} \right\} \quad (4.41)$$

in which $\mathbf{R}^n$ and $\mathbf{R}^{n-1}$ are the residuals of (4.40) at n -th and $(n-1)$ -th load increments, respectively.

The derivatives of $\mathbf{R}^m$ at the equilibrium of the m -th load increment with respect to ρ_e can be expanded as

$$\frac{\partial \mathbf{R}^m}{\partial \rho_e} = \frac{\partial \mathbf{F}_{ext}^m}{\partial \rho_e} - \int_{\Omega} \mathbf{B}_u^T \frac{\partial \boldsymbol{\sigma}^m}{\partial \rho_e} d\Omega - \mathbf{K}_u^m \frac{\partial \mathbf{u}^m}{\partial \rho_e}. \quad (4.42)$$

With (4.42), the derivatives of (4.41) can be reformulated as

$$\begin{aligned} \frac{\partial \bar{J}}{\partial \rho_e} = \frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ \left(\frac{\partial \mathbf{F}_{ext,E}^n}{\partial \rho_e} \right)^T (\Delta \mathbf{u}_E^n + \lambda_{1,E}^n) + \left(\frac{\partial \mathbf{F}_{ext,E}^{n-1}}{\partial \rho_e} \right)^T (\Delta \mathbf{u}_E^n + \lambda_{2,E}^n) \right. \\ - (\lambda_1^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma^n}{\partial \rho_e} d\Omega - (\lambda_2^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma^{n-1}}{\partial \rho_e} d\Omega \\ - (\mathbf{K}_{u,FE}^n \lambda_{1,E}^n + \mathbf{K}_{u,FF}^n \lambda_{1,F}^n)^T \frac{\partial \mathbf{u}_F^n}{\partial \rho_e} \\ \left. - (\mathbf{K}_{u,FE}^{n-1} \lambda_{2,E}^n + \mathbf{K}_{u,FF}^{n-1} \lambda_{2,F}^n)^T \frac{\partial \mathbf{u}_F^{n-1}}{\partial \rho_e} \right\}. \end{aligned} \quad (4.43)$$

In order to eliminate the unknowns as shown in (3.51), we choose

$$\begin{aligned} \lambda_{1,E}^n &= -\Delta \mathbf{u}_E^n, & \lambda_{1,F}^n &= (\mathbf{K}_{u,FF}^n)^{-1} \mathbf{K}_{u,FE}^n \Delta \mathbf{u}_E^n \\ \lambda_{2,E}^n &= -\Delta \mathbf{u}_E^n, & \lambda_{2,F}^n &= (\mathbf{K}_{u,FF}^{n-1})^{-1} \mathbf{K}_{u,FE}^{n-1} \Delta \mathbf{u}_E^n. \end{aligned} \quad (4.44)$$

Then we can obtain the final objective derivative

$$\frac{\partial \bar{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_1^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma^n}{\partial \rho_e} d\Omega + (\lambda_2^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma^{n-1}}{\partial \rho_e} d\Omega \right\}. \quad (4.45)$$

For each element e , (4.45) can be re-written as

$$\begin{aligned} \alpha_e = \sum_{n=1}^{n_{load}} (\Delta \alpha_e)^n = -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_{1,e}^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma_e^n}{\partial \rho_e} d\Omega \right. \\ \left. + (\lambda_{2,e}^n)^T \int_{\Omega} \mathbf{B}_u^T \frac{\partial \sigma_e^{n-1}}{\partial \rho_e} d\Omega \right\}, e = 1, \dots, N_e, \end{aligned} \quad (4.46)$$

in which $(\cdot)_e$ is the element component of $(\cdot)$. For the sake of simplicity, we use α_e and α to represent element sensitivity and vector of all element sensitivities.

As shown also in Section 3.4, in order to remove instabilities such as checkerboard patterns and to avoid mesh-dependency in topology optimization process, element sensitivities are smoothed by means of a filtering scheme as (3.61). Finally, the OC method is employed to update the design variables.

4.3.2 Numerical example

In this section we present a 2D example to illustrate the method. For this purpose, a specimen with two asymmetrical notches, as described in Fig. 4.2(a), is considered. Plain strain is assumed. For the sake of simplicity of the topology process, uniform meshes of quadrilateral bilinear elements with element size $h_e = 0.4$ mm are used, as shown in Fig. 4.2(b), where the red meshes at the notches are removed from the finite element mesh. The boundary conditions are as follows: on the lower end ($y = 0$), the y -displacement are fixed, while the x -displacement are free and the node ($x = 0, y = 0$) is fixed. On the upper end, the x -displacement are free, while the y -displacement are prescribed to an increasing value of $\bar{U}$ with $\Delta\bar{U} = 0.005$ mm during the simulation. The incremental loading process goes on until the reaction force is below a prescribed value, indicating that the structure is fully broken. The characteristic length scale parameter ℓ_d for damage problem and ℓ_p for plastic problem are set to be $\ell_d = h_e$ and $\ell_p = 2h_e$, respectively. The filter radius r_{min} for topology process is chosen as $r_{min} = 2h_e$. The material parameters are shown in Table 4.2.

Table 4.2 Material parameters used in the numerical simulations

Name	Symbol	Matrix	Inclusion
Shear modulus	κ	27.28 GPa	70.3 GPa
Bulk modulus	μ	71.66 GPa	136.5 GPa
Yield stress	σ_Y	0.345 GPa	0.443 GPa
Hardening modulus	H	0.25 GPa	0.3 GPa
Fracture energy threshold	ψ_c	0.03 GPa	0.04 GPa

Fig. 4.3 shows the crack propagation, equivalent plastic strains and corresponding load-displacement curve of the asymmetrically notched specimen without the reinforced material. It can be seen that the equivalent plastic strain is maximum at both notches and localization branches form between the notches. The cracks initiate at both notch roots and propagate within the plastic strain localization band and eventually merge leading to complete failure. Similar simulation results can also be found in [9, 145].

Fig. 4.4 shows the evolution histories of inclusion topologies. Here, the inclusion volume fraction is set to $f^{inc} = 5\%$. As expected, the fracture resistance of the composite structure increases with accumulation of the inclusion material around the crack paths and reduction of intermediate densities. The external work finally converges to an almost constant value of 7.72 J. Detailed propagation of the crack phase field corresponding to its load-displacement

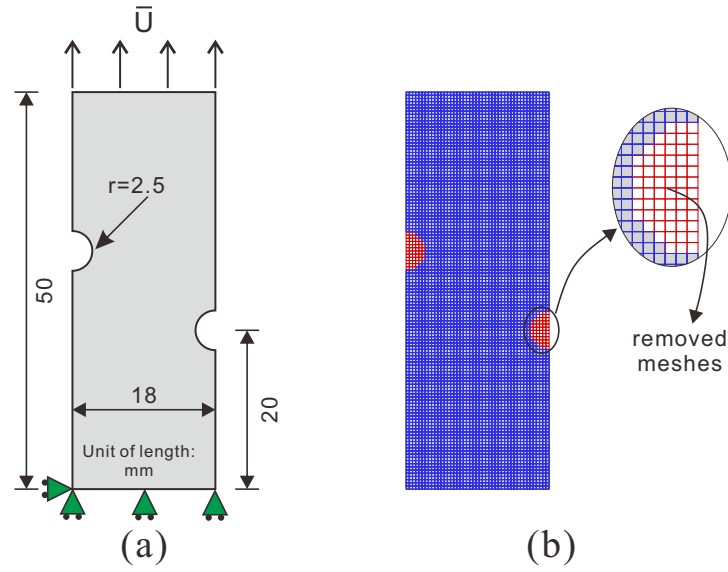


Fig. 4.2 Asymmetrically notched specimen: (a) geometry and boundary conditions; (b) finite element model.

curve for the optimized design is shown in Fig. 4.5. As can be observed from Fig. 4.5, the cracks initiate at both notch roots and go through the inclusion phase near the notches and then propagate following the inclusion surface until reaching the final failure.

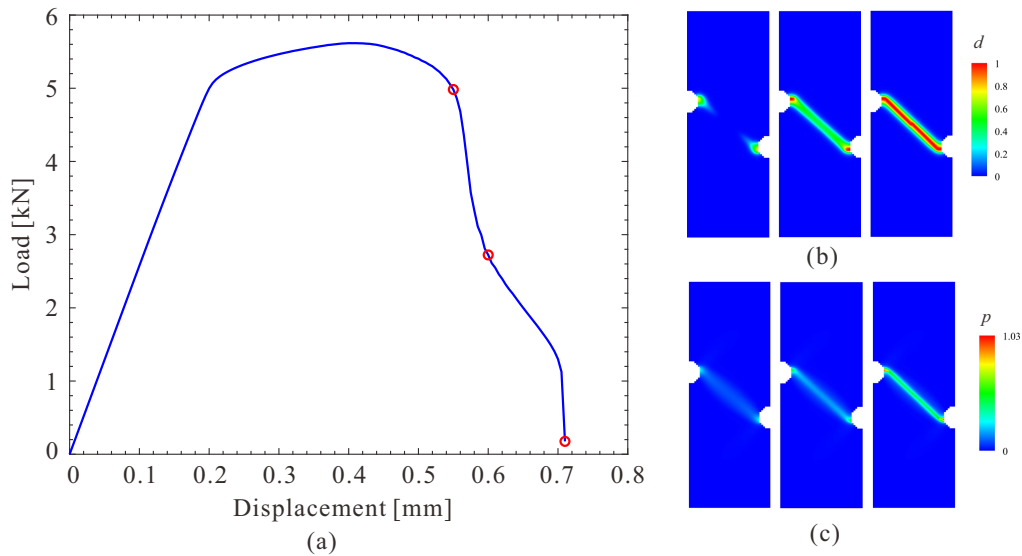


Fig. 4.3 Asymmetrically notched specimen without inclusion material: (a) load-displacement curve; (b) crack propagation and (c) equivalent plastic strains for $\bar{U} = 0.55$ mm, $\bar{U} = 0.6$ mm and $\bar{U} = 0.71$ mm.

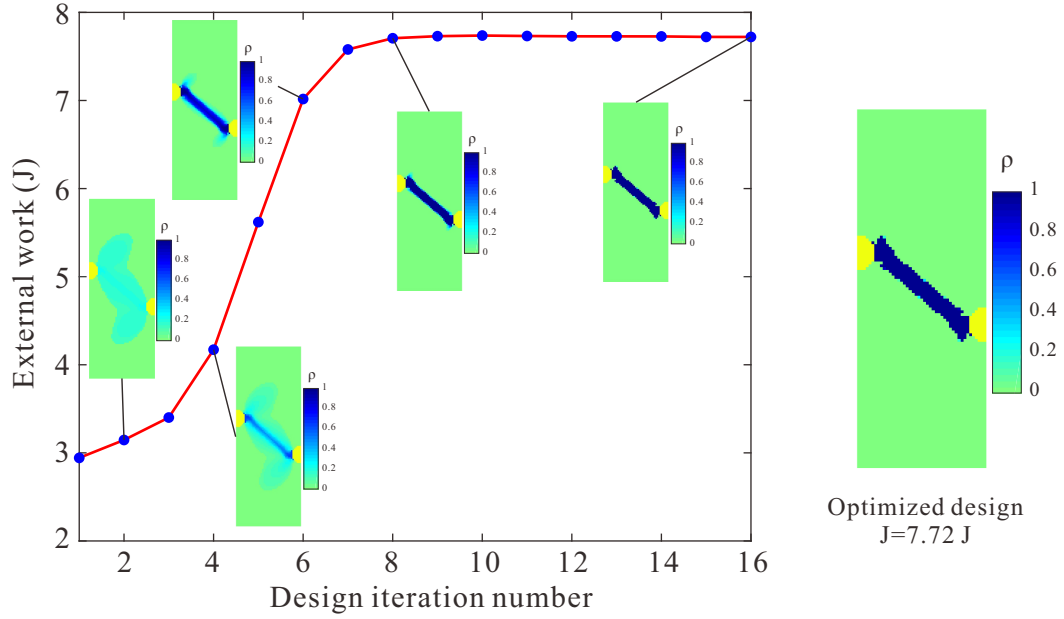


Fig. 4.4 Asymmetrically notched specimen. Evolution of inclusion topologies ($f^{inc} = 5\%$).

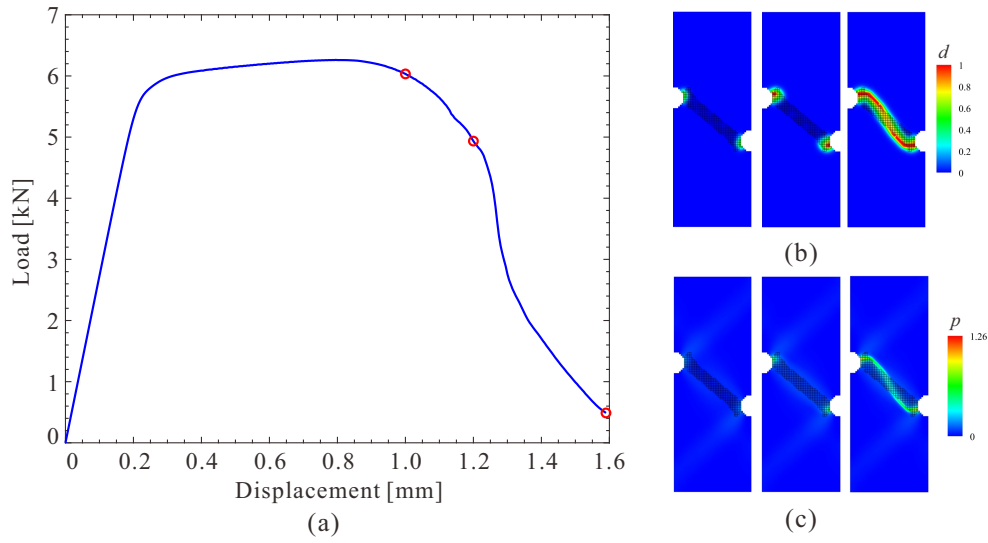


Fig. 4.5 Asymmetrically notched specimen: (a) load-displacement curve, (b) crack propagation and (c) equivalent plastic strains for the optimized design for $\bar{U} = 1$ mm, $\bar{U} = 1.2$ mm and $\bar{U} = 1.59$ mm. The inclusion meshes are shown for 2D visualization.

To illustrate the effectiveness of the proposed approach for improving the fracture resistance not simply by setting the inclusion at the crack path obtained from homogeneous sample (in other words, it is not easy to guess a good design which has the similar fracture

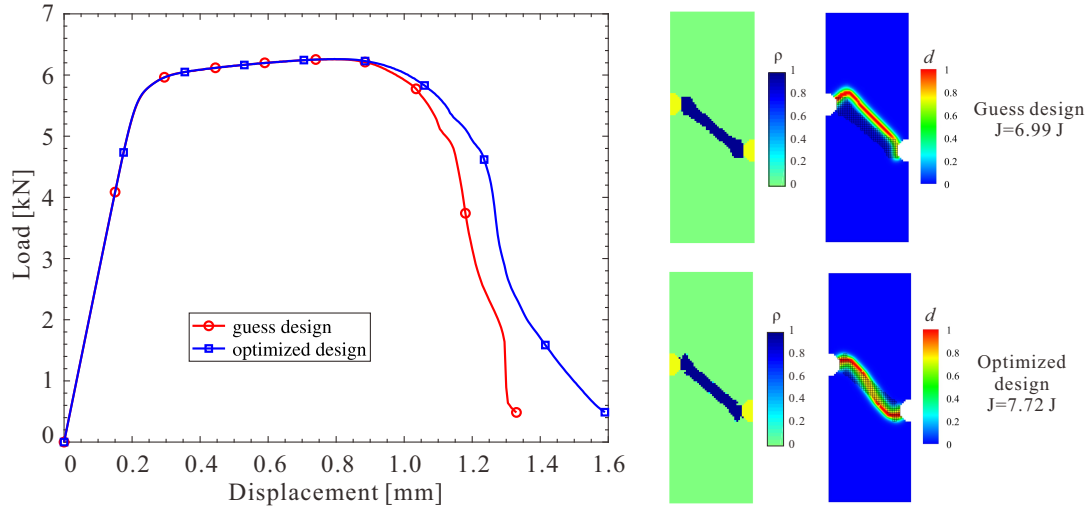


Fig. 4.6 Comparison of optimized design and guess design. The inclusion meshes are shown for 2D visualization.

resistance to the optimized design), we compare the optimized design with a guess design which is obtained by putting the inclusion at the crack path obtained from homogeneous sample. The guess design and corresponding comparisons can be found in Fig. 4.6. It can be observed that the fracture resistance of the optimized design is 10% higher as compared with the guess design.

The fracture resistance of the optimized design is further validated through another comparison study. With the same inclusion volume fraction $f^{inc} = 5\%$, another two topology optimizations using the same parameter setting have been carried out by considering only linear elastic behavior or elastoplastic behavior without accounting for crack propagation: elastic design and plastic design. Detailed comparison of these three designs is shown in Fig. 4.7. From both load–displacement curves and design objective values, the ductile design is greater 76% and 55% as compared with the elastic design and plastic design, respectively.

4.4 Topology optimization with interfaces

In this section, we present a topology optimization framework for maximizing the ductile fracture resistance, considering the interfaces in the heterogeneous structure. For the sake of simplicity, BESO was used here. The elastoplastic ductile fracture model with interfaces introduced in Section 4.2 is employed for modeling of fracture. Extended BESO method in [176, 49] is adopted to redistribute the inclusion phase with constant volume fraction. In

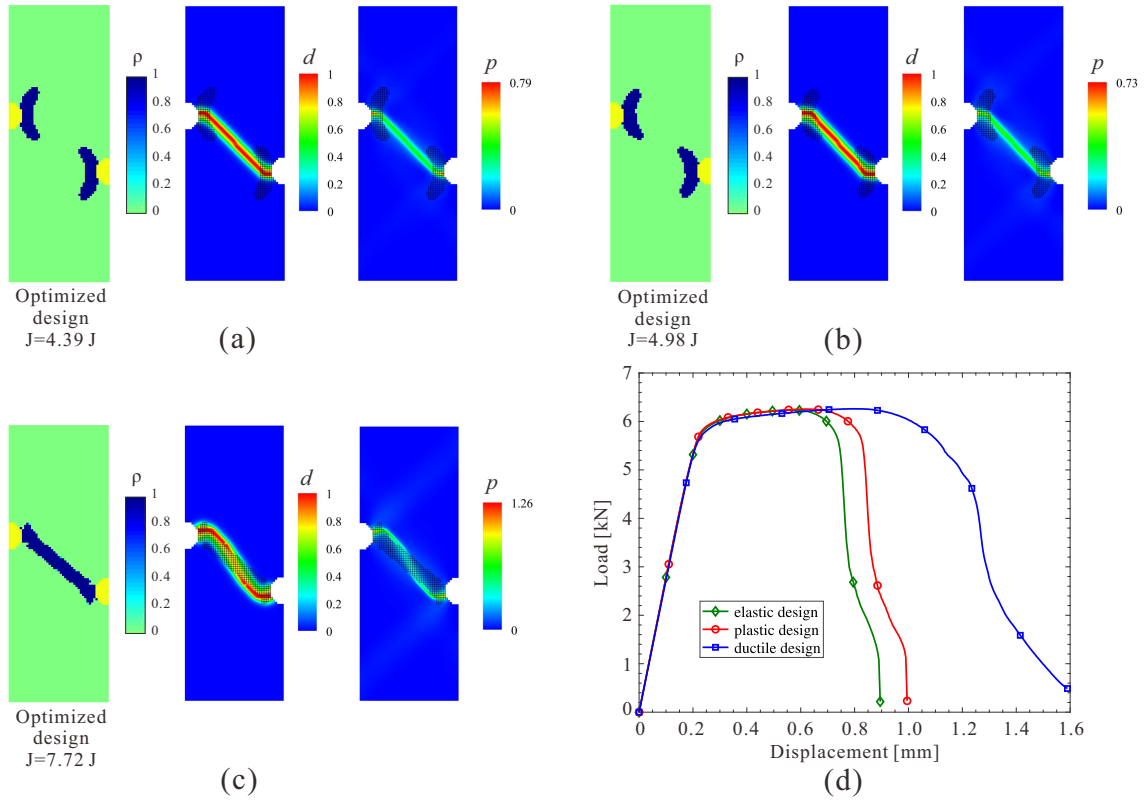


Fig. 4.7 Optimized design and corresponding final crack phase field and equivalent plastic strain: (a) elastic design; (b) plastic design and (c) ductile design, (d) load-displacement curves. The inclusion meshes are shown for 2D visualization.

the following, the topology optimization formulation is proposed in 4.4.1, then a numerical example is presented in Section 4.4.2 to show the robustness of the approach.

4.4.1 Topology optimization formulation

In order to clearly show the interfaces between matrix and inclusion phase, we use a discrete topology design variable $\rho_e \in \{0; 1\}$ indicates the associated material phase (matrix/inclusion) of the e -th element. The new material interpolations for the two-phase material are defined as

$$\begin{cases} \mu_e = \rho_e \mu_{inc} + (1 - \rho_e) \mu_{mat} \\ \kappa_e = \rho_e \kappa_{inc} + (1 - \rho_e) \kappa_{mat} \\ \sigma_{Y,e} = \rho_e \sigma_{Y,inc} + (1 - \rho_e) \sigma_{Y,mat} \\ h_e = \rho_e h_{inc} + (1 - \rho_e) h_{mat} \\ \psi_{c,e} = \rho_e \psi_{c,inc} + (1 - \rho_e) \psi_{c,mat} \end{cases} \quad (4.47)$$

As in Section 4.3, we optimize the total mechanical work to represent the optimization of the the fracture resistance. The optimization problem based on the discrete definition is then defined as follows:

$$\begin{aligned} & \max_{\rho} : J(\rho, \mathbf{u}, \mathbf{p}, \mathbf{d}) \\ & \text{subject to} : \mathbf{R} = 0 \\ & : \sum_{e=1}^{N_e} \rho_e v_e / (\sum_{e=1}^{N_e} v_e) = f^{inc} \\ & : \rho_e = 0 \text{ or } 1, e = 1, \dots, N_e. \end{aligned} \quad (4.48)$$

Above, $\mathbf{R}$ denotes the nodal residual force, when considering the interfaces, $\mathbf{R}$ is defined by [49]:

$$\mathbf{R} = \mathbf{F}_{ext} - \sum_{e=1}^{N_e} \rho_e \int_{\Omega_e} \mathbf{B}_u^T \sigma_e d\Omega_e, \quad (4.49)$$

Based on the sensitivity analysis as formulated in Section 4.3.1.2, the derivative of the total mechanical work J in (4.39) with respect to the topology design variable ρ_e can be stated as:

$$\frac{\partial \bar{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_{1,e}^n)^T \int_{\Omega_e} \mathbf{B}_u^T \sigma_e^n d\Omega_e + (\lambda_{2,e}^n)^T \int_{\Omega_e} \mathbf{B}_u^T \sigma_e^{n-1} d\Omega_e \right\}. \quad (4.50)$$

Above, λ_1^n and λ_2^n can be solve by:

$$\begin{aligned} \lambda_{1,E}^n &= -\Delta \mathbf{u}_E^n, & \lambda_{1,F}^n &= (\mathbf{K}_{u,FF}^n)^{-1} \mathbf{K}_{u,FE}^n \Delta \mathbf{u}_E^n \\ \lambda_{2,E}^n &= -\Delta \mathbf{u}_E^n, & \lambda_{2,F}^n &= (\mathbf{K}_{u,FF}^{n-1})^{-1} \mathbf{K}_{u,FE}^{n-1} \Delta \mathbf{u}_E^n, \end{aligned} \quad (4.51)$$

where $\mathbf{K}_u$ is given in (4.24).

The extended BESO method developed in [176, 49] is then employed here to update the design variables. In this method, the sensitivity numbers associated with the relative ranking of the element sensitivities are chosen to determine material phase exchange. When uniform meshes are used, the sensitivity numbers for the considered objective are defined as the following using the element sensitivity computed from (4.50):

$$\alpha_e = \begin{cases} \left(\frac{\partial \bar{J}}{\partial \rho_e} \right)^\eta, & \text{if } \rho_e = 1 \\ 0, & \text{if } \rho_e = 0 \end{cases} \quad (4.52)$$

in which η is a numerical damping coefficient. When $\eta = 1$, we recover the conventional sensitivity numbers for linear elastic designs [178]. In the presence of dissipative effects,

the sensitivity numbers vary by several orders of magnitude resulting in instabilities of the topology evolution process, especially when removing certain structural branches. For this reason, the sensitivity numbers are damped in this work with $\eta = 0.5$ as suggested in [177].

In order to remove instabilities such as checkerboard patterns and to avoid mesh-dependency in topology optimization process, element sensitivities are smoothed by means of a filtering scheme introduced in (3.61) in Section 3. Then the current sensitivity numbers are needed to be averaged with their historical information to improve the design convergence

$$\alpha_e^n \leftarrow \frac{(\alpha_e^n + \alpha_e^{n-1})}{2}. \quad (4.53)$$

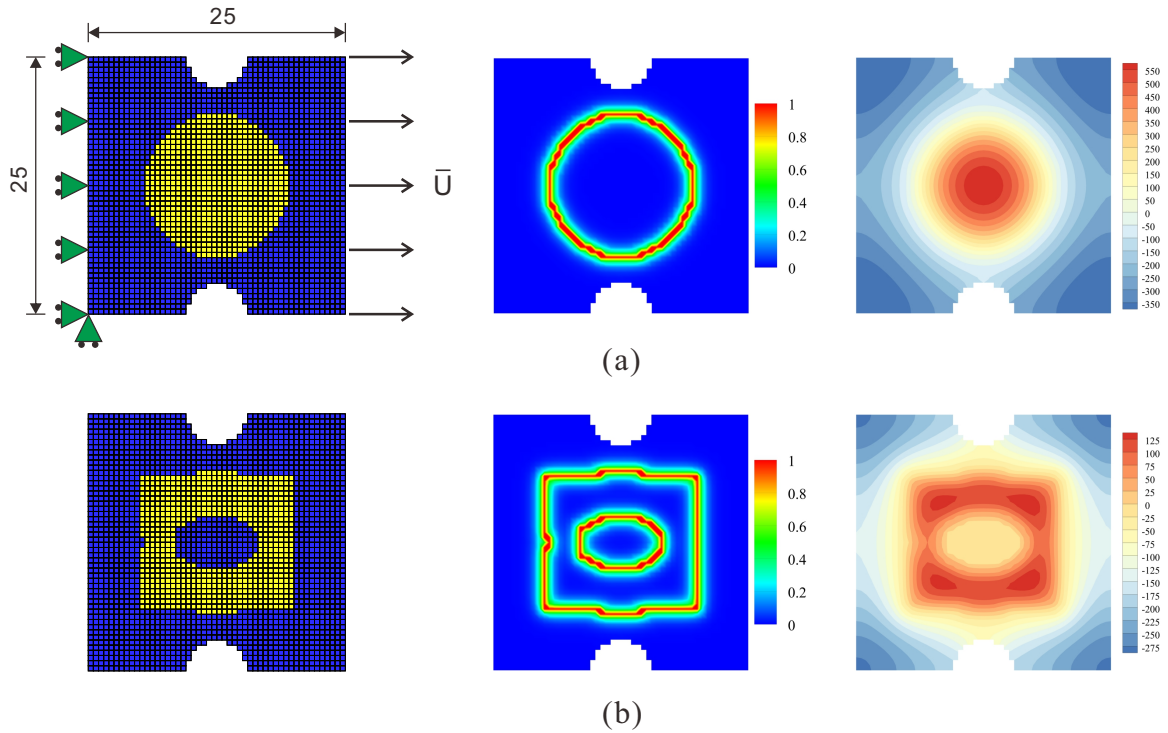


Fig. 4.8 A composite specimen with two symmetrical notches: inclusion shape (left), interfacial damage (center) and level-set function (right) for (a) initial design and (b) final design.

4.4.2 Numerical example

In this section, we present a 2D example to show the effectiveness of the method. For this purpose, a composite specimen with two symmetrical notches and a single fiber, as described in Fig. 4.8(a), is considered. Plain strain is assumed. For the sake of simplicity of topology

process, uniform meshes of quadrilateral bilinear elements with element size $h_e = 0.5$ mm are used. The boundary conditions are as follows: on the left end ($x = 0$), the x -displacement are fixed, while the y -displacement are free and the node ($x = 0, y = 0$) is fixed. On the right end, the y -displacement are free, while x -displacement are prescribed to an increasing value of $\bar{U}$ with $\Delta\bar{U} = 0.005$ mm during the simulation. The same stopping criterion based on reaction force indicating that the structure is fully broken is used. The characteristic length scale parameter ℓ_d for damage problem and ℓ_p for plastic problem are set to be $\ell_d = h_e$ and $\ell_p = 2h_e$, respectively. The filter radius r_{min} for topology process is chosen as $r_{min} = 6h_e$. The material parameters are shown in Table 4.2. Besides, the parameters related to interface are: $g_c^I = 0.1$ MPa, $t_u = 0.2$ MPa and $\ell_\beta = h = h_e$.

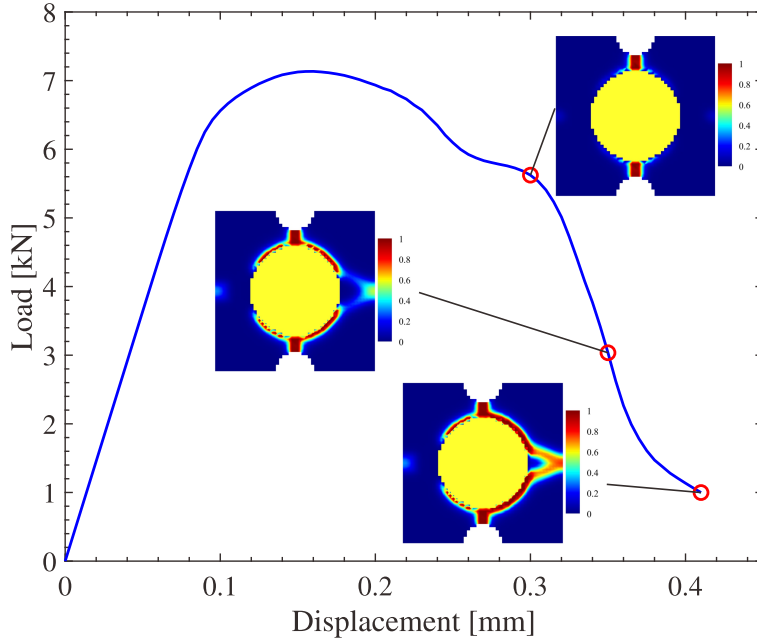


Fig. 4.9 Load-displacement curve and crack evolution for the initial design in the specimen with two symmetrical notches: (a) $\bar{U} = 0.3$ mm; (b) $\bar{U} = 0.35$ mm; (c) $\bar{U} = 0.41$ mm.

During the optimization process, the inclusion volume fraction f^{inc} is maintained constant ($f^{inc} = 0.258$). Fig. 4.8(b) shows the final design of inclusion topology. It is observed that the inclusion phase on the center moves outside, and finally distributes into a square-shape with an approximate ellipsoidal hole. Detailed propagation of the phase field crack of the initially and finally designed composite structure is shown in Fig. 4.9 and Fig. 4.10, respectively. In Fig. 4.9, we can see that the cracks initiate from the notch tips and propagate vertically to the surface of the inclusion phase and then propagate following the surface, finally interact at the right end of the specimen resulting in final failure of structure. From Fig. 4.10, we can

observe that the cracks also initiate from the notch tips and propagate vertically to the surface of the inclusion phase, while then another two cracks initiate from the top and bottom corner of the right surface of the inclusion phase and then interact with the crack initiating from the right end of the specimen, finally the cracks follow and interact at the surface of inclusion phase resulting in the fully broken state of the structure. We can see that the propagation of the cracks in final design structure meets more obstacles than that in initial design structure. Fig. 4.11 shows comparison of load-displacement curves and final crack patterns for initial and final design. Here, the fracture resistance of the final design is 13% higher as compared with the initial design.

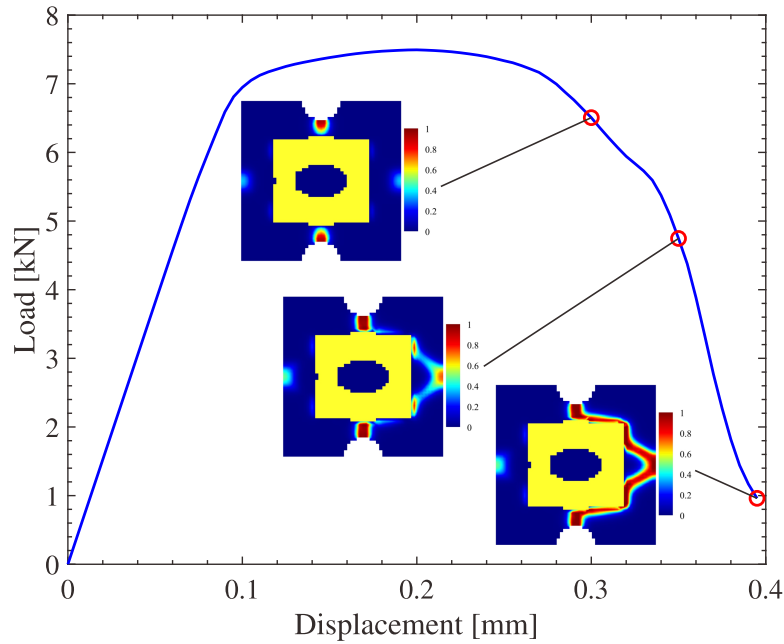


Fig. 4.10 Load-displacement curve and crack evolution for the final design in the specimen with two symmetrical notches: (a) $\bar{U} = 0.3$ mm; (b) $\bar{U} = 0.35$ mm; (c) $\bar{U} = 0.395$ mm.

4.5 Topology optimization of elastoplastic periodic structures with interfaces

In this section, we extend the topology optimization framework of optimal fracture resistance to elastoplastic periodic composites, considering the interfacial damage in the structure. The ductile phase field method presented in Section 4.2 is employed for modeling fracture propagation in the composite. Here, the composite is assumed to be composed of the substructure

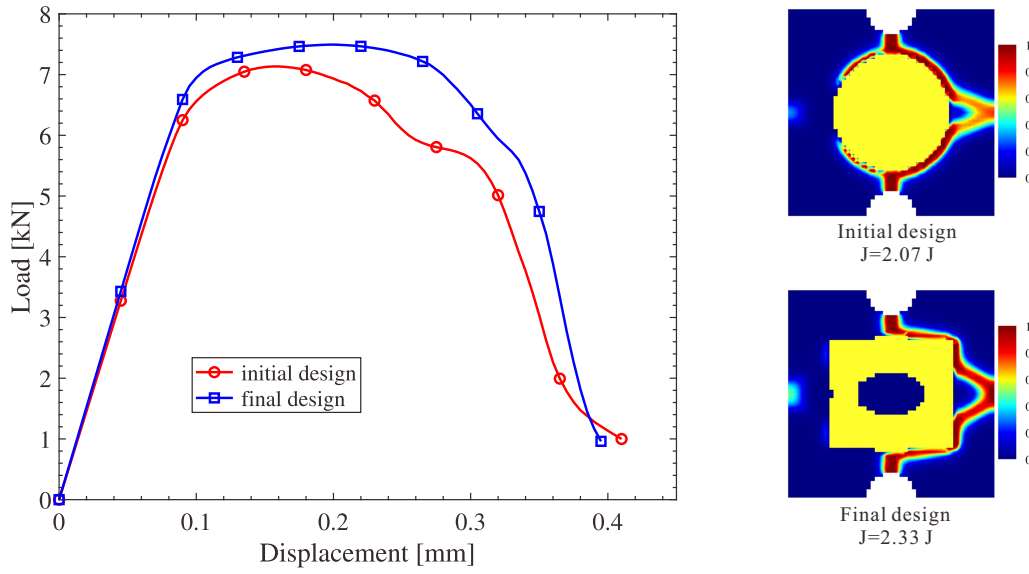


Fig. 4.11 Load-displacement curves and final crack pattern for initial and final design in the specimen with two symmetrical notches.

or representative volume element (RVE) periodically. Therefore, the optimization is carried out only on the RVE, but takes into account the response of the whole composite specimen to maximize its fracture resistance. Extended BESO method in 4.4.1 is adopted to redistribute the inclusion phase in the RVE with constant volume fraction. In the following, Section 4.5.1 provides the topology optimization model for maximizing the fracture resistance of periodic composites, then a numerical example is presented in Section 4.5.2 to show the efficiency of the approach.

4.5.1 Topology optimization formulation

In this section, the optimization problem for finding the optimal material distribution or topology of the inclusion phase within the RVE of the periodic composites. It is assumed that the total number of substructures/RVEs in the composites is N_k . The fracture resistance maximization problem then can be formulated using the design variable ρ_e^k , where k and e denote the substructure number and the element number in each substructure, respectively.

The optimization problem is then defined as follows:

$$\begin{aligned}
& \max_{\{\rho^1, \dots, \rho^k\}} : J(\rho, \mathbf{u}, \mathbf{p}, \mathbf{d}) \\
& \text{subject to : } \mathbf{R} = 0 \\
& : \sum_{e=1}^{N_e} \rho_e^k v_e^k / (\sum_{e=1}^{N_e} v_e^k) = f^{inc}, k = 1, \dots, N_k \\
& : \rho_e^1 = \dots = \rho_e^k, e = 1, \dots, N_e \\
& : \rho_e^k = 0 \text{ or } 1, e = 1, \dots, N_e,
\end{aligned} \tag{4.54}$$

where J is known as the fracture energy which is calculated by using numerical integration as (4.39). R denotes the nodal residual force in (4.49). v_e^k is the volume (area in 2D) of the e -th element in the k -th RVE, and N_e is the number of elements in each RVE. The condition $\rho_e^1 = \dots = \rho_e^k, e = 1, \dots, N_e$ ensures that the composites are periodic during the whole optimization process. The same material interpolation model as (4.47) is employed.

Based on the sensitivity analysis as formulated in Section 4.3.1.2, the derivative of the total mechanical work J with respect to the topology design variable ρ_e can be stated as:

$$\frac{\partial \bar{J}}{\partial \rho_e} = -\frac{1}{2} \sum_{n=1}^{n_{load}} \left\{ (\lambda_{1,e}^n)^T \int_{\Omega_e} \mathbf{B}_u^T \sigma_e^n d\Omega_e + (\lambda_{2,e}^n)^T \int_{\Omega_e} \mathbf{B}_u^T \sigma_e^{n-1} d\Omega_e \right\}. \tag{4.55}$$

Above, λ_1^n and λ_2^n can be solved as (4.51).

However, since the considered composites are periodic in this scheme, and the optimization process is carried out only within the substructure/RVE. Therefore, the element sensitivity numbers at the same location in each substructure need to be consistent to enforce the periodic array of the substructures. They are then defined as the sum of the sensitivity of corresponding elements in all substructures, i.e. the sensitivity number ρ_e is formulated as [48]:

$$\alpha_e = \sum_{k=1}^{N_k} \frac{\partial \bar{J}}{\partial \rho_e^k}. \tag{4.56}$$

As a result, the above sensitivity information takes into account the fracture response of the whole periodic composite.

Following Section 4.4.1, the sensitivity numbers associated with the relative ranking of the element sensitivities are treated with the damping as (4.52). In order to avoid checkerboard patterns, the above formulated sensitivity numbers are then smoothed by means of a filtering scheme as (3.61). Due to the discrete nature of design variable of the adopted method and to

avoid oscillations in evolutionary history of the design objective value, the current sensitivity number are further averaged with its historical information as (4.53).

4.5.2 Numerical example

This section presents a 2D example to show the effectiveness of the method in the topology of periodic structure. For this purpose, the composite structure in Section 4.4.2 is employed to reproduce a periodic structure, as described in Fig. 4.12(a). Plain strain is assumed. The boundary conditions are same as Section 4.4.2 as follows: on the left end ($x = 0$), the x -displacement are fixed, while the y -displacement are free and the node ($x = 0, y = 0$) is fixed. On the right end, the y -displacement are free, while x -displacement are prescribed to an increasing value of $\bar{U}$ with $\Delta\bar{U} = 0.005$ mm during the simulation. The same parameters as shown in Section 4.4.2 are used.

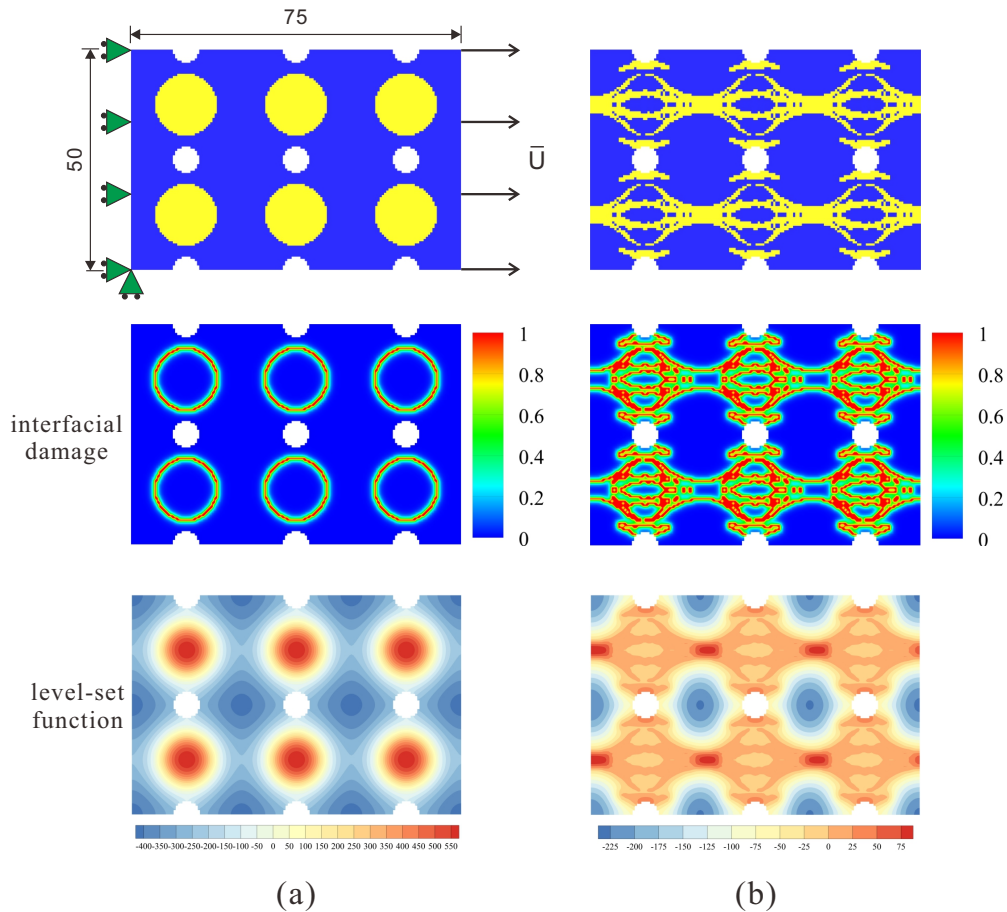


Fig. 4.12 A periodic specimen: inclusion shape (top), interface damage (center) and level-set function (bottom) for (a) initial design and (b) final design.

During the optimization process, the inclusion volume fraction f^{inc} is maintained constant. Based on their sensitivity numbers, the inclusion phase will be redistributed within the periodic cell by the extended BESO method so as to improve the fracture resistance of the whole periodic composite. Fig. 4.12(b) shows the final design of inclusion topology. We can see that the inclusion phase on the center moves to the notch tips and to the left and right end of the periodic cell, and finally distributes a complex composite structure. Detailed propagation of the phase field crack of the initially and finally designed composite structure is shown in Fig. 4.13 and Fig. 4.14, respectively. In Fig. 4.13, we can see that the cracks initiate from all the notch tips at the same time, then the two cracks initiating from the right hole propagate following the surface of inclusions, finally interact at the right end of the specimen resulting in final failure of structure. From Fig. 4.14, we can observe that the cracks initiate from the inclusion surface and propagate following the surface of inclusions and then continue to propagate until reaching the right end of the specimen. Fig. 4.15 shows comparison of load-displacement curves and final crack patterns for initial and final design. Here, the fracture resistance of the final design is 48% higher as compared with the initial design.

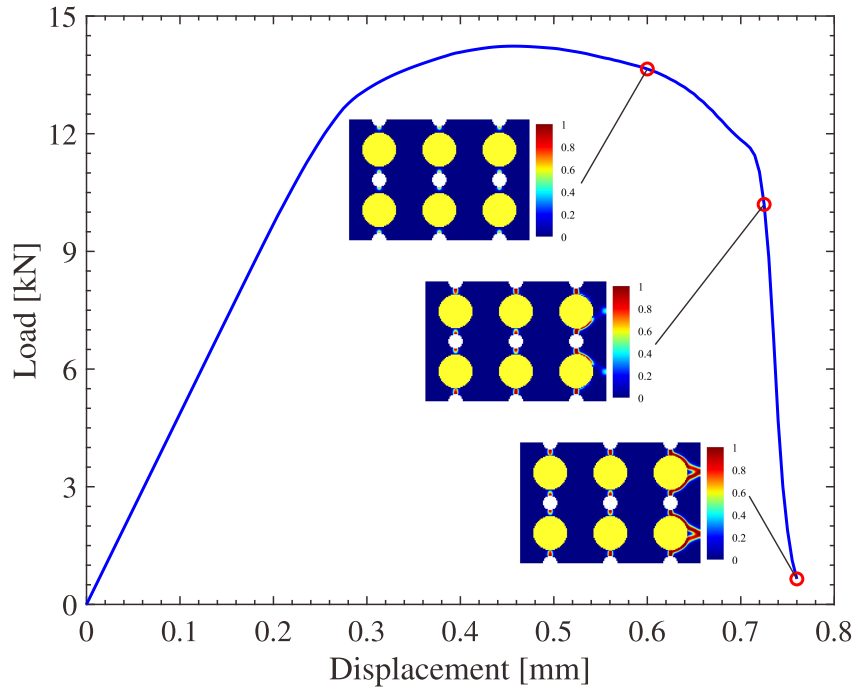


Fig. 4.13 Load-displacement curve and crack evolution for the initial design in the periodic specimen: (a) $\bar{U} = 0.6$ mm; (b) $\bar{U} = 0.725$ mm; (c) $\bar{U} = 0.76$ mm.

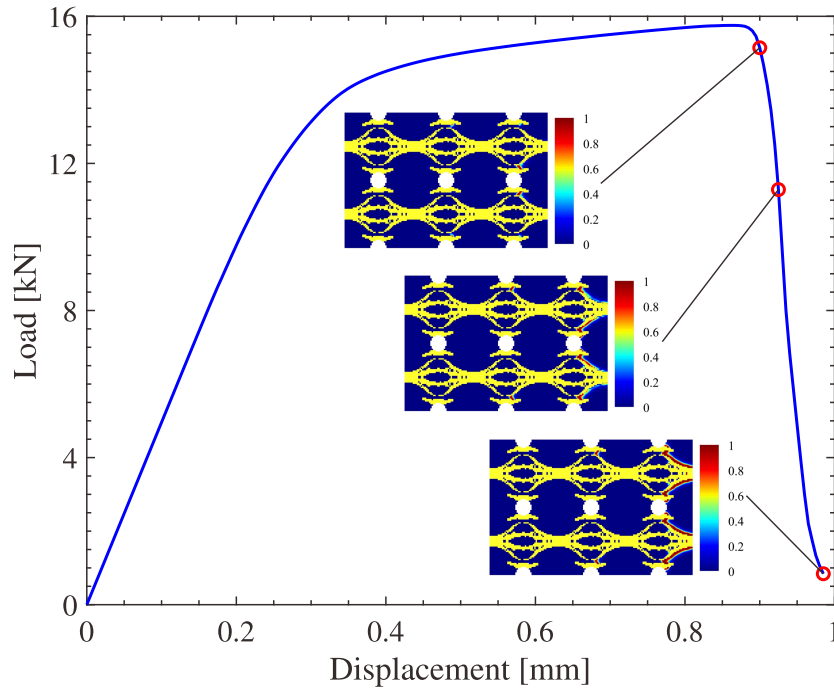


Fig. 4.14 Load-displacement curve and crack evolution for the final design in the periodic specimen: (a) $\bar{U} = 0.9$ mm; (b) $\bar{U} = 0.925$ mm; (c) $\bar{U} = 0.985$ mm.

4.6 Conclusion

In this chapter, we have developed topology optimization procedure for maximizing the fracture resistance of elastoplastic composites. A plasticity gradient phase field model [145] has been applied to better constrain the damage zone within the plastic zone. Interfacial damage has been taken into account through a regularized description of interfaces, and a diffuse weighting function to differentiate the bulk and interfacial behaviors, following [130]. Three cases have been investigated: (i) the case without considering interfacial damage between inclusion and matrix phase; (ii) the case considering interfacial damage between inclusion and matrix phase and (iii) the case considering interfacial damage for periodic structures. Three numerical tests have been presented to demonstrate the potential of the proposed topology optimization framework. In all cases, it has been shown that significant improvement of the fracture resistance of the considered composite structures can also be achieved for final designs when compared to the initial designs.

To summarize, the following original contributions have been introduced in this chapter: (i) a framework for modeling interfacial damage interacting with bulk ductile fracture within the gradient plasticity phase field method and (ii) a topology optimization of ductile

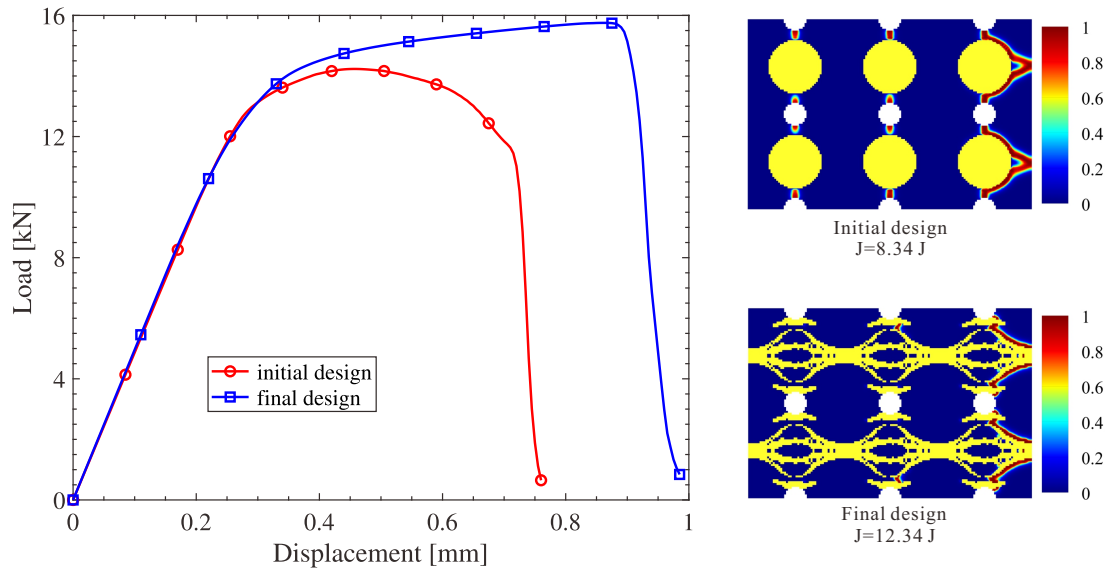


Fig. 4.15 Load-displacement curves and final crack pattern for initial and final design in the periodic specimen.

fracture resistance for elastoplastic composites with the proposed phase field model. Finally, the present framework seems to be very promising for improving fracture resistance of elastoplastic composites where both interfacial damage and bulk ductile fracture occur.

Chapter 5

A phase field anisotropic damage model for 3D printed elastoplastic materials

5.1 Introduction

In this chapter, we propose a damage model able to describe the behavior of polymer structures obtained by 3D printing processes, and which are formed by a layered structure. Such layered structure induces a preferential crack propagation direction along weak planes associated with the process, and related e.g. to a higher porosity between each layer of deposited powder or in polymer fuse deposition modeling. In addition to the induced anisotropic damage model, the behavior can be elastoplastic when the sample is loaded in a direction parallel to the layers, but brittle along a direction perpendicular to the layers. To our best knowledge, a model able to take into account both these characteristics is not available in the literature. The objective of this chapter is then to propose such model. A first contribution then consists into developing a full anisotropic elastoplastic phase field damage model, such that depending on the orientation and on the chosen parameters, the behavior can be differentiated into elastoplastic or quasi-brittle, depending on the underlying layers direction. A second contribution is an original methodology to construct the elastic energy functional within the phase field model by means of numerical calculations on a Representative Volume Element (RVE). Then, instead of using an empirical model, this elastic function is fully consistent with the full-field response of the microstructure. Numerical examples are provided to illustrate the capabilities of the present model.

5.2 Phase field approach to anisotropic damage in 3D printed elastoplastic materials

Phase-field models based on the variational formulation for anisotropic fracture have recently gained popularity, for example in [89, 168], where an anisotropic fracture energy was employed to simulate crack propagation in polycrystals [45, 125]. In [3], R. Alessi and F. Freddi used phase field model to investigate the complex failure process of unidirectional hybrid laminates. More recently in [28], J. Bleyer and R. Alessi proposed an anisotropic brittle fracture model to simulate the longitudinal/transverse damage in unidirectional fiber-reinforced composites.

5.2.1 Damage variables

We consider a 3D printed elastoplastic material in plane stress conditions, as described in Fig. 5.1(a), where the material frame (e_1, e_2) has an angle θ with respect to the global frame (e_x, e_y) . When the material is loaded in tension there are two different damage mechanisms: (i) the first one, as shown in Fig. 5.1(b), corresponds to failure oriented along e_1 occurring in the interface between two layers, called interfacial damage and represented by an associated damage variable α and (ii) the second one, Fig. 5.1(c), corresponds to failure oriented along e_2 in the layers, called bulk fracture and represented by d .

In order to capture the directional fracture θ and d in the global frame (e_x, e_y) , two anisotropic crack surface density functions extended from (2.3) are written by the following expressions:

$$\gamma_\alpha(\alpha) = \frac{\alpha^2}{2\ell_\alpha} + \frac{\ell_\alpha}{2} \omega_\alpha : (\nabla \alpha \otimes \nabla \alpha), \quad (5.1)$$

$$\gamma_d(d) = \frac{d^2}{2\ell_d} + \frac{\ell_d}{2} \omega_d : (\nabla d \otimes \nabla d), \quad (5.2)$$

where ℓ_α and ℓ_d are the length scale parameter of regularization for α and d , respectively. More explanation on this point can be found in Chapter 2. ω_α and ω_d are two second-order structural tensors, being invariant with respect to rotation of frame (e_1, e_2) .

In order to make the energy release rate orientation-dependent, the tensors ω_α and ω_d can be defined by [45, 125]:

$$\omega_\alpha = \mathbf{1} + \xi_\alpha (\mathbf{1} - \mathbf{M}_\alpha \otimes \mathbf{M}_\alpha), \quad (5.3)$$

$$\omega_d = \mathbf{1} + \xi_d (\mathbf{1} - \mathbf{M}_d \otimes \mathbf{M}_d), \quad (5.4)$$

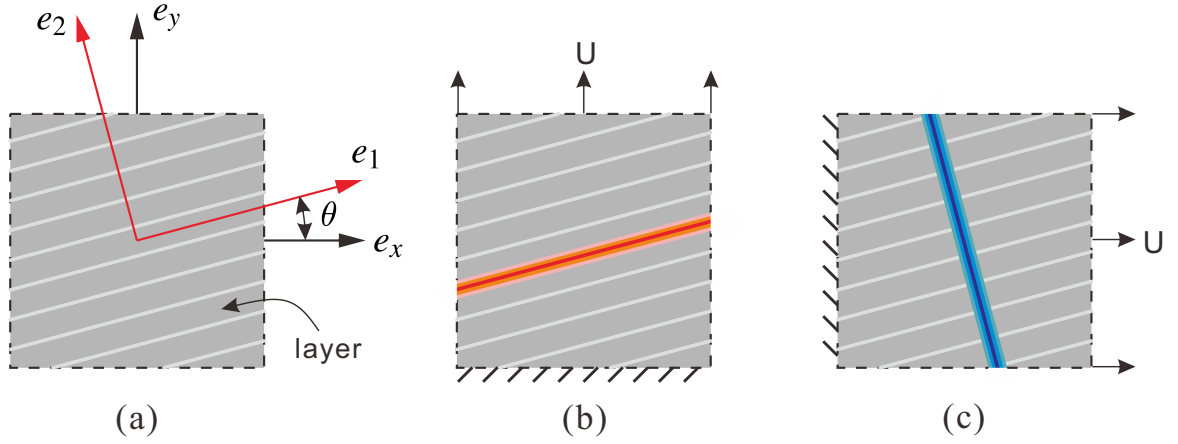


Fig. 5.1 Illustration of 3D printed materials for (a) layer direction, (b) interfacial damage and (c) bulk fracture.

where $\mathbf{M}_\alpha$ and $\mathbf{M}_d$ denote the unit vectors normal to e_1 and e_2 , respectively. $\xi_\alpha, \xi_d \gg 1$ are used to prevent damage α and d to develop on planes not normal to $\mathbf{M}_\alpha$ and $\mathbf{M}_d$, respectively. An estimation of the anisotropy introduced in the surface energy by this formulation can be found in [124].

5.2.2 Variational formulation

To construct the anisotropic damage model which can be quasi-brittle or elastoplastic depending on the orientation, we introduce two modifications as compared to the model in Chapter 2. First, the elastic strain density function is now dependent on the intra-layer damage variable α , as discussed in more details in the following. Second, an additional crack functional associated with α is added. The new proposed energy functional is in the form:

$$W(\mathbf{u}, p, d, \alpha) = \int_{\Omega} \psi^e(\boldsymbol{\varepsilon}(\mathbf{u}), p, d, \alpha) d\Omega + \int_{\Omega} [\psi^p(p) + \psi^d(d) + \psi^\alpha(\alpha)] d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} d\Omega, \quad (5.5)$$

where $\psi^p(p)$ is the stored plastic energy density function and has been defined in (2.31). $\psi^\alpha(\alpha)$ and $\psi^d(d)$ are the damage dissipative potentials with respect to α and d , respectively. They are defined as

$$\psi^\alpha(\alpha) = g_c^\alpha \gamma_\alpha(\alpha), \quad \psi^d(d) = g_c^d \gamma_d(d), \quad (5.6)$$

g_c^α and g_c^d are the fracture toughnesses with respect to α and d , respectively. We introduce the elastic strain density function ψ^e in the form

$$\psi^e(\boldsymbol{\varepsilon}(\mathbf{u}), p, d, \alpha) = \frac{1}{2}(\boldsymbol{\varepsilon}^e)^T \mathbf{C}(\alpha, d) \boldsymbol{\varepsilon}^e, \quad (5.7)$$

where $\mathbf{C}(\alpha, d)$ is the matrix form of elasticity tensor corresponding to the vector of elastic strain components $\boldsymbol{\varepsilon}^e = [\varepsilon_{11}^e, \varepsilon_{22}^e, 2\varepsilon_{12}^e]^T$ in the material frame (e_1, e_2) . The dependence to θ defining the angle between e_1 and the printed layer direction will be discussed in section 5.3.1.

In the reference frame (e_1, e_2) , we assume that the damage-dependent elasticity matrix is given by:

$$\mathbf{C}(\alpha, d) = g(d) \mathbf{C}_\alpha(\alpha), \quad (5.8)$$

where $g(d)$ has been defined in (2.30). $\mathbf{C}_\alpha(\alpha)$ is the interfacial damage-dependent elasticity matrix. A detailed description for the numerical computation of $\mathbf{C}_\alpha(\alpha)$, based on a numerical homogenization method, is provided in Section 5.3.

It should be noted that $\mathbf{C}_\alpha(\alpha)$ in this work is constructed by taking into account the real mechanical reactions of a RVE from 3D printed materials, unlike in [28], where the anisotropic brittle fracture model is based on an empirical damage-dependent elasticity tensor.

5.2.2.1 Irreversibility condition

The irreversibility condition is prescribed on the bulk fracture d and interfacial damage α . For bulk fracture irreversibility condition, it can be found in (2.8). For interfacial damage irreversibility condition, it can be expressed with the similar manner to the plastic irreversibility condition in (4.3).

5.2.2.2 First-order stability condition

The first order stability condition (see [113, 114, 143]) is expressed by:

$$D_{\delta \mathbf{u}} W(\mathbf{u}, p, d, \alpha) + D_{\delta p} W(\mathbf{u}, p, d, \alpha) + D_{\delta d} W(\mathbf{u}, p, d, \alpha) + D_{\delta \alpha} W(\mathbf{u}, p, d, \alpha) \geq 0. \quad (5.9)$$

With (5.5), (5.9) yields:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta \mathbf{u}) d\Omega + \int_{\Omega} \left(-\sqrt{\frac{3}{2}} \boldsymbol{\sigma} : \hat{\mathbf{n}} + \frac{\partial \psi^p}{\partial p} \right) \delta p d\Omega +$$

$$\int_{\Omega} \left(\frac{\partial \psi^e}{\partial d} + \frac{\partial \psi^d}{\partial d} \right) \delta d d\Omega + \int_{\Omega} \left(\frac{\partial \psi^e}{\partial \alpha} + \frac{\partial \psi^\alpha}{\partial \alpha} \right) \delta \alpha d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta \mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta \mathbf{u} d\Omega \geq 0 \quad (5.10)$$

where ε^e has been expressed in (2.12) and

$$\boldsymbol{\sigma} = \frac{\partial \psi^e}{\partial \varepsilon^e} = g(d) \mathbf{C}_\alpha(\alpha) \varepsilon^e. \quad (5.11)$$

Then, the following results stem out:

- For $\delta p = \delta d = \delta \alpha = 0$, we obtain (2.14).
- For $\delta d = \delta \alpha = 0$ and $\delta \mathbf{u} = \mathbf{0}$, we obtain (2.15)-(2.17).
- For $\delta p = \delta \alpha = 0$ and $\delta \mathbf{u} = \mathbf{0}$, we obtain (2.18) and (2.19).
- For $\delta p = \delta d = 0$ and $\delta \mathbf{u} = \mathbf{0}$, we obtain:

$$\int_{\Omega} \left(\frac{\partial \psi^e}{\partial \alpha} + \frac{\partial \psi^\alpha}{\partial \alpha} \right) \delta \alpha d\Omega \geq 0 \quad (5.12)$$

which is the weak form of the damage criterion. In local form, it can be expressed as:

$$F^\alpha(\alpha) = - \left(\frac{\partial \psi^e}{\partial \alpha} + \frac{\partial \psi^\alpha}{\partial \alpha} \right) \leq 0 \text{ in } \Omega. \quad (5.13)$$

5.2.2.3 Energy balance

Similarly than in Chapter 2, the consistency conditions for plasticity, bulk damage and interfacial damage are obtained as:

$$F^p(p) \dot{p} = 0, \quad F^d(d) \dot{d} = 0, \quad F^\alpha(\alpha) \dot{\alpha} = 0. \quad (5.14)$$

5.2.2.4 Alternate minimization

With a similarly staggered alternate minimization algorithm in Chapter 2, the weak forms for displacement problem, plastic problem, bulk fracture problem and interfacial damage problem are obtained:

- Minimization with respect to the displacement field, the weak form for displacement problem as in (2.24) is obtained.
- Minimization with respect to the equivalent plastic strain p , the weak form for plastic problem as in (2.25) is obtained.

- Minimization with respect to the bulk fracture d , the weak form for bulk fracture problem as in (2.26) is obtained.
- Minimization with respect to the interfacial damage α :

$$D_{\delta\alpha}W(\mathbf{u}, p, d, \alpha) = \int_{\Omega} \left(\frac{\partial \psi^e}{\partial \alpha} + \frac{\partial \psi^\alpha}{\partial \alpha} \right) \delta\alpha d\Omega = 0, \quad (5.15)$$

which is the weak form for interfacial damage problem.

More specifically, the staggered procedure to solve the four problems is summarized in Table 5.1.

Table 5.1 Problems to be solved in the staggered procedure

Displacement problem and plastic problem: given d and α , solve for $\mathbf{u}$:

$$\int_{\Omega} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^e(\delta\mathbf{u}) d\Omega - \int_{\partial\Omega_F} \mathbf{F} \cdot \delta\mathbf{u} dS - \int_{\Omega} \mathbf{f} \cdot \delta\mathbf{u} d\Omega = 0$$

$$\boldsymbol{\sigma} = g(d)\mathbf{C}_\alpha(\alpha)\boldsymbol{\varepsilon}^e$$

$$F^p(p) = \sqrt{\frac{3}{2}}\|\mathbf{s}\| - (\sigma_Y + Hp) \leq 0$$

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{p}\sqrt{\frac{3}{2}}\frac{\mathbf{s}}{\|\mathbf{s}\|} \text{ with } \dot{p} \geq 0$$

Bulk fracture problem: given $\mathbf{u}$ and α , solve for d :

$$\int_{\Omega} \left[\left(2\mathcal{H}(\mathbf{u}) + \frac{g_c^d}{\ell_d} \right) d\delta d + g_c^d \ell_d \nabla d \omega_d \nabla(\delta d) \right] d\Omega = \int_{\Omega} 2\mathcal{H}(\mathbf{u}) \delta d d\Omega$$

$$\mathcal{H}(\mathbf{u}) = \max_{s \in [0,1]} \psi_0^e(\mathbf{u}, s) \text{ with } \psi_0^e = \frac{1}{2} \boldsymbol{\varepsilon}^e \mathbf{C}_\alpha(\alpha) \boldsymbol{\varepsilon}^e$$

Interfacial damage problem: given $\mathbf{u}$ and d , solve for α :

$$\int_{\Omega} \left[\frac{1}{2} g(d) \boldsymbol{\varepsilon}^e \frac{\partial \mathbf{C}_\alpha}{\partial \alpha} \boldsymbol{\varepsilon}^e + \frac{g_c^\alpha}{\ell_\alpha} \alpha \delta \alpha + g_c^\alpha \ell_\alpha \nabla \alpha \omega_\alpha \nabla(\delta \alpha) \right] d\Omega = 0.$$

5.3 Construction of $\mathbf{C}_\alpha(\alpha)$ based on a numerical homogenization method

A major difficulty for this proposed model is to determine the influence of interfacial damage evolution on the elasticity matrix $\mathbf{C}_\alpha(\alpha)$ in (5.8). In this section, we propose a novel approach to construct $\mathbf{C}_\alpha(\alpha)$ based on a numerical homogenization method.

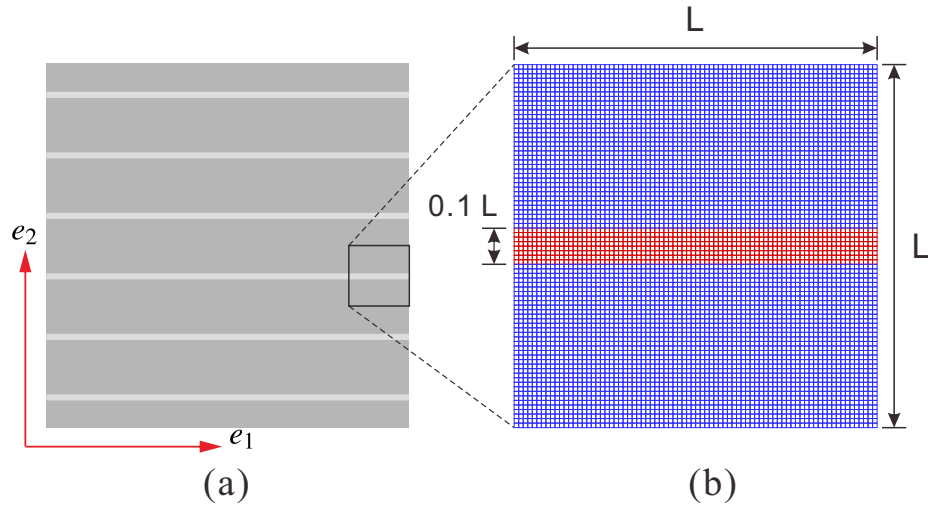


Fig. 5.2 (a) 3D printed material in the frame (e_1, e_2) ; (b) Representative volume element geometry and FE mesh.

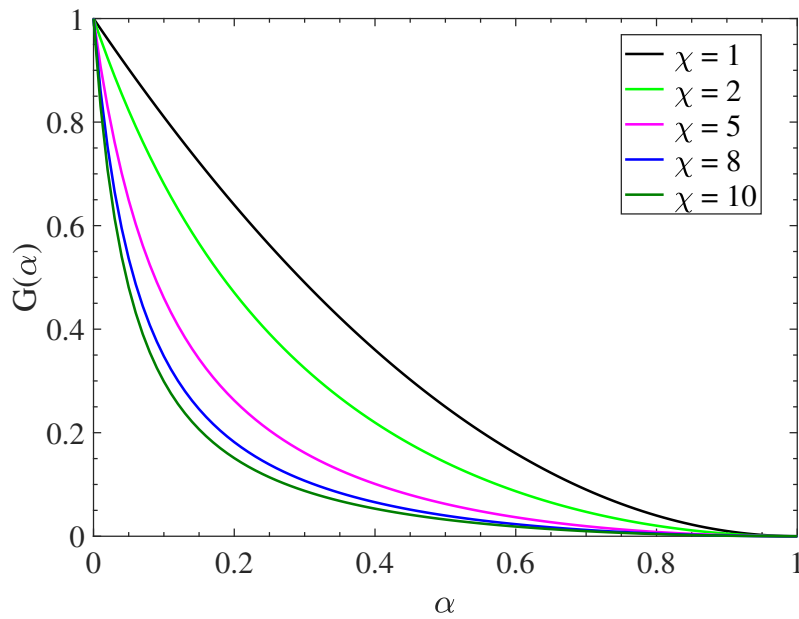


Fig. 5.3 The degradation function $G(\alpha)$ for various parameter χ .

We consider a 3D printed material in the frame (e_1, e_2) , as described in Fig. 5.2(a). An RVE with FE mesh is shown in Fig. 5.2(b), where the blue mesh corresponds to the layers and the red mesh corresponds to an interface between two layers. In order to simulate the degradation of the interface domain caused by the evolution of interfacial damage, we define

the Young's modulus E_I for interface mesh as

$$E_I(\alpha) = G(\alpha)E, \quad G(\alpha) = \frac{(1-\alpha)^2}{\chi - (\chi-1)(1-\alpha)^2} \text{ with } \chi \geq 1, \quad (5.16)$$

where the degradation function $G(\alpha)$ is found from [6]. Fig. 5.3 shows the performance of $G(\alpha)$ with different parameter χ . The Poisson's ratio ν_I for interface mesh is assumed as $\nu_I = \nu$.

With the plane stress assumption, the elasticity matrix for the interface mesh can be expressed as

$$\mathbf{C}_I(\alpha) = \frac{E_I(\alpha)}{1-\nu_I^2} \begin{bmatrix} 1 & \nu_I & 0 \\ \nu_I & 1 & 0 \\ 0 & 0 & \frac{1-\nu_I}{2} \end{bmatrix}. \quad (5.17)$$

5.3.1 Strain approach

A localization problem based on strains, i.e., assuming that the RVE is subjected to a homogeneous strain field is used here. An effective elasticity tensor is computed for each given value of α , which defines the local elasticity tensor in the RVE $\mathbf{C}^0(\mathbf{x})$ according to (5.21). Then, the displacement solution of the localization problem can be expressed as [186]

$$\mathbf{u}(\mathbf{x}) = \underbrace{\begin{bmatrix} \mathbf{u}^{(11)}(\mathbf{x}) & \mathbf{u}^{(22)}(\mathbf{x}) & \mathbf{u}^{(12)}(\mathbf{x}) \end{bmatrix}}_{\mathbf{U}} \underbrace{\begin{bmatrix} \bar{\epsilon}_{11} \\ \bar{\epsilon}_{22} \\ 2\bar{\epsilon}_{12} \end{bmatrix}}_{[\bar{\epsilon}]}, \quad (5.18)$$

where $[\bar{\epsilon}]$ is the macroscopic strain of the RVE in vector form, and $\mathbf{u}^{(ij)}(\mathbf{x})$ is the FEM solution of the localization problem for the corresponding macroscopic strain component $\bar{\epsilon}_{ij} = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}$ and $\begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$, prescribed through periodic boundary conditions over the nodes of the external boundary of the RVE mesh. A detailed description on how to prescribe the periodic boundary conditions is provided in Section 5.3.2.

Then in each element, we can obtain the stress:

$$[\boldsymbol{\sigma}(\mathbf{x})] = \mathbf{C}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{U}^e [\bar{\epsilon}], \quad (5.19)$$

where $\mathbf{C}(\mathbf{x})$ is the elasticity matrix for plane stress conditions, and $\mathbf{B}(\mathbf{x})$ is a matrix of displacement shape function derivatives, and $\mathbf{U}^e$ is the element component of $\mathbf{U}$. With the

spatial average of (5.19), we obtain macroscopic stress of the RVE in vector form

$$[\bar{\sigma}] = \left(\underbrace{\frac{1}{V} \int_{\Omega^e} \mathbf{C}(\mathbf{x}) \mathbf{B}(\mathbf{x}) \mathbf{U}^e d\Omega^e}_{\bar{\mathbf{C}}^0} \right) [\bar{\epsilon}], \quad (5.20)$$

where

$$\bar{\mathbf{C}}^0 = \frac{1}{V} \int_{\Omega^e} \mathbf{C}(\mathbf{x}) \mathbf{B}(\mathbf{x}) \mathbf{U}^e d\Omega^e \quad (5.21)$$

is the effective elasticity matrix.

Then, we can obtain $\mathbf{C}_\alpha(\alpha)$ through polynomial fitting of the evolution of $\bar{\mathbf{C}}$ with respect to the interfacial damage $\alpha \in [0, 1]$. A detailed numerical example on specialization of $\mathbf{C}_\alpha$ is provided in Section 5.5.1. For an arbitrary rotation angle θ , the final effective elasticity tensor is given by

$$C_{ijkl}(\theta) = R_{ip}(\theta) R_{jq}(\theta) R_{kr}(\theta) R_{ls}(\theta) C_{pqrs}^0, \quad (5.22)$$

with

$$\mathbf{R}(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (5.23)$$

5.3.2 Periodic boundary conditions

In this section, we detail how to prescribe the periodic boundary conditions over the nodes of the external boundary of the RVE mesh. Compared to other types of boundary conditions, it ensures that the obtained effective properties converge with respect to a single periodic cell.

Considering two nodes m and n on opposite faces of the RVE, the displacements on the two nodes have the forms:

$$u_i(\mathbf{x}^m) = \bar{\epsilon}_{ij} x_j^m + \tilde{u}_i(\mathbf{x}^m) \quad (5.24)$$

and

$$u_i(\mathbf{x}^n) = \bar{\epsilon}_{ij} x_j^n + \tilde{u}_i(\mathbf{x}^n). \quad (5.25)$$

As the fluctuation $\tilde{\mathbf{u}}$ is periodic on $\partial\Omega$, we have

$$\tilde{u}_i(\mathbf{x}^m) = \tilde{u}_i(\mathbf{x}^n). \quad (5.26)$$

Then, we can obtain

$$u_i(\mathbf{x}^m) - u_i(\mathbf{x}^n) = \bar{\varepsilon}_{ij}(x_j^m - x_j^n). \quad (5.27)$$

Based on a technique of Lagrange multipliers to ensure the constrained minimization problem, we can add the periodicity constraints in (5.27) into the linear system for displacement solving as (see [186] for more details):

$$\begin{bmatrix} \mathbf{K} & \mathbf{P}^T \\ \mathbf{P} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \Lambda \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{R} \end{bmatrix} \quad (5.28)$$

where $\mathbf{K}$ is the stiffness matrix obtained after discretization of the elastic problem in Section 5.3.1 before prescribing the Dirichlet boundary conditions, $\mathbf{P}$ is a matrix relating the coupled nodes indices to the whole set of nodes indices, Λ is the vector of Lagrange multipliers associated with the periodicity constraints, and $\mathbf{R}$ is the vector containing $\bar{\varepsilon}_{ij}(x_j^m - x_j^n)$ for all coupled nodes.

It should be noted that four nodes on the corners in Fig. 5.2(b) should be prescribed through kinematically uniform boundary conditions to prevent matrix singularity when solving (5.28).

5.4 Numerical implementation

In this section, we detail the FEM discretizations for displacement, bulk damage and interfacial damage problems.

5.4.1 Displacement problem

We refer to sections 2.2.3.1 and 2.2.3.2, where the procedure is identical than for the present problem.

5.4.2 Bulk damage problem

The discretization of bulk damage problem in Table 5.1 results into the following discrete system of equations:

$$\mathbf{K}_d \mathbf{d} = \mathbf{F}_d \quad (5.29)$$

in which

$$\mathbf{K}_d = \int_{\Omega} \left[\left(2\mathcal{H} + \frac{g_c^d}{\ell_d} \right) \mathbf{N}_d^T \mathbf{N}_d + g_c^d \ell_d \mathbf{B}_d^T \boldsymbol{\omega}_d \mathbf{B}_d \right] d\Omega \quad (5.30)$$

and

$$\mathbf{F}_d = \int_{\Omega} 2\mathbf{N}_d^T \mathcal{H} d\Omega, \quad (5.31)$$

where $\mathcal{H}$ is given in Table 5.1.

5.4.3 Interfacial damage problem

The discretization of interfacial damage problem in Table 5.1 results into the following discrete system of equations:

$$\mathbf{K}_{\alpha}\alpha + \mathbf{F}_{\alpha}(\alpha) = \mathbf{0} \quad (5.32)$$

in which

$$\mathbf{K}_{\alpha} = \int_{\Omega} \left(\frac{g_c^{\alpha}}{\ell_{\alpha}} \mathbf{N}_d^T \mathbf{N}_d + g_c^{\alpha} \ell_{\alpha} \mathbf{B}_d^T \omega_{\alpha} \mathbf{B}_d \right) d\Omega \quad (5.33)$$

and

$$\mathbf{F}_{\alpha}(\alpha) = \int_{\Omega} \frac{1}{2} g(d) \varepsilon^e \frac{\partial \mathbf{C}_{\alpha}}{\partial \alpha} \varepsilon^e d\Omega. \quad (5.34)$$

Note that in general, (5.32) is a nonlinear problem and must be solved through a standard Newton-type iteration as used in Section 2.2.3.2. In section 5.5.1, we will fit a quadratic model to the components $\mathbf{C}(\alpha)$ to keep (5.32) linear.

In the present work, a staggered scheme is employed, where at each load increment the displacement problem is solved for fixed bulk and interfacial damage field which is known from the previous time step. The bulk damage problem is then solved with the new displacement field and previous interfacial damage field. Finally, the interfacial damage problem is solved with the new displacement field and bulk damage field.

5.5 Numerical examples

For all of the following numerical examples, a mesh of 4-node quadrilateral elements and plane stress assumption has been used. The material parameters for layer are as follows (unless otherwise stated): $E = 10$ GPa, $\nu = 0.25$, $\sigma_Y = 0.08$ GPa and $H = 0.1$ GPa. The fracture toughness for bulk fracture and interfacial damage are $g_c^d = 2 \times 10^{-3}$ kN/mm and $g_c^{\alpha} = 1 \times 10^{-3}$ kN/mm, respectively. The length scale parameters for bulk damage and interfacial damage are $\ell_d = \ell_{\alpha} = 0.2$ mm. $\xi_{\alpha} = \xi_d = 30$ is used.

5.5.1 Specialization of $\mathbf{C}_\alpha$

As mentioned above, to maintain the problem related to α as linear, we introduce a quadratic fit of the different components of $\bar{\mathbf{C}}(\alpha)$. Here the material parameters of the interface elements in Fig. 5.2(b) have been defined in Section 5.3 as: $E_I(\alpha) = G(\alpha)E$ and $\nu_I = \nu$. The effective elasticity matrix is computed by the above procedure as shown in Section 5.3. The evolution of the different effective components are depicted in Fig. 5.4. We can see that the effective elasticity components $\bar{C}_{12}$, $\bar{C}_{22}$ and $\bar{C}_{33}$ decrease to zero when $\alpha = 1$, and the effective elasticity component $\bar{C}_{11}$ decreases slightly to a nonzero constant when $\alpha = 1$.

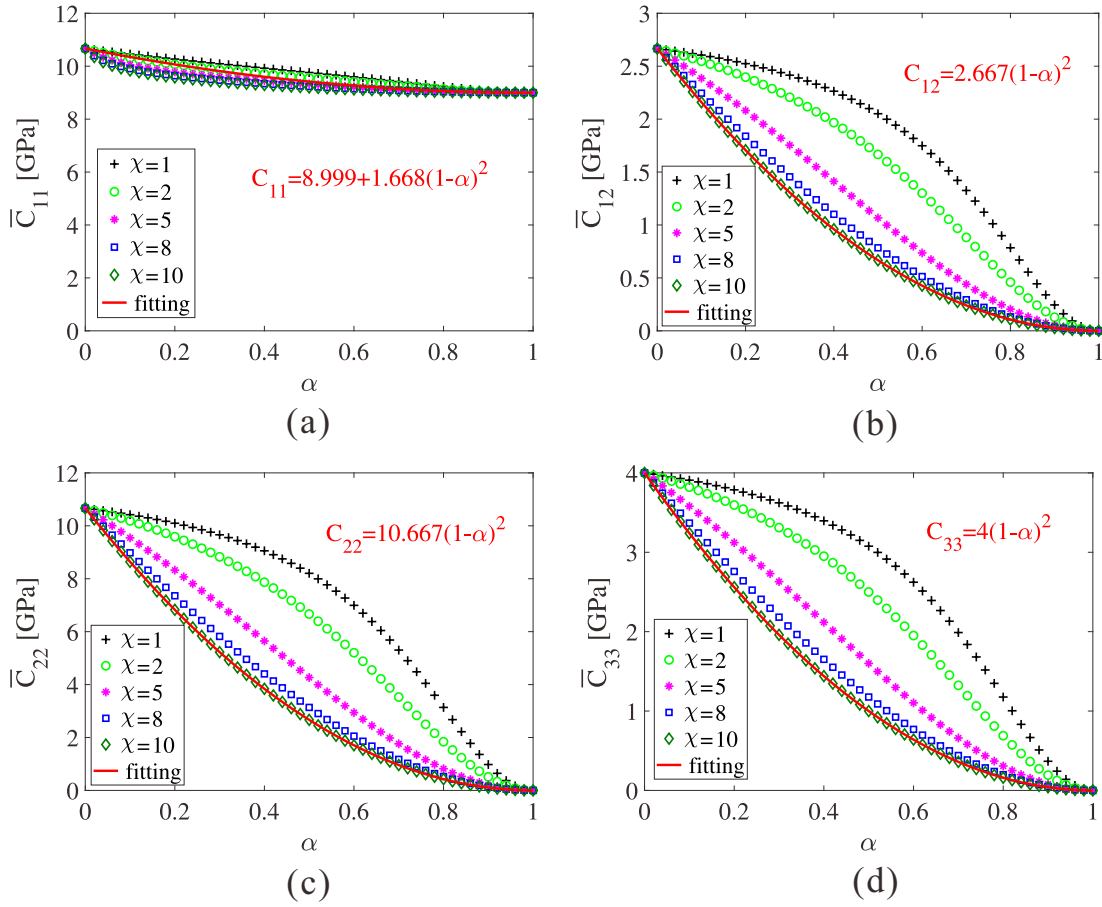


Fig. 5.4 Evolution of $\bar{\mathbf{C}}$ with respect to the interfacial damage α .

In order to ensure the properties: (i) $0 \leq \alpha \leq 1$ and (ii) $\alpha \rightarrow 1$ for $\mathcal{H} \rightarrow \infty$ when solving (5.32), a second-order function as

$$\mathbf{C}_{ij}(\alpha) = a_1 + a_2(1 - \alpha)^2 \quad (5.35)$$

is employed to interpolate the evolution of the effective elastic components which are thought as a function of α , as shown in Fig. 5.4, where the $\mathbf{C}_\alpha$ is obtained as

$$\mathbf{C}_\alpha(\alpha) = \mathbf{C}(\alpha) = \begin{bmatrix} 8.999 + 1.668(1 - \alpha)^2 & 2.667(1 - \alpha)^2 & 0 \\ 2.667(1 - \alpha)^2 & 10.667(1 - \alpha)^2 & 0 \\ 0 & 0 & 4(1 - \alpha)^2 \end{bmatrix}. \quad (5.36)$$

It can be seen that the interpolation function (5.35) still can provide a very satisfying performance in fitting the computing data when $\chi = 10$, especially for the effective elasticity components $\bar{\mathbf{C}}_{12}$, $\bar{\mathbf{C}}_{22}$ and $\bar{\mathbf{C}}_{33}$.

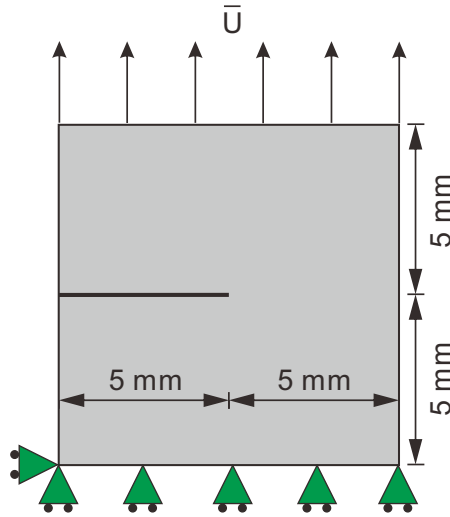


Fig. 5.5 One-notch square plate: the geometry and boundary conditions.

5.5.2 One-notch square plate

In this example, we investigate this proposed model with an one-notch square plate, as shown in Fig. 5.5. The boundary conditions are as follows: on the lower end ($y = 0$), the y -displacement are fixed, while the x -displacement are free and the node ($x = 0, y = 0$) is fixed. On the upper end, the x -displacement are free, while the y -displacement are prescribed to an increasing value of $\bar{U}$ with $\Delta\bar{U} = 5 \times 10^{-4}$ mm during the simulation.

Fig. 5.6 shows the load-displacement curves for different layer directions. It can be seen that the curves for $\theta = 0^\circ$ and $\theta = 30^\circ$ are very close, and the curve for $\theta = 60^\circ$ shows a higher peak load and the three curves all do not perform a significant plastic stage, while for $\theta = 90^\circ$ the curve shows a long plastic stage before the final failure of the plate. Fig. 5.7 shows the final interfacial damage and bulk crack for different layer directions. We

can see that, for $\theta = 0^\circ$ and $\theta = 30^\circ$, the directions of interfacial crack are the same to the layer directions, and the final failure of the plate is caused by the evolution of the interfacial damage. For $\theta = 60^\circ$, the interfacial crack and bulk crack both occur, while the failure of the plate is mainly caused by the evolution of the interfacial damage (when the interfacial crack reaches the top boundary, the bulk crack initiates and propagates vertically to the layer direction causing the final failure of the plate). For $\theta = 90^\circ$, after a long plastic stage, the evolution of the bulk crack perpendicular to the layer direction causes the final failure of the plate.

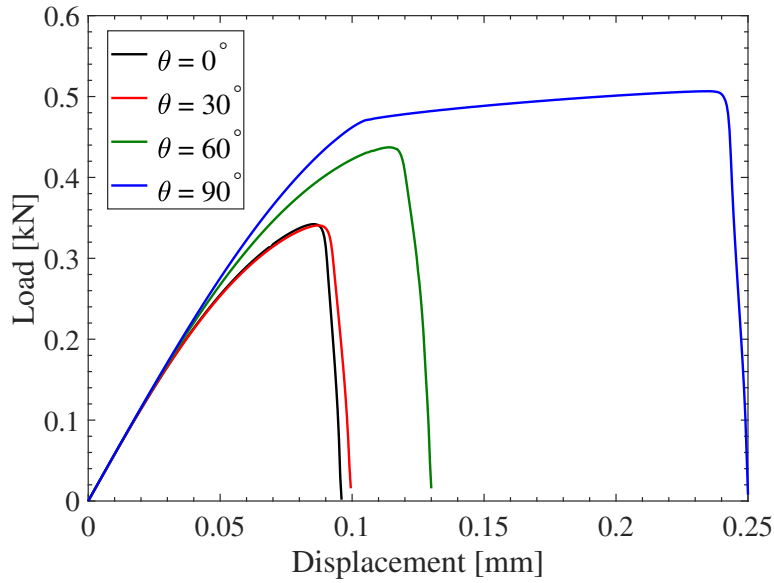


Fig. 5.6 One-notch square plate. Load-displacement curves for different layer directions.

We can note that the present model is able to describe an elastoplastic-damage model when the sample is loaded in one direction, while the response is quasi-brittle in the other direction.

5.5.3 Two-notch specimen

In this next example, we investigate this proposed model with a two-notch specimen, as shown in Fig. 5.8(a). The boundary conditions are the same as the example in Section 5.5.2. The spatial discretization of the model comprises 10,803 4-node quadrilateral elements, with refinement in the central region where the crack is expected to propagate (see Fig. 5.5.2(b)).

The load-displacement curves for different layer directions are shown in Fig. 5.9. We can see that the peak load increases with the rise of layer directions, and the curves for

all four layer directions do not show a significant plastic stage. Fig. 5.10 shows the final interfacial damage and bulk crack for different layer directions. It can be seen that when $\theta = 0^\circ$, $\theta = 30^\circ$ and $\theta = 60^\circ$, the failure of the structure is mainly caused by the evolution of the interfacial crack, and for $\theta = 90^\circ$ the bulk crack perpendicular to the layer direction causes the final failure of the structure.

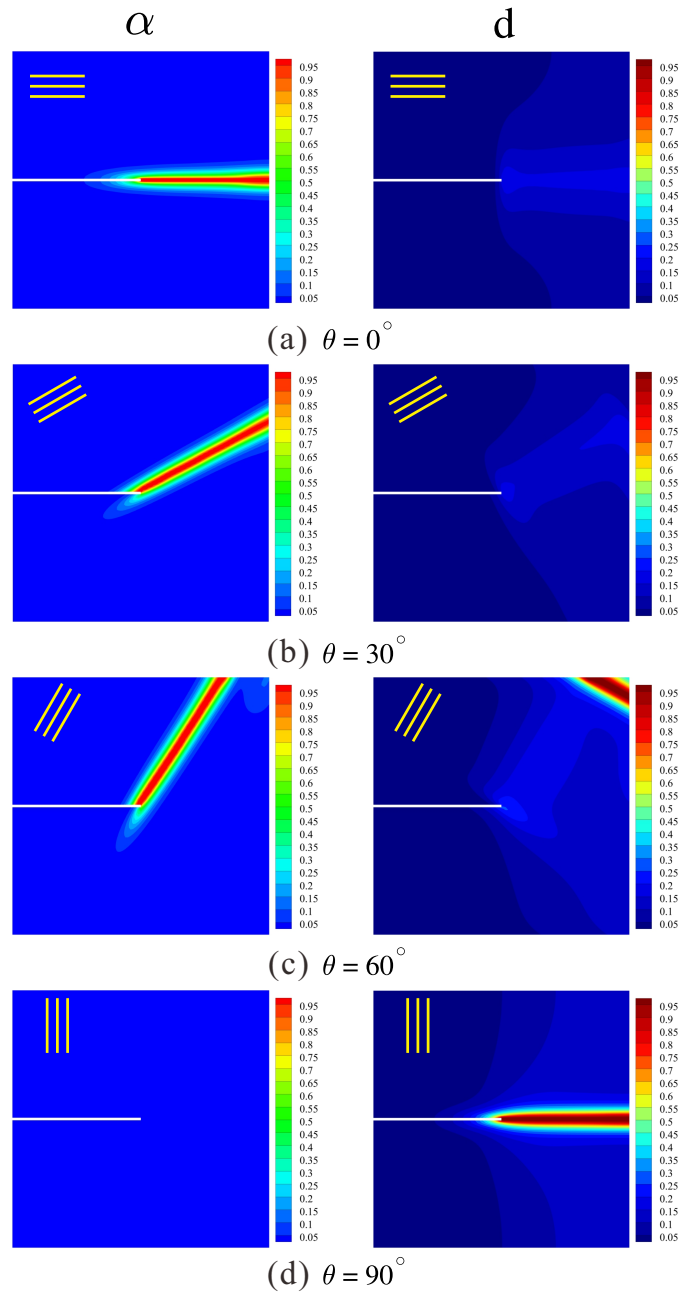


Fig. 5.7 One-notch square plate. Final interfacial damage and bulk crack for different layer directions.

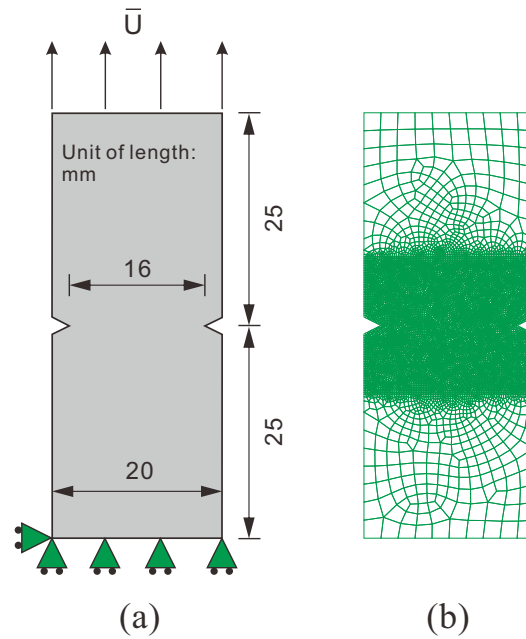


Fig. 5.8 Two-notch specimen: (a) geometry and boundary conditions; (b) finite element model.

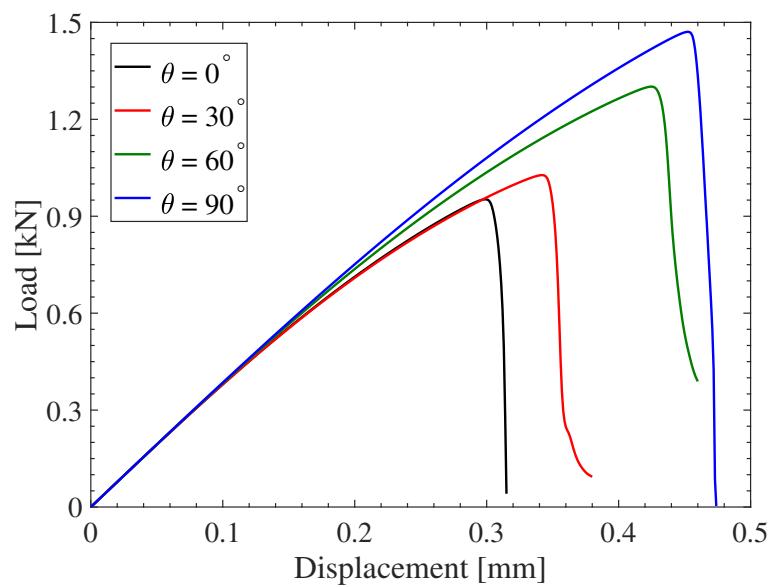


Fig. 5.9 Two-notch specimen. Load-displacement curves for different layer directions.

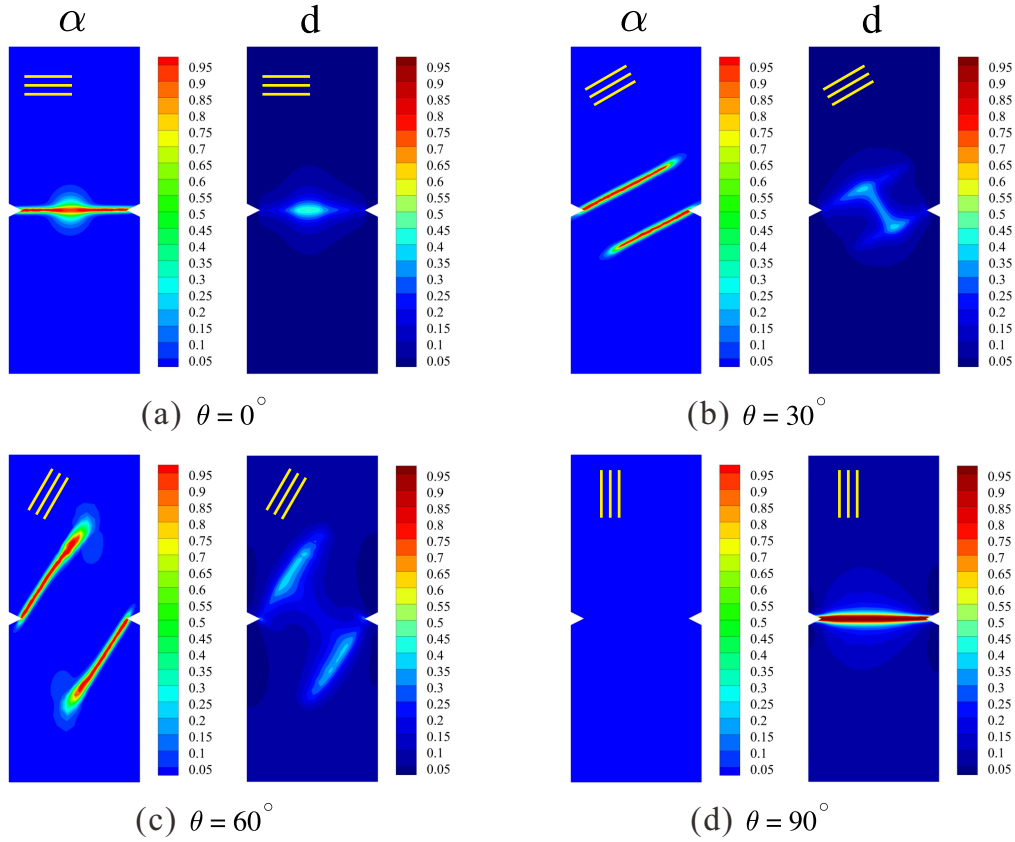


Fig. 5.10 Two-notch specimen. Final interfacial damage and bulk crack for different layer directions.

5.5.4 Two-hole specimen

In this last example, we investigate this proposed model with a relatively complex structure, e.g., a structure with two asymmetric holes, as shown in Fig. 5.11(a). The boundary conditions are same to the example in Section 5.5.2. The spatial discretization of the model comprises 13,839 4-node quadrilateral elements, with refinement around the holes where the crack is expected to propagate, see Fig. 5.11(b).

Fig. 5.12 shows the load-displacement curves for different layer directions. It can be seen that compared to the curves for $\theta = 0^\circ$, $\theta = 30^\circ$ and $\theta = 60^\circ$, the curve for $\theta = 90^\circ$ shows a plastic stage before the final failure of the structure. Fig. 5.13 shows the final interfacial damage and bulk crack for different layer directions. We can see that the bulk cracks and interfacial cracks both initiate from the hole notches, and the evolution of interfacial cracks cause the final failure of the structure for $\theta = 0^\circ$, $\theta = 30^\circ$ and $\theta = 60^\circ$, and for $\theta = 90^\circ$ it is the bulk crack perpendicular to the layer direction that causes the final failure of the structure.

As a conclusion, we can note that the present model is able to describe a complex anisotropic response of a layered structure, differentiating quasi-brittle and elastoplastic damage behavior according to the layer direction, even in complex geometries.

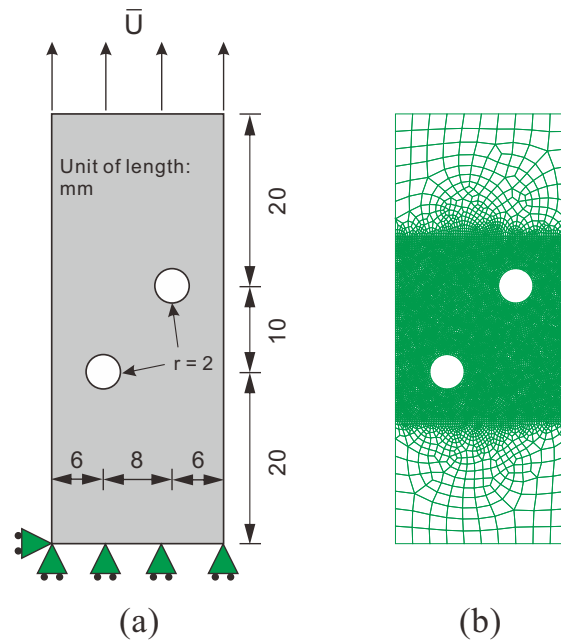


Fig. 5.11 Two-hole specimen: (a) geometry and boundary conditions; (b) finite element model.

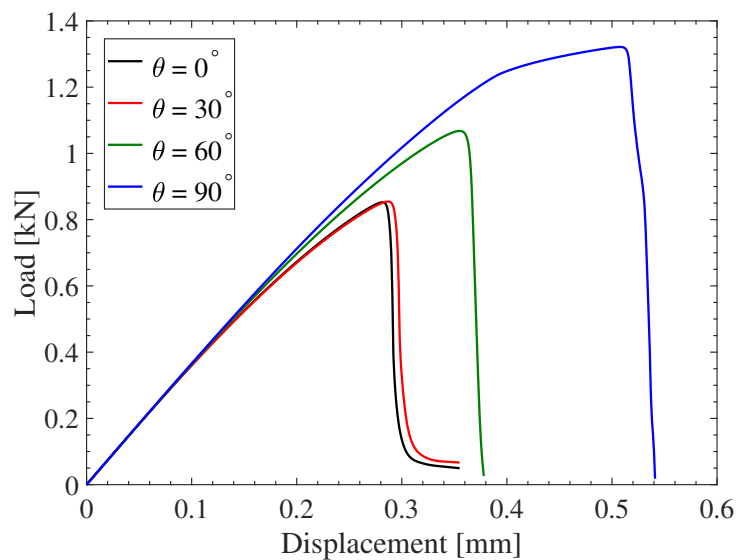


Fig. 5.12 Two-hole specimen. Load-displacement curves for different layer directions.

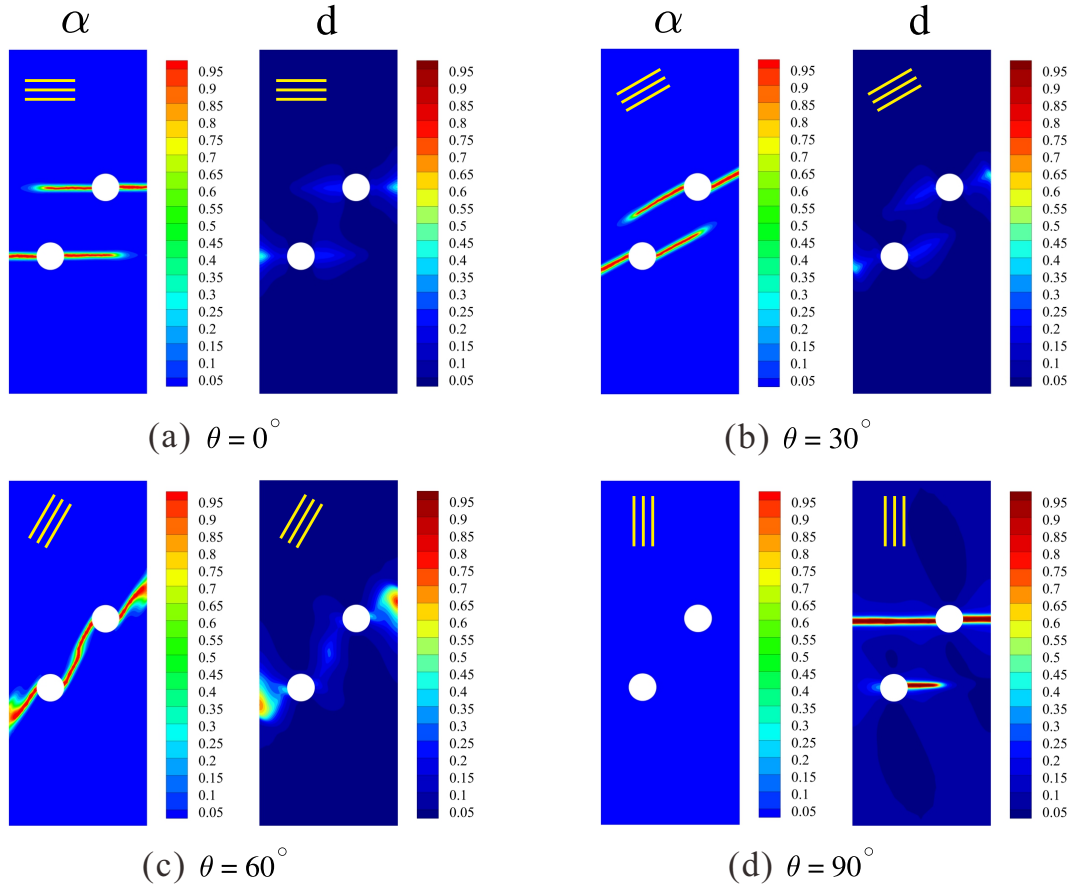


Fig. 5.13 Two-hole specimen. Final interfacial damage and bulk crack for different layer directions.

5.5.5 Removing constraint on the bulk crack direction

In this section, the model without constraining the bulk crack direction is investigated by simply setting $\xi_d = 0$ in (5.4). In order to delay the initiation of the bulk crack and let the results be more reasonable, a new fracture toughness $g_c^d = 4 \times 10^{-3}$ kN/mm is used. The results for one-notch square plate are shown in Fig. 5.14 and 5.15. For the two-notch specimen and the two-hole specimen, the length scale parameters for bulk damage and interfacial damage are $\ell_d = \ell_\alpha = 0.4$ mm. The results for these two specimens are shown in Fig. 5.16-Fig. 5.19.

As can be seen from Fig. 5.14 and 5.15, the cracks in Fig. 5.15 are very similar to the results in Fig. 5.7 except that the bulk crack for $\theta = 60^\circ$ is not vertical to the layer direction. Compared to Fig. 5.6, the curve in Fig. 5.14 for $\theta = 90^\circ$ shows a long softening stage after the peak force, unlike in Fig. 5.6, where the curve has a sharp degraded process, inducing

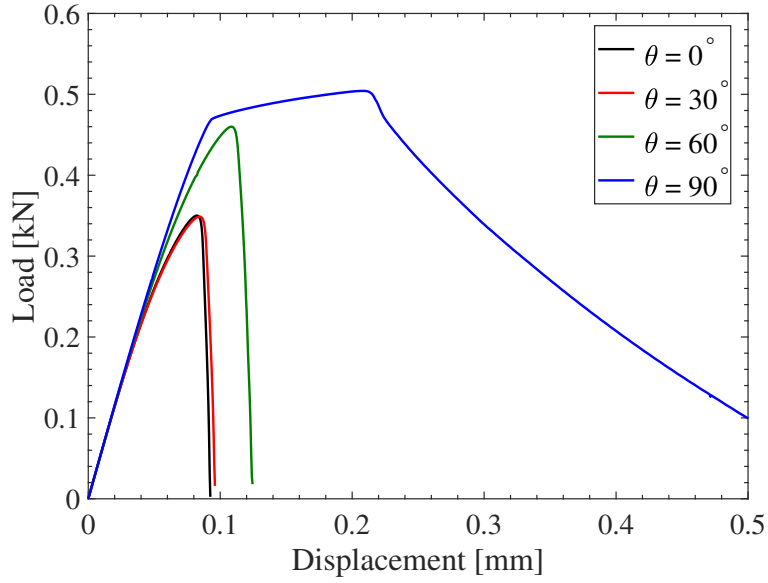


Fig. 5.14 One-notch square plate. Load-displacement curves for different layer directions with $\xi_d = 0$.

more dissipation. Then, removing the bulk crack direction constraint allows more flexibility when identifying elastoplastic-damage processes.

The results in Fig. 5.16 and 5.17 are very similar to the results in Fig. 5.9 and 5.10, here we do not talk about them. In Fig. 5.19, it can be seen that for $\theta = 90^\circ$, the failure of the sample is caused by both the interfacial cracks and the bulk crack, unlike the results in Fig. 5.13.

5.6 Conclusion

In this chapter, a phase field model for anisotropic, elastoplastic damage model of crack propagation in layered 3D printed structures has been proposed. As compared to available anisotropic phase field models for fracture available in the literature, we have introduced two main contributions. First, we have extended the phase field anisotropic models for fracture to elastoplastic behaviors, which is done here for the first time, to our best knowledge. Secondly, the elasticity density function is identified from numerical calculations on an RVE. We have uses a quadratic fit for the different elasticity components with respect to the layer damage variable, which maintains the linearity of the problems in the staggered procedure. As a result, the procedure allows describing different damage behaviors according to the local strain field with respect to a given orientation of the 3D printed layered structure, quasi-

brittle, elastoplastic with damage, or a combination of both in complex configurations. A short perspective of this work will be the identification of the model and its validation on experimental 3D printed layered samples.

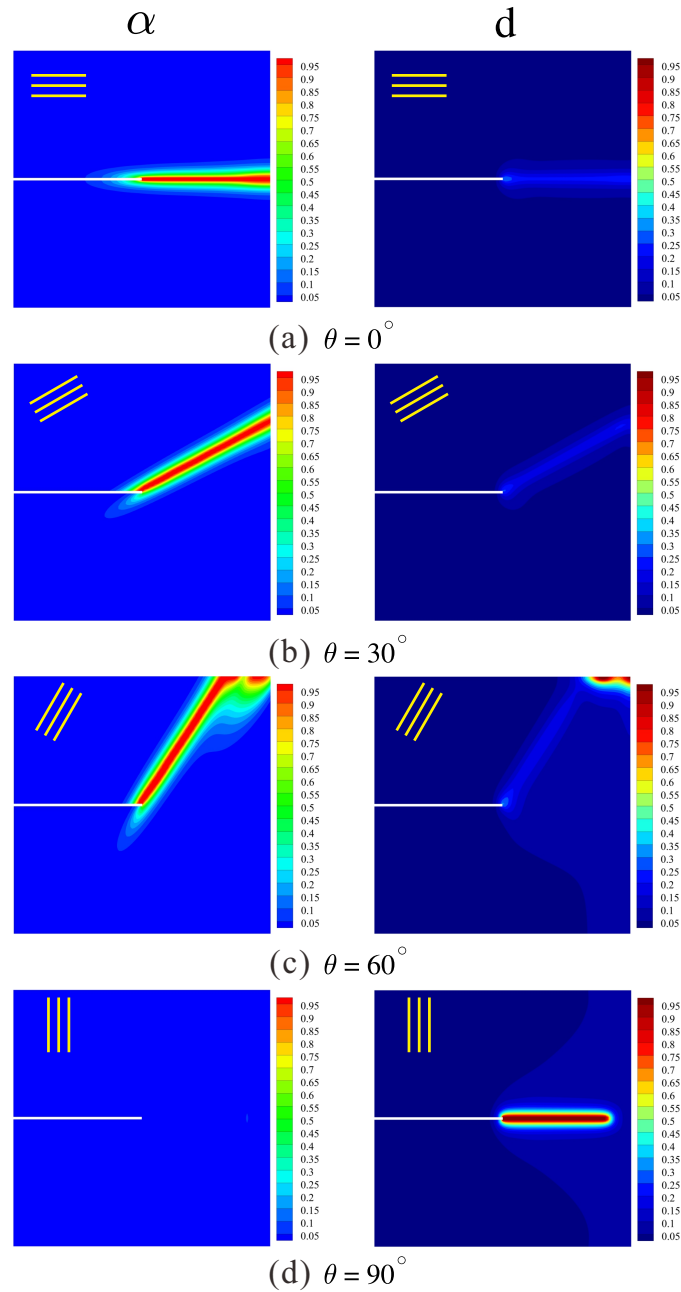


Fig. 5.15 One-notch square plate. Final interfacial damage and bulk crack for different layer directions with $\xi_d = 0$.

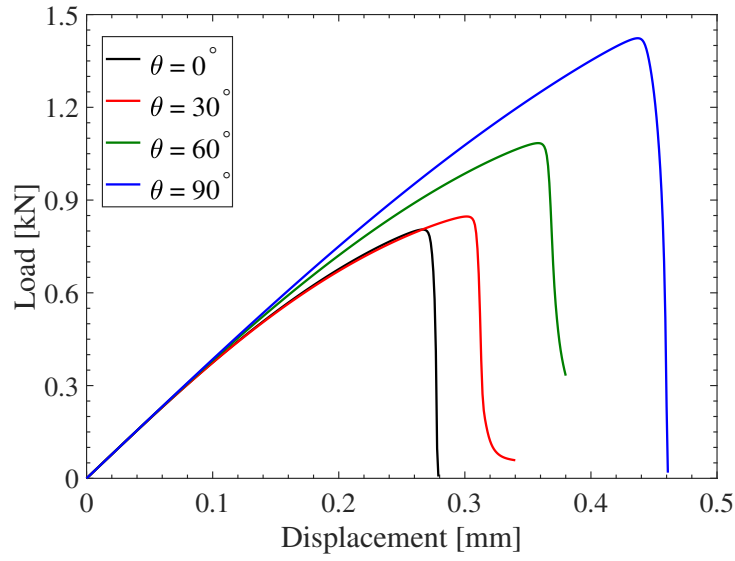


Fig. 5.16 Two-notch specimen. Load-displacement curves for different layer directions with $\xi_d = 0$.

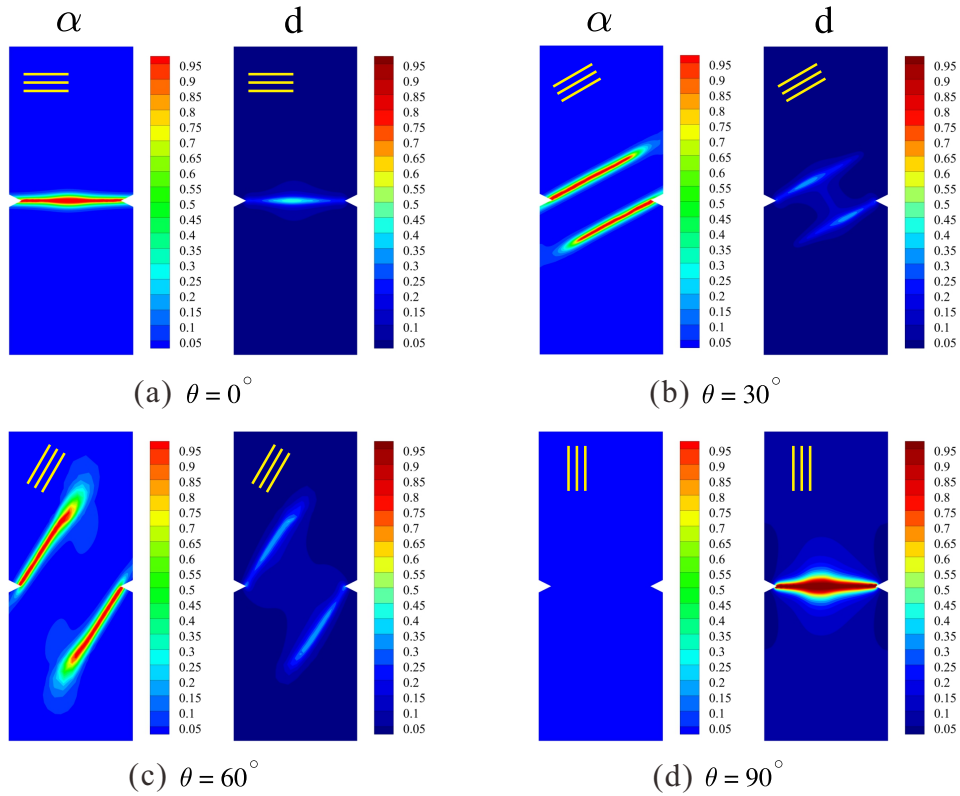


Fig. 5.17 Two-notch specimen. Final interfacial damage and bulk crack for different layer directions with $\xi_d = 0$.

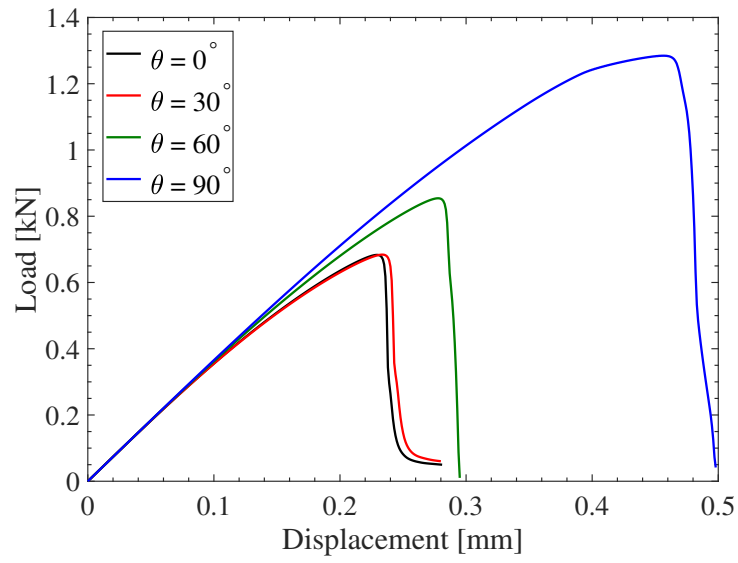


Fig. 5.18 Two-hole specimen. Load-displacement curves for different layer directions with $\xi_d = 0$.

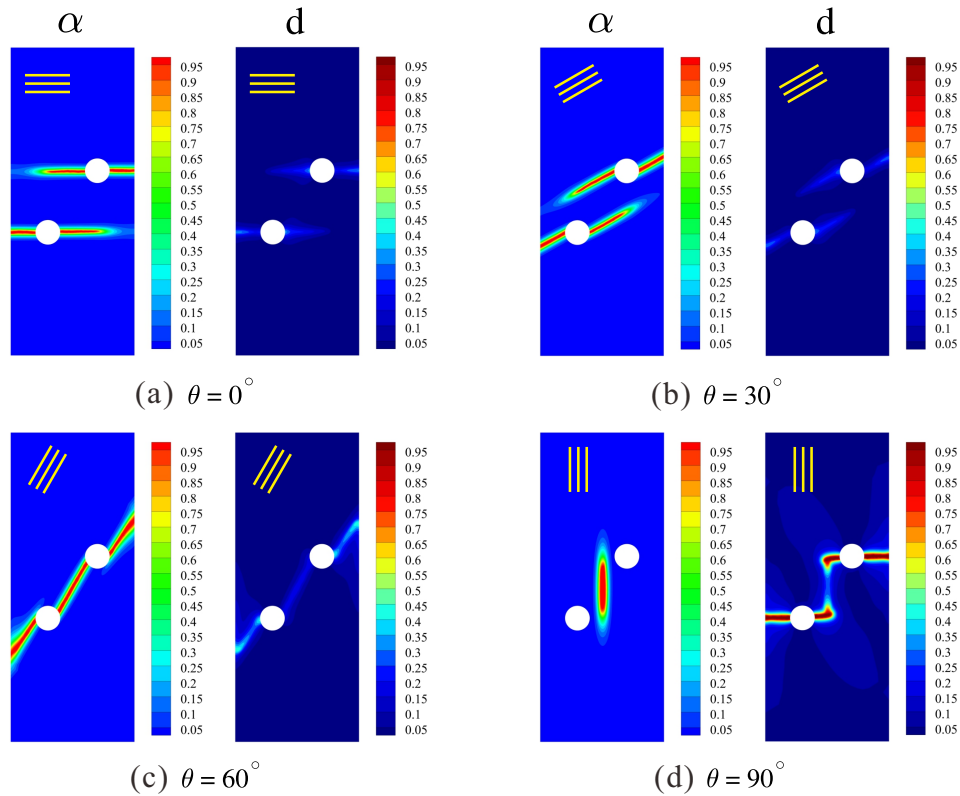


Fig. 5.19 Two-hole specimen. Final interfacial damage and bulk crack for different layer directions with $\xi_d = 0$.

Chapter 6

Micro cracking simulations in image-based models of 3D-printed composite microstructures

6.1 Introduction

In this chapter, we investigate crack propagation in realistic microstructures obtained by segmented images arising from X-Ray micro-tomography (XR- μ CT) images. More specifically, the material is a 3D printed composite, with polymer matrix, and embedding glass fibers. The material is obtained by Selective Laser Sintering (SLS) of PA12 polymer powder embedding glass fibers and additive particles. This material is investigated within the ANR MMELED Project, whose objective is to understand the damage mechanisms in 3D printed composites used in aircraft industry. The samples have been provided by Weare Aerospace Company. An experimental analysis conducted at Navier Laboratory (M. Bornert, T.X. Le and P. Aimedieu) has shown that the material was composed of 5 phases, including: the polymer (PA12) matrix, glass fibers, pores, iron particles and additive particles, which could be flame retardant (see Fig. 6.1). The objective of this chapter is to show the capability of the elastoplastic phase field model developed in this thesis to conduct crack propagation simulations in realistic image-based models of microstructures, and to provide preliminary results regarding the sensitivity of the response of the Representative Volume Element with respect to material parameters and orientation of the microstructures.

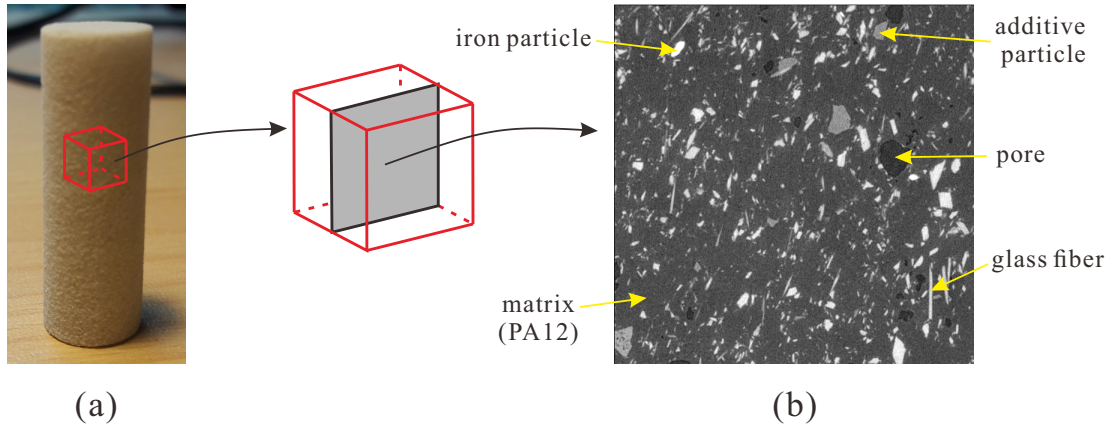


Fig. 6.1 3D printed polymer composite: (a) sample (b) XR- μ CT image (grey image) of its microstructure.

6.2 Obtaining realistic microstructures by XR- μ CT

In this section, we briefly describe the procedure used to obtain the realistic microstructural model used in the simulations from XR- μ CT. The tomography and segmentation processes are introduced in Section 6.2.1 and 6.2.2 respectively. Section 6.2.3 introduces the construction of the finite element mesh.

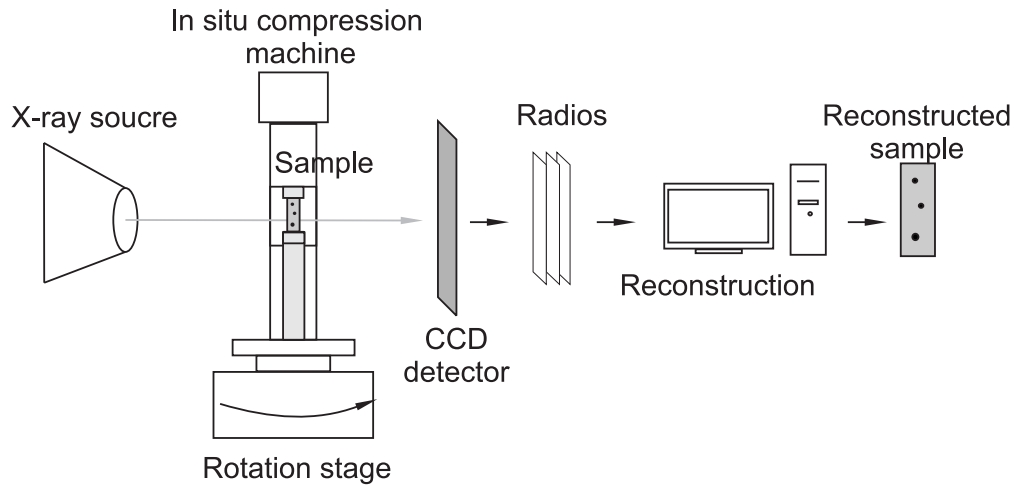
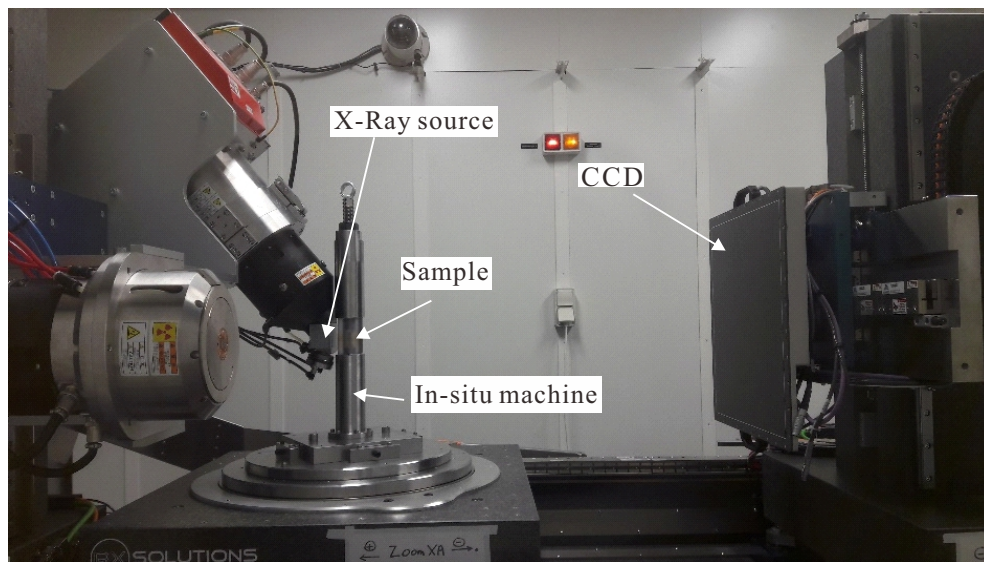


Fig. 6.2 Schematic illustration of the in-situ compression test in a XR- μ CT device. [123].



(a)



(b)

Fig. 6.3 (a) In-situ compression machine and (b) in-situ compression test combined with XR- μ CT at Laboratoire Navier.

6.2.1 Tomography

Nowadays XR- μ CT is widely developed for material science. This nondestructive technique is used for visualizing interior features of solid materials or structures, and for obtaining information on their 3D geometries. The XR- μ CT is based on X-ray radiography: an X-ray beam is sent on the sample and the transmitted beam is recorded on a detector. The ratio of the number of transmitted to incident photons, according to Beer-Lambert law, is related to the integral of the absorption coefficient of the material μ along the path that the photons follow through the sample:

$$I = I_0 \exp(-\mu x), \quad (6.1)$$

where I_0 and I are the initial intensity of X-rays and the X-ray intensity measured after crossing the object, respectively. In Eq. (6.1) x is the path length of the X-rays through the object and μ is the linear attenuation coefficient. X-ray absorption is a function of the nature of the atoms constitutive of the material and their number as well as the energy of the rays. Using the detector which is generally a combination of a scintillator (a system that converts X-ray energy into visible light) and a CCD sensor in modern tomographs, we can record a series of radiographs corresponding to various angular positions of the sample in the beam. Those radiographs are used by a reconstruction software to obtain a three dimensional image, which is related to the heterogeneous distribution of μ . A schematic illustration of an XR- μ CT experiment setup is depicted in Fig. 6.2.

The CT images of this work were captured on the XR- μ CT laboratory scanner available at Navier Laboratory (Ultratom from RX-Solution) by Prof. Michel Bornert, Dr. Thi Xiu Le and P. Aimedieu, through a collaboration within the ANR MMELED project. A view of the in-situ experiments conducted on the laboratory tomograph is depicted in Fig. 6.3.

6.2.2 Segmentation

As shown in Fig. 6.1(b), the 3D printed polymer composite specimen is composed of five phases: a polymer PA12 matrix, pores, glass fibers, iron and additive particles. The detailed segmentation procedures for these five phases is described as follows:

- Grey images are attributed to pure phases (5 phases) and interphase phases (10 phases). Volume fractions of each phase is evaluated. The reader is referred to [86] for more details of this procedure.
- Each fiber particle, including pure phase and surrounding interphase, is represented by equivalent parallelepiped by considering the partial volume effect.

- Some voxels are added around pure pores, iron and additive particle phases under the constraint of their volume fractions, and the remaining voxels are added to the pure matrix phase.

An example of 2D segmented result is shown in Fig. 6.4.

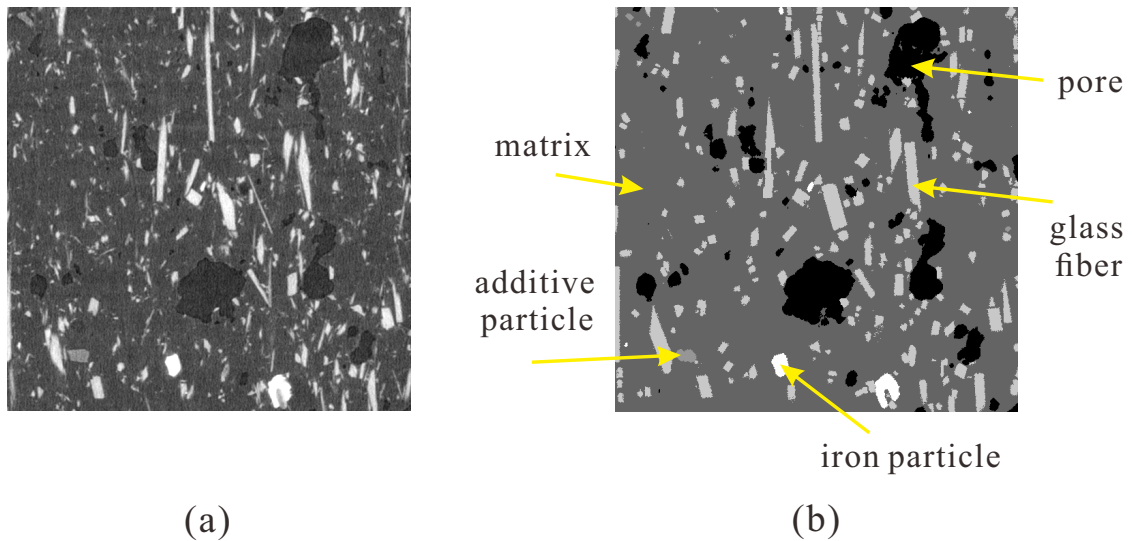


Fig. 6.4 (a) Grey image and (b) Segmented image.

6.2.3 Construction of the microstructural mesh

In this work, a software was used to construct unstructured meshes where the interfaces are explicitly meshed, from the voxel-based images. Today several softwares are capable to perform such task automatically, like e.g. Cgal, Tetgen, Iso2mesh and AVIZO, among others. In the present work, through a collaboration with LEM3 Lab., Lorraine University (M. Nouari, B. Haddag, H. Makich), the Avizo[®] software has been used to construct a mesh from the previous CT images, see Fig. 6.5, where pore phases were not meshed. Examples of simulations using this unstructured mesh are presented in Section 6.3.

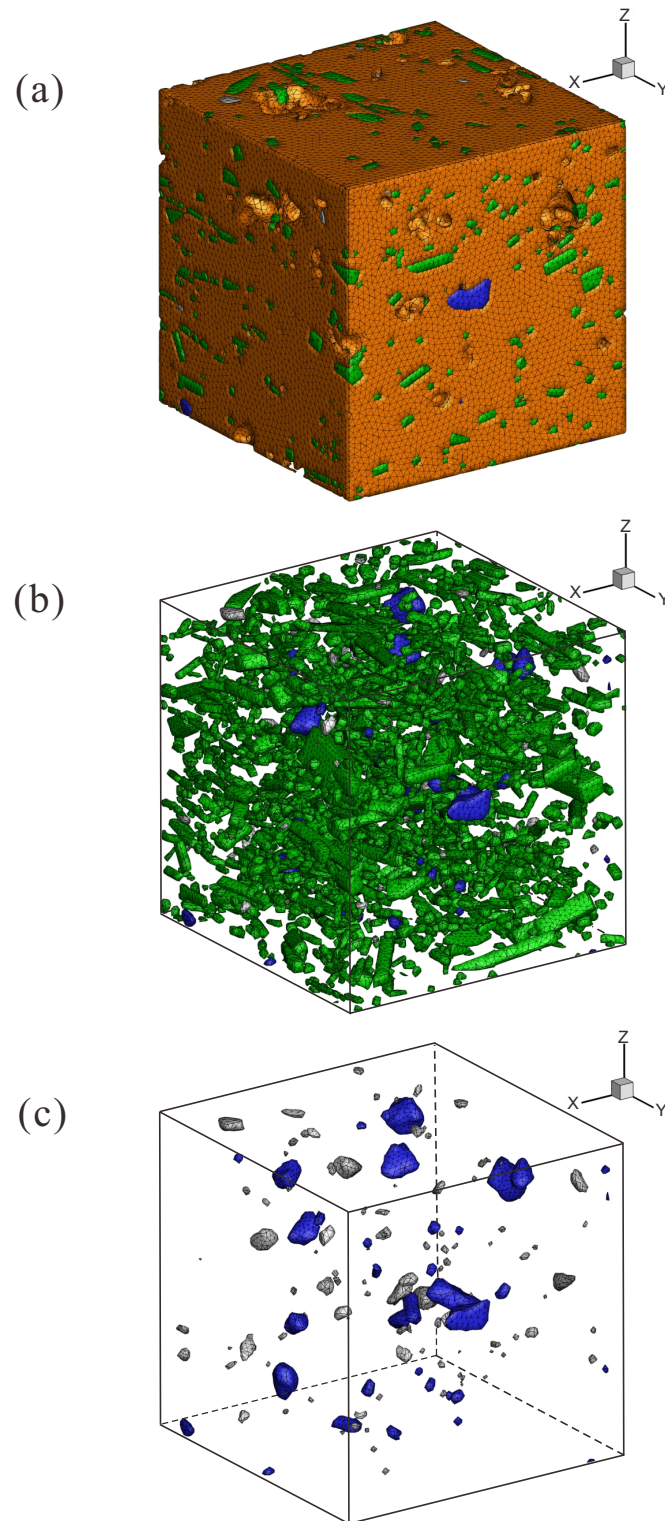


Fig. 6.5 (a) Whole mesh model; (b) mesh model for glass fibers (green), iron particles (grey) and additive particles (blue); (c) mesh model for iron particles (grey) and additive particles (blue).

Table 6.1 Material parameters used in the numerical simulations

Name	Symbol	Matrix	Fiber	Iron	Additive	Unit
Young's modulus	E	1.7	55	120	3	GPa
Poisson's ratio	ν	0.32	0.25	0.3	0.25	[—]
Yield stress	σ_Y	0.1	—	—	—	GPa
Hardening modulus	H	0.25	—	—	—	GPa
Fracture toughness	g_c	7	60	500	10	N/mm

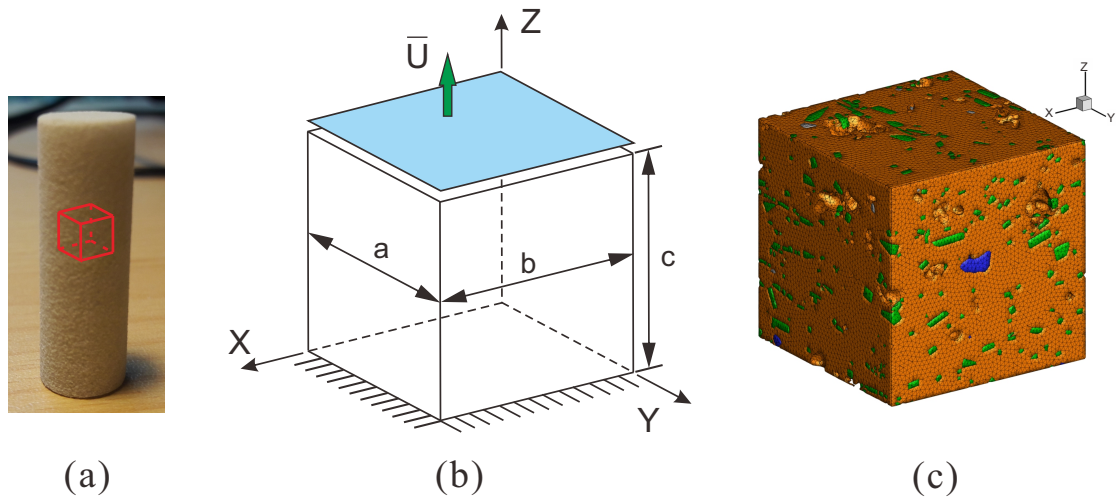


Fig. 6.6 Traction test of a microtomography image-based polymer composite sample in 3D: (a) Sample; (b) geometry of the sub-volume extracted from the sample and boundary conditions; (c) whole mesh model (see Fig. 6.5 for more details).

6.3 Numerical simulations

In this section, the above realistic microstructural models (see Fig. 6.6) are used to conduct crack propagation simulations. Note that even though experimental in-situ results are readily available, at the time this chapter is written we lacked time to perform rigorous comparisons between experiments and simulations. Then, we only present simulations where the boundary conditions do not represent the conditions in the experiments. The objective here is more to demonstrate the capability of such model to represent complex fracture mechanisms in realistic microstructures rather than to provide direct comparisons with experiments. Such comparisons are reported to future short-term works.

The dimensions of the microstructure are $a = b = c = 4$ mm. The boundary conditions are as follows: on the lower end ($z = 0$), the (x, y, z) -displacements are fixed. On the upper end, the (x, y) -displacements are free, while the z -displacements are prescribed to an increasing value of $\bar{U}$ with $\Delta\bar{U} = 5 \times 10^{-4}$ mm during the simulation. The mesh model has 697,659 tetrahedral elements. The material parameters are taken from the literature and are detailed in Table 6.1, here the matrix (PA12) is thought as an elastoplastic brittle fracture behaviour, and the glass fiber, iron and additive particles are thought as elastic brittle fracture behavior. The regularization length is taken as $\ell = 0.05$ mm.

Fig. 6.7 shows the load-displacement curve for the 3D microstructure problem in tension. We can see that the curve has an obvious plastic hardening stage before the final failure of the microstructure. The corresponding cracks are depicted in Fig. 6.8. Here for the sake of clear visualization, only the crack phase field with values higher than 0.9 is plotted. For the sake of clarity, we plot the crack path within several planes. The results are depicted in Fig. 6.9. We observe that the crack initiates from the boundaries of the pores, and then propagates into the matrix, surrounding the particles and fibers.

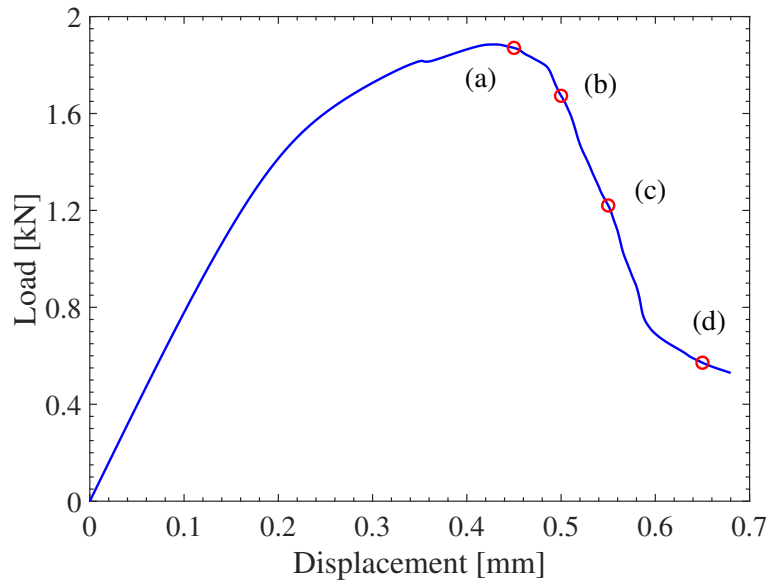


Fig. 6.7 The load-displacement curve for the 3D microstructure problem in tension.

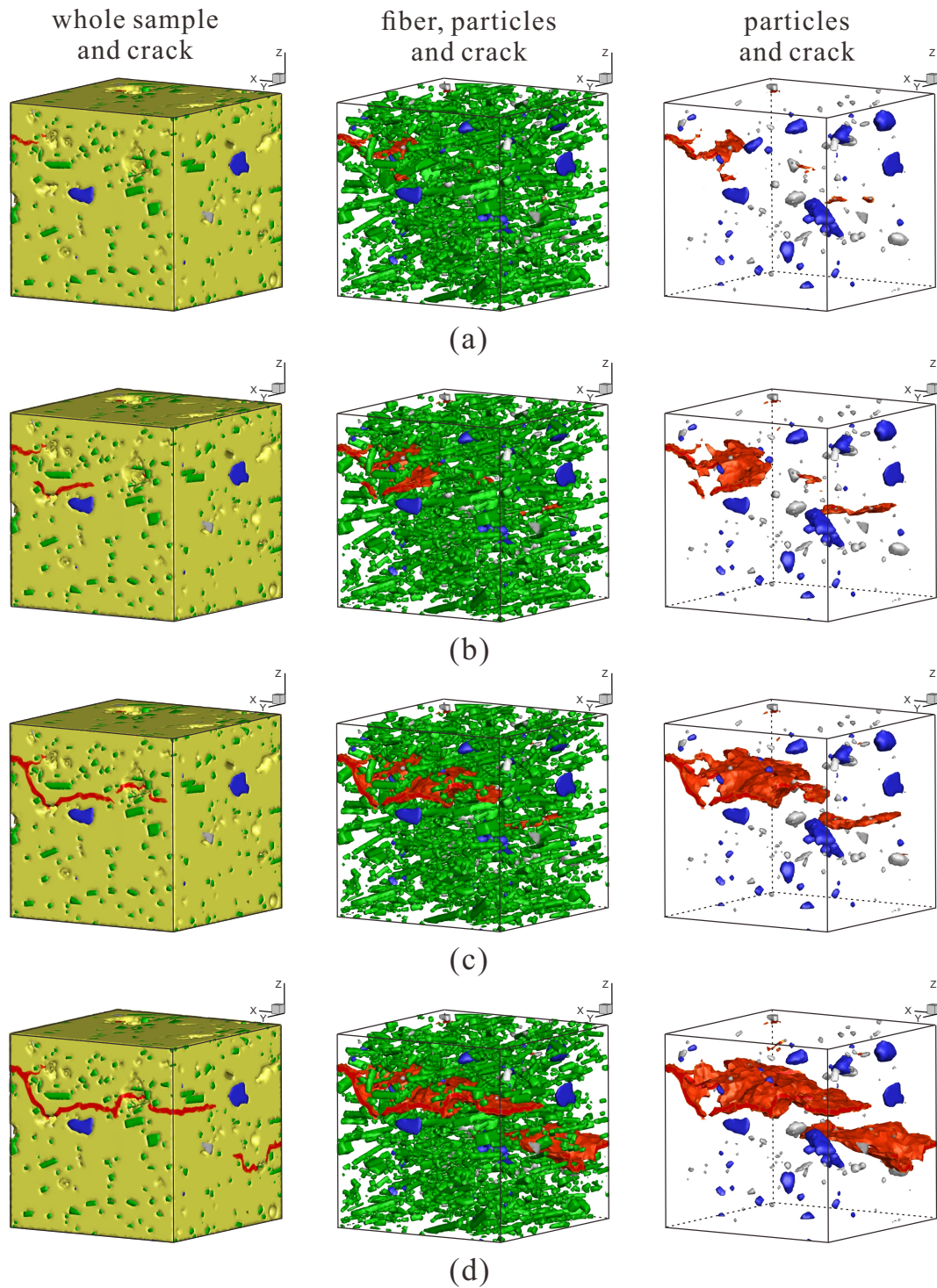


Fig. 6.8 Traction test of a microtomography image-based polymer composite sample in 3D. Evolution of the crack phase field for an applied traction displacement U : (a) $\bar{U} = 0.45$ mm, (b) $\bar{U} = 0.5$ mm, (c) $\bar{U} = 0.55$ mm and (d) $\bar{U} = 0.65$ mm. The yellow, green, grey, blue and red refer to the PA12 matrix, the glass fiber, the iron particle, the additive particle and the crack, respectively.

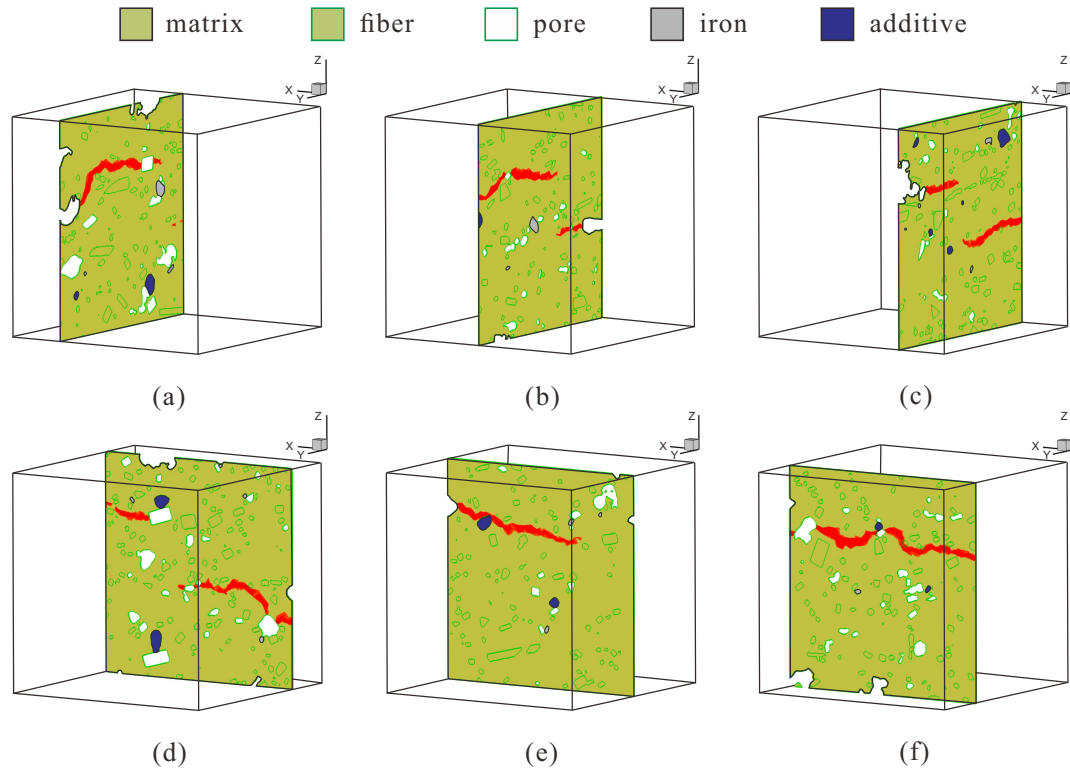


Fig. 6.9 Crack phase field for $\bar{U} = 0.65$ mm in different planes: (a) $x = 3$ mm, (b) $x = 2$ mm, (c) $x = 1$ mm, (d) $y = 1$ mm, (e) $y = 2$ mm and (f) $y = 3$ mm.

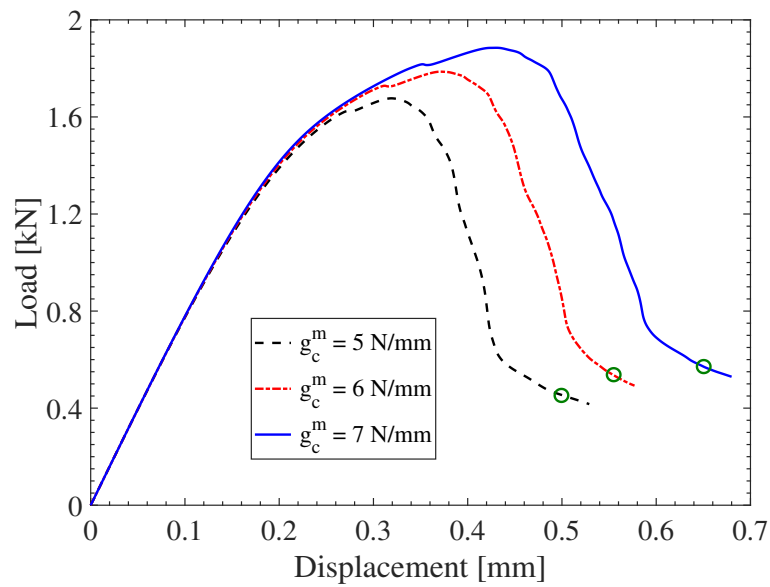


Fig. 6.10 Comparison of load-displacement curves for different g_c^m .

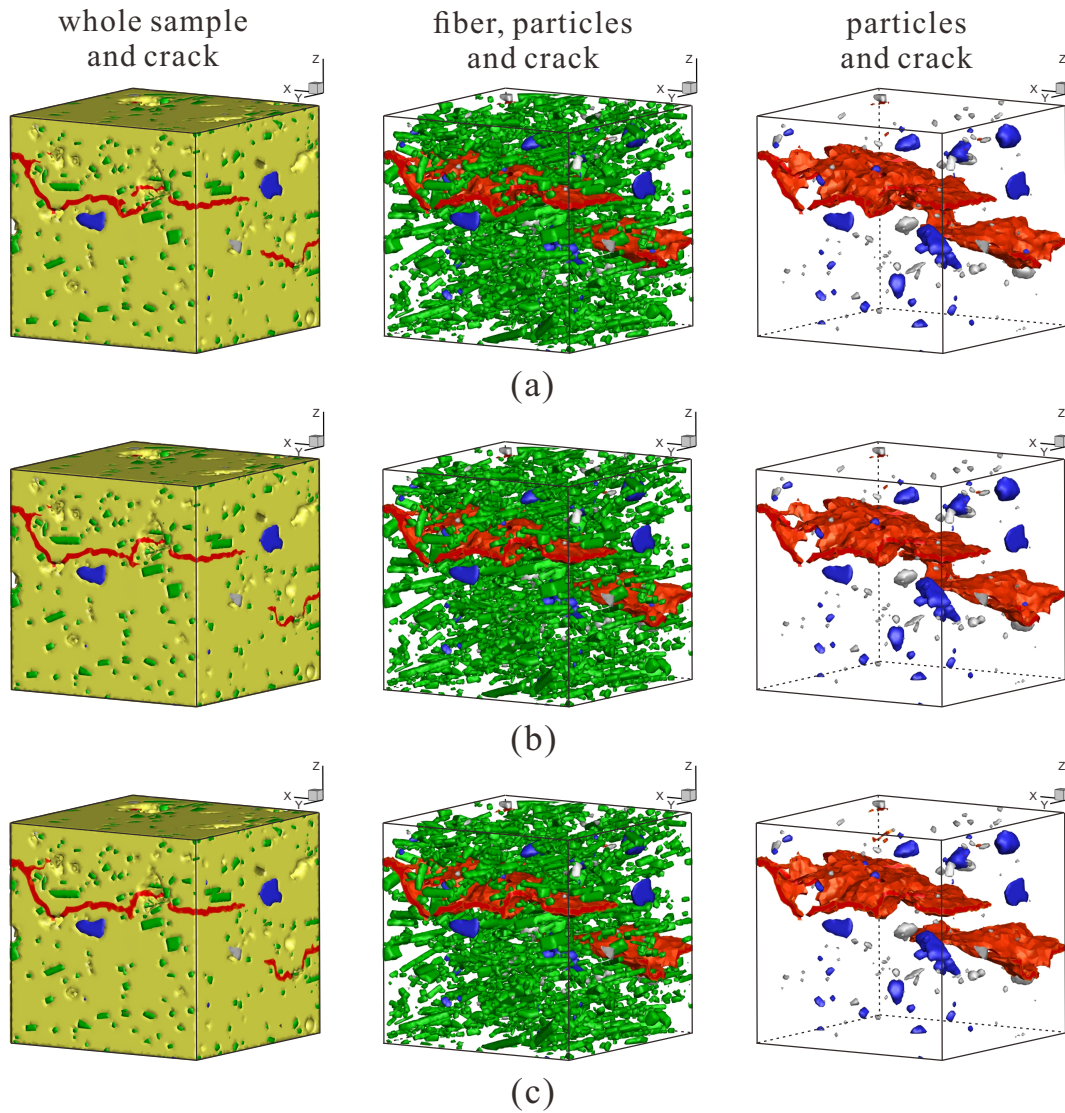


Fig. 6.11 Crack phase fields for (a) $g_c^m = 5$ N/mm, (b) $g_c^m = 6$ N/mm (c) $g_c^m = 7$ N/mm. The yellow, green, grey, blue and red refer to the PA12 matrix, the glass fiber, the iron particle, the additive particle and the crack, respectively.

This complex and realistic elastoplastic example has been run on a Matlab code and on a workstation with 24 cores, 768 Go Ram and 2.70 GHz processor. The computational time is about 168 h (only 12 cores in this workstation were used). It should be noted that the assembly of the different matrices (e.g. $\mathbf{K}_{\text{tan}}$ in (2.51) and $\mathbf{K}_d$ in (2.55)) is parallelized [47], and an iterative Biconjugate gradient stabilized solver [150] was used to solve the largest systems (2.50) and (2.54). Each assembly of the different matrices only costs several

seconds, and most of computational time (about 95% of total time) was used to solve the largest system (2.50).

To investigate the effect of the fracture toughness of matrix (g_c^m), two additional simulations are conducted with $g_c^m = 5$ N/mm and $g_c^m = 6$ N/mm respectively. The load-displacement curves are shown in Fig. 6.10. The different crack phase fields are shown in Fig. 6.11. It can be observed that an increase of g_c^m increases the plastic hardening stage and delays the initiation of crack.

We can then observe that the different g_c^m do not have a significant influence on the response of curve after the peak load, and the final crack phase fields are very similar, as shown in Fig. 6.11.

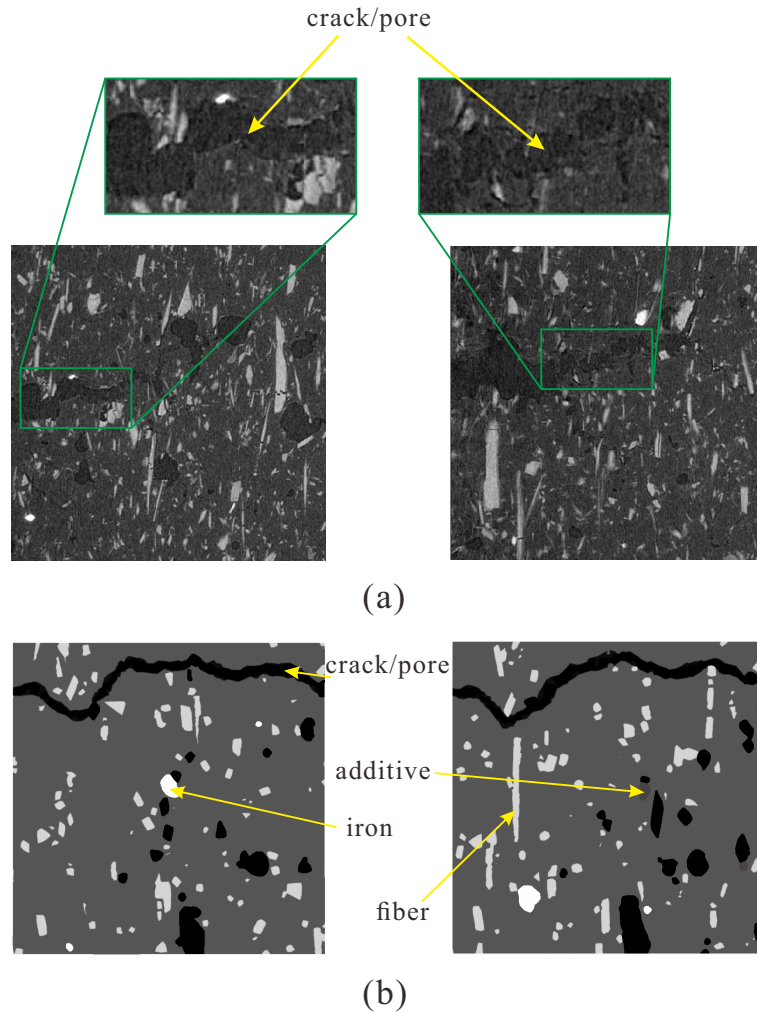


Fig. 6.12 Comparison of crack in (a) grey images obtained from in-situ tests and (b) numerical simulation (“y-direction” in the following).

To illustrate the capability of the proposed model to describe qualitatively the local damage mechanisms in the 3D printed polymer-glass fibers composite, a comparison of crack obtained from in-situ tests and numerical simulation is performed in Fig. 6.12. The in-situ test, conducted by Xiu Le and Michel Bornert at Navier Lab. involves the compression of a cylindrical sample. For the sake of brevity and due to the fact that the next results do not intend to provide rigorous comparisons between simulations and experiments, the details of this test are reported to a separated work. After a given load, buckling occurs and lateral cracking is observed due to a state of local tension during the bending of the sample. The simulation involves a pure tension test of the cubic RVE. Then, the mechanical state is not exactly the same than in the experiment. In addition, the geometry of the microstructure is also not in the same location of the sample. From Fig. 6.12(a), it can be seen that the cracks, which surround the particles and glass fibers and connect the existing pores, cause the final failure of microstructures. The simulations in Fig. 6.12(b). provide a qualitative comparison, where we can note that local microcracks also merge to form a macro crack.

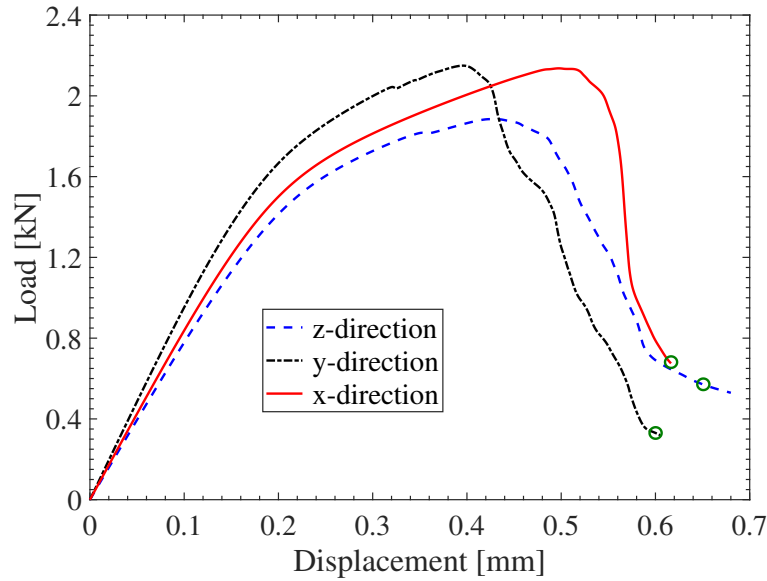


Fig. 6.13 Comparison of load-displacement curves for different loading direction.

Finally, we investigate the effects of the printing orientation to the mechanical response of the microstructure. Then, two additional simulations with $g_c^m = 7 \text{ N/mm}$ are performed: (i) in the first one, called “y-direction”, the boundary conditions are as follows: on the plane $y = 0$, the (x, y, z) -displacements are fixed, on the plane $y = \max(y)$, the (x, z) -displacements are free, while the y -displacements are prescribed to an increasing value of $\bar{U}$, and (ii) in the second one, called “x-direction”, the (x, y, z) -displacements are fixed on the plane $x = 0$,

on the plane $x = \max(x)$, the (y, z) -displacements are free, while the x -displacements are prescribed to an increasing value of $\bar{U}$. Fig. 6.13 shows the comparison of load-displacement curves for different loading direction. We can see a clear effect of the orientation from the numerical simulations on the mechanical response. First, the effective elastic moduli are different. Then, according to the orientation, different plastic stage and different damage response are found. This can be explained by the fact that the 3D-printed material has an anisotropic microstructure due to the manufacturing process: (a) the fibers are oriented in the plane associated with each layer during the laser sintering process and (b) after each path of the laser, a roller compress the powder and then induces a preferential orientation of the fibers in the plane of the layer. We can see that such model where the microstructure directly arises from the experimental XR- μ CT allows capturing such anisotropic effect on the mechanical response.

6.4 Conclusion

In this chapter, we have conducted crack propagation simulations in image-based models of realistic microstructures from 3D printed polymer-glass fibers composite. The elastoplastic phase field model developed in Chapter 2 has been employed. Due to lack of time, we were not able to perform quantitative comparisons with in-situ tests. However, our contribution in this chapter was to conduct crack propagation in elastoplastic microstructures with realistic geometries arising from XR-micro CT images, and to show that we could qualitatively reproduce some complex microstructural damage mechanisms such as diffuse crack interactions merging into more macro cracks and capturing the effects of the anisotropic microstructure induced by the manufacturing process. More rigorous comparisons with in-situ experiments are reported to short-term perspective of this thesis work.

Computationally, we have observed that even though the assembly of the different matrices is parallelized, and an iterative Biconjugate gradient stabilized solver was used to solve the largest systems, such simulations still remain computationally highly demanding. Here most of computational time about 95% of total time was used to solve the linear system of FEM equations. We believe that there remains significant room for improvement in term of time reduction, by employing e.g. parallel solving of the linear system. Several solutions could be explored, like AMG (Algebraic Multigrid method) [182, 25].

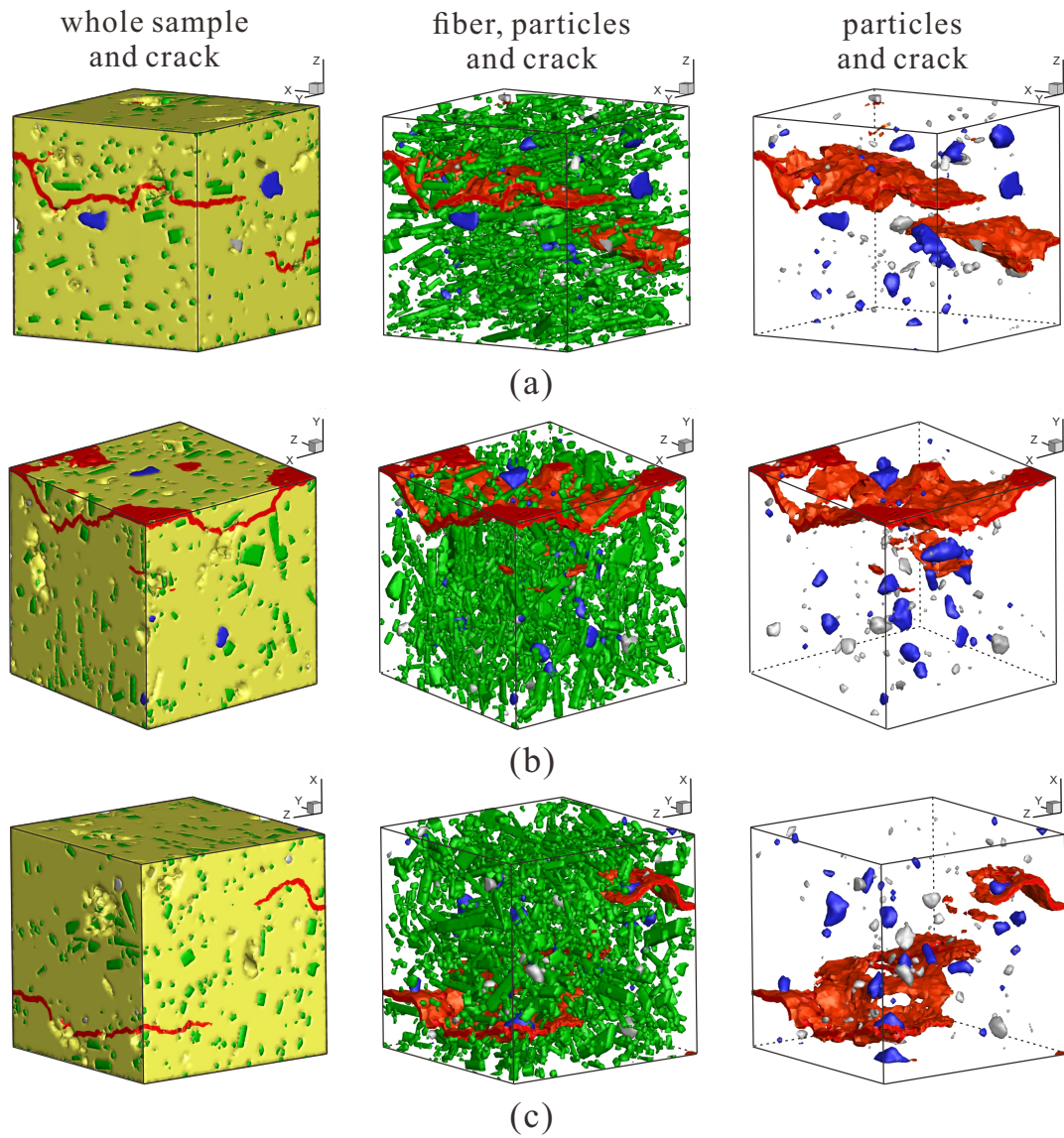


Fig. 6.14 Crack phase fields for different loading direction: (a) z-direction, (b) y-direction and (c) x-direction. The yellow, green, grey, blue and red refer to the PA12 matrix, the glass fiber, the iron particle, the additive particle and the crack, respectively.

Chapter 7

Conclusions and perspectives

7.1 General conclusions

In the present thesis work, we have investigated the modeling of crack propagation in quasi-brittle and elastoplastic micro-structured materials. The main contributions deal with the development of interfacial damage within elastoplastic phase field crack models, topology optimization of heterogeneous materials with respect to crack resistance in quasi-brittle and elastoplastic composites, modeling of cracks in 3D printed materials using anisotropic phase field models, and modeling of cracks in image-based models of elastoplastic 3D printed composite microstructures. The detailed contributions developed in this thesis are summarized as follows.

First, in Chapter 2, we have validated available elastoplastic phase fields models for crack propagation with respect to experimental results on original configurations. We have then extended the elastoplastic brittle phase field method to consider interfacial damage. For this purpose, the energetic formulation has been modified by adding: (i) a strain density depending of the displacement jump related to matrix/inclusions decohesion; (ii) a modified description of the total energy involving a regularized approximation of the singular strain part along the interfaces and (iii) the use of a regularized description of interfaces through diffuse weighting functions which are introduced in the energetic formulation to differentiate the bulk and interfacial damage mechanisms. In that manner, different damage mechanisms can be associated with interfaces as compared to the bulk.

In Chapter 3, we have proposed for the first time a framework combining SIMP topology optimization and phase field method to maximize the fracture resistance of composites (two-phase materials) structures. It has been demonstrated that the continuous density representation obtained by the SIMP method allows a good convergence of the scheme and improves the fracture resistance of a structure embedding a reinforcement phase (inclusion)

for a fixed volume fraction. 2D and 3D applications have been presented, involving a complex 3D application with 1,176,000 eight-node cubic elements. Such 3D application can be dealt with owing to the fast convergent process of the proposed SIMP topology optimization framework.

In Chapter 4, we have developed a topology optimization procedure for maximizing the fracture resistance of elastoplastic composites. A plasticity gradient phase field model with damage-plasticity coupling has been applied to better constrain the damage zone within the plastic zone. Interfacial damage has been taken into account through a regularized description of interfaces. We have then combined it with a topology optimization for maximizing the fracture resistance of elastoplastic composites for the first time to our best knowledge.

In Chapter 5, with the aim of modeling 3D printed layered polymer-glass fibers composites, a phase field model for anisotropic, elastoplastic damage model of crack propagation has been proposed. The added-value as compared to available anisotropic phase field models for fracture is as follows: first, we have extended the anisotropic phase field models for fracture to elastoplastic behaviors, which is done here for the first time, to our best knowledge. Secondly, the elastic strain density function is here identified from numerical calculations on an RVE. We have used a quadratic fit for the different components of the elastic tensor with respect to a layer damage variable, which maintains the linearity of the problems in the staggered procedure.

Finally in Chapter 6, we have investigated the crack propagation in microstructural models obtain from experimental images of elastoplastic 3D-printed polymer composite, by using the elastoplastic phase field model introduced in Chapter 2. The studied polymer composite has five phases: matrix (PA12), glass fibers, pores, iron particles and additive particles. The image-based model in this work has been constructed by XR- μ CT and can be used to define position and geometry of each phase within the microstructure. The preliminary calculations have provided encouraging results which will be the basis for future studies, with the aim to characterize and understand the damage mechanisms in 3D-printed composites.

7.2 Perspectives

There are many potential research directions from the results and methodologies developed in this work, which are listed as follows:

- The elastoplastic brittle phase field model presented in Chapter 2 could be extended by employing a Drucker–Prager type plasticity model to simulate elastoplastic brittle fracture in pressure-sensitive geological materials. In the present work, we have used a von Mises yield criterion which is a pressure insensitive yield criterion.

- In the present topology optimization work, the damage and plasticity constraints are taken into account implicitly as the regularized fracture and plasticity problem are solved in a staggered solving procedure. These two constraints are not explicitly used in the sensitivity analysis process. Thus, developing a new framework to explicitly use these two constraints in the sensitivity analysis is another possible extension of this work.
- The constructed phase field model for anisotropic, elastoplastic damage model of crack propagation in layered 3D printed structures still requires identification and validation from experiments. Such study combining the present numerical simulations and experiments on 3D-printed samples of composites is a short-range perspective of this work.
- Combining XR- μ CT images and in-situ experimental tests to identify and validate crack propagation in elastoplastic models of 3D-printed microstructures is another challenging and exciting follow-up of this work. Using the developed microstructural models, direct comparisons of crack paths could be conducted between simulations and in-situ tests, using techniques developed in previous studies like e.g. using sub-volume method, image-correlation techniques and inverse approaches (see e.g. [126]).
- Finally, a longer-term perspective will be to identify damage models for 3D-printed composites, and use them in topology optimization procedures to design new materials and structures with tailored mechanical and physical properties, including resistance to damage.

References

- [1] Aldakheel, F. (2016). *Mechanics of nonlocal dissipative solids: gradient plasticity and phase field modeling of ductile fracture*. Stuttgart: Institut für Mechanik (Bauwesen), Lehrstuhl I, Universität Stuttgart.
- [2] Alessi, R. (2013). *Variational approach to fracture mechanics with plasticity*. PhD thesis, Ecole Polytechnique X.
- [3] Alessi, R. and Freddi, F. (2017). Phase-field modelling of failure in hybrid laminates. *Composite Structures*, 181:9–25.
- [4] Alessi, R., Marigo, J.-J., Maurini, C., and Vidoli, S. (2018). Coupling damage and plasticity for a phase-field regularisation of brittle, cohesive and ductile fracture: one-dimensional examples. *International Journal of Mechanical Sciences*, 149:559–576.
- [5] Alessi, R., Marigo, J.-J., and Vidoli, S. (2014). Gradient damage models coupled with plasticity and nucleation of cohesive cracks. *Archive for Rational Mechanics and Analysis*, 214(2):575–615.
- [6] Alessi, R., Marigo, J.-J., and Vidoli, S. (2015). Gradient damage models coupled with plasticity: variational formulation and main properties. *Mechanics of Materials*, 80:351–367.
- [7] Ambati, M. (2017). *Phase-field Modeling and Computations of Brittle and Ductile Fracture for Solids and Shells*. Technische Universität Carolo-Wilhelmina zu Braunschweig.
- [8] Ambati, M. and De Lorenzis, L. (2016). Phase-field modeling of brittle and ductile fracture in shells with isogeometric nurbs-based solid-shell elements. *Computer Methods in Applied Mechanics and Engineering*, 312:351–373.
- [9] Ambati, M., Gerasimov, T., and De Lorenzis, L. (2015a). Phase-field modeling of ductile fracture. *Computational Mechanics*, 55(5):1017–1040.
- [10] Ambati, M., Gerasimov, T., and De Lorenzis, L. (2015b). A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics*, 55(2):383–405.
- [11] Ambati, M., Gerasimov, T., and de Lorenzis, L. (2015c). A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics*, 55(2):383–405.

- [12] Ambrosio, L. and Tortorelli, V. M. (1990). Approximation of functional depending on jumps by elliptic functional via t-convergence. *Communications on Pure and Applied Mathematics*, 43(8):999–1036.
- [13] Amin, A. R., Kao, Y.-T., Tai, B. L., and Wang, J. (2017). Dynamic response of 3d-printed bi-material structure using drop weight impact test. In *International Manufacturing Science and Engineering Conference*, volume 50732, page V002T01A021. American Society of Mechanical Engineers.
- [14] Amir, O. (2013). A topology optimization procedure for reinforced concrete structures. *Computers & Structures*, 114:46–58.
- [15] Amir, O. and Sigmund, O. (2013). Reinforcement layout design for concrete structures based on continuum damage and truss topology optimization. *Structural and Multidisciplinary Optimization*, 47(2):157–174.
- [16] Amor, H., Marigo, J.-J., and Maurini, C. (2009). Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments. *Journal of the Mechanics and Physics of Solids*, 57(8):1209–1229.
- [17] Andreassen, E., Clausen, A., Schevenels, M., Lazarov, B. S., and Sigmund, O. (2011). Efficient topology optimization in matlab using 88 lines of code. *Structural and Multidisciplinary Optimization*, 43(1):1–16.
- [18] Asareh, I., Kim, T.-Y., and Song, J.-H. (2018). A linear complete extended finite element method for dynamic fracture simulation with non-nodal enrichments. *Finite Elements in Analysis and Design*, 152:27–45.
- [19] Babout, L., Maire, E., and Fougères, R. (2004). Damage initiation in model metallic materials: X-ray tomography and modelling. *Acta Materialia*, 52(8):2475–2487.
- [20] Badnava, H., Etemadi, E., and Msekh, M. (2017). A phase field model for rate-dependent ductile fracture. *Metals*, 7(5):180.
- [21] Barenblatt, G. (1959). Concerning equilibrium cracks forming during brittle fracture. the stability of isolated cracks. relationships with energetic theories. *Journal of Applied Mathematics and Mechanics*, 23(5):1273–1282.
- [22] Bažant, Z. P. and Becq-Giraudon, E. (2002). Statistical prediction of fracture parameters of concrete and implications for choice of testing standard. *Cement and concrete research*, 32(4):529–556.
- [23] Bažant, Z. P. and Jirásek, M. (2002). Nonlocal integral formulations of plasticity and damage: survey of progress. *Journal of engineering mechanics*, 128(11):1119–1149.
- [24] Bažant, Z. P. and Oh, B. H. (1983). Crack band theory for fracture of concrete. *Matériaux et construction*, 16(3):155–177.
- [25] Bell, W., Olson, L., and Schroder, J. (2011). Pyamg: Algebraic multigrid solvers in python v2. 0. *h ttp://www.pyamg.org*.

- [26] Bendsøe, M. and Sigmund, O. (2003). Theory, methods and applications. *Topology optimization*. Springer, Berlin.
- [27] Bernard, P.-E., Moës, N., and Chevaugeon, N. (2012). Damage growth modeling using the thick level set (tls) approach: Efficient discretization for quasi-static loadings. *Computer Methods in Applied Mechanics and Engineering*, 233:11–27.
- [28] Bleyer, J. and Alessi, R. (2018). Phase-field modeling of anisotropic brittle fracture including several damage mechanisms. *Computer Methods in Applied Mechanics and Engineering*, 336:213–236.
- [29] Borden, M., Verhoosel, C., Scott, M., Hughes, T., and Landis, C. (2012a). A phase-field description of dynamic brittle fracture. *Computer Methods in Applied Mechanics and Engineering*, 217:77–95.
- [30] Borden, M. J., Hughes, T. J., Landis, C. M., Anvari, A., and Lee, I. J. (2016). A phase-field formulation for fracture in ductile materials: Finite deformation balance law derivation, plastic degradation, and stress triaxiality effects. *Computer Methods in Applied Mechanics and Engineering*, 312:130–166.
- [31] Borden, M. J., Hughes, T. J., Landis, C. M., and Verhoosel, C. V. (2014). A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework. *Computer Methods in Applied Mechanics and Engineering*, 273:100–118.
- [32] Borden, M. J., Verhoosel, C. V., Scott, M. A., Hughes, T. J., and Landis, C. M. (2012b). A phase-field description of dynamic brittle fracture. *Computer Methods in Applied Mechanics and Engineering*, 217:77–95.
- [33] Borst, R. d., Sluys, L. J., Muhlhaus, H.-B., and Pamin, J. (1993). Fundamental issues in finite element analyses of localization of deformation. *Engineering Computations: Int J for Computer-Aided Engineering*, 10(2):99–121.
- [34] Bouchard, P.-O., Bourgeon, L., Lachapele, H., Maire, E., Verdu, C., Forestier, R., and Logé, R. E. (2008). On the influence of particle distribution and reverse loading on damage mechanisms of ductile steels. *Materials Science and engineering: A*, 496(1-2):223–233.
- [35] Bourdin, B., Francfort, G., and Marigo, J. (2008a). *The Variational Approach to Fracture*. Springer-Verlag, Berlin.
- [36] Bourdin, B., Francfort, G. A., and Marigo, J.-J. (2000). Numerical experiments in revisited brittle fracture. *Journal of the Mechanics and Physics of Solids*, 48(4):797–826.
- [37] Bourdin, B., Francfort, G. A., and Marigo, J.-J. (2008b). The variational approach to fracture. *Journal of elasticity*, 91(1-3):5–148.
- [38] Bourdin, B., Larsen, C. J., and Richardson, C. L. (2011). A time-discrete model for dynamic fracture based on crack regularization. *International journal of fracture*, 168(2):133–143.

- [39] Broumand, P. and Khoei, A. (2013). The extended finite element method for large deformation ductile fracture problems with a non-local damage-plasticity model. *Engineering Fracture Mechanics*, 112:97–125.
- [40] Buhl, T., Pedersen, C. B., and Sigmund, O. (2000). Stiffness design of geometrically nonlinear structures using topology optimization. *Structural and Multidisciplinary Optimization*, 19(2):93–104.
- [41] Buljac, A., Navas, V.-M. T., Shakoor, M., Bouterf, A., Neggers, J., Bernacki, M., Bouchard, P.-O., Morgeneyer, T. F., and Hild, F. (2018). On the calibration of elastoplastic parameters at the microscale via x-ray microtomography and digital volume correlation for the simulation of ductile damage. *European Journal of Mechanics-A/Solids*, 72:287–297.
- [42] Chaboche, J.-L. (1988). Continuum damage mechanics: Part ii—damage growth, crack initiation, and crack growth.
- [43] Challis, V. J., Roberts, A. P., and Wilkins, A. H. (2008). Fracture resistance via topology optimization. *Structural and Multidisciplinary Optimization*, 36(3):263–271.
- [44] Choo, J. and Sun, W. (2018). Coupled phase-field and plasticity modeling of geological materials: From brittle fracture to ductile flow. *Computer Methods in Applied Mechanics and Engineering*, 330:1–32.
- [45] Clayton, J. and Knap, J. (2015). Phase field modeling of directional fracture in anisotropic polycrystals. *Computational Materials Science*, 98:158–169.
- [46] Cornetti, P. and Carpinteri, A. (2011). Modelling the frp-concrete delamination by means of an exponential softening law. *Engineering Structures*, 33(6):1988–2001.
- [47] Cuvelier, F., Japhet, C., and Scarella, G. (2013). An efficient way to perform the assembly of finite element matrices in matlab and octave. *arXiv preprint arXiv:1305.3122*.
- [48] Da, D. and Yvonnet, J. (2020). Topology optimization for maximizing the fracture resistance of periodic quasi-brittle composites structures. *Materials*, 13(15):3279.
- [49] Da, D., Yvonnet, J., Xia, L., and Li, G. (2018). Topology optimization of particle-matrix composites for optimal fracture resistance taking into account interfacial damage. *International Journal for Numerical Methods in Engineering*, 115(5):604–626.
- [50] De Borst, R. (1991). Simulation of strain localization: a reappraisal of the cosserat continuum. *Engineering computations*.
- [51] de Souza Neto, E. A., Peric, D., and Owen, D. R. (2011). *Computational methods for plasticity: theory and applications*. John Wiley & Sons.
- [52] Doan, D. H., Bui, T. Q., Duc, N. D., and Fushinobu, K. (2016). Hybrid phase field simulation of dynamic crack propagation in functionally graded glass-filled epoxy. *Composites Part B: Engineering*, 99:266–276.
- [53] Duda, F. P., Ciarbonetti, A., Sánchez, P. J., and Huespe, A. E. (2015). A phase-field/gradient damage model for brittle fracture in elastic–plastic solids. *International Journal of Plasticity*, 65:269–296.

- [54] Dugdale, D. S. (1960). Yielding of steel sheets containing slits. *Journal of the Mechanics and Physics of Solids*, 8(2):100–104.
- [55] Ehlers, W. and Luo, C. (2017). A phase-field approach embedded in the theory of porous media for the description of dynamic hydraulic fracturing. *Computer Methods in Applied Mechanics and Engineering*, 315:348–368.
- [56] Etse, G. and Willam, K. (1999). Failure analysis of elastoviscoplastic material models. *Journal of engineering mechanics*, 125(1):60–69.
- [57] Francfort, G. A. and Marigo, J.-J. (1998). Revisiting brittle fracture as an energy minimization problem. *Journal of the Mechanics and Physics of Solids*, 46(8):1319–1342.
- [58] Gao, Y., Lin, Q., Bijeljic, B., and Blunt, M. J. (2017). X-ray microtomography of intermittency in multiphase flow at steady state using a differential imaging method. *Water Resources Research*, 53(12):10274–10292.
- [59] Gauthier, R. (2017). *Crack propagation mechanisms in human cortical bone on different paired anatomical locations: biomechanical, tomographic and biochemical approaches*. PhD thesis.
- [60] Georgiadis, A., Berg, S., Makurat, A., Maitland, G., and Ott, H. (2013). Pore-scale micro-computed-tomography imaging: Nonwetting-phase cluster-size distribution during drainage and imbibition. *Physical Review E*, 88(3):033002.
- [61] Ghajari, M., Iannucci, L., and Curtis, P. (2014). A peridynamic material model for the analysis of dynamic crack propagation in orthotropic media. *Computer Methods in Applied Mechanics and Engineering*, 276:431–452.
- [62] Giry, C., Dufour, F., and Mazars, J. (2011). Stress-based nonlocal damage model. *International Journal of Solids and Structures*, 48(25-26):3431–3443.
- [63] Goswami, S., Anitescu, C., Chakraborty, S., and Rabczuk, T. (2020). Transfer learning enhanced physics informed neural network for phase-field modeling of fracture. *Theoretical and Applied Fracture Mechanics*, 106:102447.
- [64] Grassl, P. and Jirásek, M. (2004). On mesh bias of local damage models for concrete. *Fracture mechanics of concrete structures*, pages 323–337.
- [65] Gu, G. X., Dimas, L., Qin, Z., and Buehler, M. J. (2016). Optimization of composite fracture properties: Method, validation, and applications. *Journal of Applied Mechanics*, 83(7):071006.
- [66] Guinea, G., Planas, J., and Elices, M. (1994). A general bilinear fit for the softening curve of concrete. *Materials and structures*, 27(2):99–105.
- [67] Hilchenbach, C. F. and Ramm, E. (2015). Optimization of multiphase structures considering damage. *Structural and Multidisciplinary Optimization*, 51(5):1083–1096.
- [68] Hillerborg, A., Modéer, M., and Petersson, P.-E. (1976). Analysis of crack formation and crack growth in concrete by means of fracture mechanics and finite elements. *Cement and concrete research*, 6(6):773–781.

- [69] Huang, X. and Xie, Y. (2007). Convergent and mesh-independent solutions for the bi-directional evolutionary structural optimization method. *Finite Elements in Analysis and Design*, 43(14):1039–1049.
- [70] James, K. A. and Waisman, H. (2014). Failure mitigation in optimal topology design using a coupled nonlinear continuum damage model. *Computer Methods in Applied Mechanics and Engineering*, 268:614–631.
- [71] Jin, Z.-H., Paulino, G. H., and Dodds Jr, R. H. (2003). Cohesive fracture modeling of elastic–plastic crack growth in functionally graded materials. *Engineering Fracture Mechanics*, 70(14):1885–1912.
- [72] Jirásek, M. (2007). Nonlocal damage mechanics. *Revue européenne de génie civil*, 11(7-8):993–1021.
- [73] KACHANOV, L. M. (1958). Time of the rupture process under creep conditions, izy akad. *Nank SSR Otd Tech Nauk*, 8:26–31.
- [74] Kang, Z., Liu, P., and Li, M. (2017). Topology optimization considering fracture mechanics behaviors at specified locations. *Structural and Multidisciplinary Optimization*, 55(5):1847–1864.
- [75] Kao, Y.-T., Zhang, Y., Wang, J., and Tai, B. L. (2016). Loading-unloading cycles of 3d-printing built bi-material structures with ceramic and elastomer. In *International Manufacturing Science and Engineering Conference*, volume 49910, page V003T08A008. American Society of Mechanical Engineers.
- [76] Karma, A., Kessler, D. A., and Levine, H. (2001). Phase-field model of mode iii dynamic fracture. *Physical Review Letters*, 87(4):045501.
- [77] Kato, J. and Ramm, E. (2013). Multiphase layout optimization for fiber reinforced composites considering a damage model. *Engineering structures*, 49:202–220.
- [78] Khaddour, G., Riedel, I., Andò, E., Charrier, P., Bésuelle, P., Desrues, J., Viggiani, G., and Salager, S. (2018). Grain-scale characterization of water retention behaviour of sand using x-ray ct. *Acta Geotechnica*, 13(3):497–512.
- [79] Krajcinovic, D. (1983). Constitutive equations for damaging materials.
- [80] Kuhn, C., Noll, T., and Müller, R. (2016). On phase field modeling of ductile fracture. *GAMM-Mitteilungen*, 39(1):35–54.
- [81] Kulkarni, M., Matouš, K., and Geubelle, P. (2010). Coupled multi-scale cohesive modeling of failure in heterogeneous adhesives. *International Journal for Numerical Methods in Engineering*, 84(8):916–946.
- [82] Lakes, R., Nakamura, S., Behiri, J., and Bonfield, W. (1990). Fracture mechanics of bone with short cracks. *Journal of biomechanics*, 23(10):967–975.
- [83] Landis, E. N. and Keane, D. T. (1999). X-ray microtomography for fracture studies in cement-based materials. In *Developments in X-ray Tomography II*, volume 3772, pages 105–113. International Society for Optics and Photonics.

- [84] Landis, E. N., Nagy, E. N., and Keane, D. T. (2003). Microstructure and fracture in three dimensions. *Engineering Fracture Mechanics*, 70(7-8):911–925.
- [85] Lasry, D. and Belytschko, T. (1988). Localization limiters in transient problems. *International Journal of Solids and Structures*, 24(6):581–597.
- [86] Le, T. X. (2019). *Experimental study on the mechanical properties and the microstructure of methane hydrate-bearing sandy sediments*. PhD thesis, Université Paris-Est.
- [87] Le, T.-X., Bornert, M., Aïmedieu, P., Chabot, B., King, A., and Tang, A.-M. (2020). An experimental investigation on methane hydrate morphologies and pore habits in sandy sediment using synchrotron x-ray computed tomography. *Marine and Petroleum Geology*, 122:104646.
- [88] Li, B. and Maurini, C. (2019). Crack kinking in a variational phase-field model of brittle fracture with strongly anisotropic surface energy. *Journal of the Mechanics and Physics of Solids*, 125:502–522.
- [89] Li, B., Peco, C., Millán, D., Arias, I., and Arroyo, M. (2015). Phase-field modeling and simulation of fracture in brittle materials with strongly anisotropic surface energy. *International Journal for Numerical Methods in Engineering*, 102(3-4):711–727.
- [90] Li, L. and Khandelwal, K. (2017). Design of fracture resistant energy absorbing structures using elastoplastic topology optimization. *Structural and Multidisciplinary Optimization*, 56(6):1447–1475.
- [91] Li, L., Zhang, G., and Khandelwal, K. (2017). Topology optimization of energy absorbing structures with maximum damage constraint. *International Journal for Numerical Methods in Engineering*, 112(7):737–775.
- [92] Li, L., Zhang, G., and Khandelwal, K. (2018a). Failure resistant topology optimization of structures using nonlocal elastoplastic-damage model. *Structural and Multidisciplinary Optimization*, 58(4):1589–1618.
- [93] Li, P., Wu, Y., and Yvonnet, J. (2020a). A simp-phase field topology optimization framework to maximize quasi-brittle fracture resistance of 2d and 3d composites. *submitted*.
- [94] Li, P., Yvonnet, J., and Combescure, C. (2020b). An extension of the phase field method to model interactions between interfacial damage and brittle fracture in elastoplastic composites. *International Journal of Mechanical Sciences*, page 105633.
- [95] Li, P., Zhu, Q., Gu, S., and Ni, T. (2018b). A phase field method to simulate crack nucleation and crack propagation in rock-like materials. *Engineering Mechanics*, 35:41–48.
- [96] Limodin, N., Réthoré, J., Buffière, J.-Y., Gravouil, A., Hild, F., and Roux, S. (2009). Crack closure and stress intensity factor measurements in nodular graphite cast iron using three-dimensional correlation of laboratory x-ray microtomography images. *Acta materialia*, 57(14):4090–4101.

- [97] Limodin, N., Rethore, J., Buffiere, J.-Y., Hild, F., Roux, S., Ludwig, W., Rannou, J., and Gravouil, A. (2010). Influence of closure on the 3d propagation of fatigue cracks in a nodular cast iron investigated by x-ray tomography and 3d volume correlation. *Acta Materialia*, 58(8):2957–2967.
- [98] Liu, G., Li, Q., Msekh, M. A., and Zuo, Z. (2016a). Abaqus implementation of monolithic and staggered schemes for quasi-static and dynamic fracture phase-field model. *Computational Materials Science*, 121:35–47.
- [99] Liu, P., Luo, Y., and Kang, Z. (2016b). Multi-material topology optimization considering interface behavior via xfem and level set method. *Computer methods in applied mechanics and engineering*, 308:113–133.
- [100] Lotfi, H. R. and Shing, P. B. (1995). Embedded representation of fracture in concrete with mixed finite elements. *International journal for numerical methods in engineering*, 38(8):1307–1325.
- [101] Lu, S., Landis, E., and Keane, D. (2006). X-ray microtomographic studies of pore structure and permeability in portland cement concrete. *Materials and structures*, 39(6):611–620.
- [102] Mandal, T. K., Nguyen, V. P., and Wu, J.-Y. (2019). Length scale and mesh bias sensitivity of phase-field models for brittle and cohesive fracture. *Engineering Fracture Mechanics*, 217:106532.
- [103] Mathieu, F., Amedieu, P., Guimard, J.-M., and Hild, F. (2013). Identification of interlaminar fracture properties of a composite laminate using local full-field kinematic measurements and finite element simulations. *Composites Part A: Applied Science and Manufacturing*, 49:203–213.
- [104] Mediavilla, J., Peerlings, R., and Geers, M. (2006). Discrete crack modelling of ductile fracture driven by non-local softening plasticity. *International journal for numerical methods in engineering*, 66(4):661–688.
- [105] Melenk, J. M. and Babuška, I. (1996). The partition of unity finite element method: basic theory and applications. In *Research Report/Seminar für Angewandte Mathematik*, volume 1996. Eidgenössische Technische Hochschule, Seminar für Angewandte Mathematik.
- [106] Miehe, C., Aldakheel, F., and Raina, A. (2016). Phase field modeling of ductile fracture at finite strains: A variational gradient-extended plasticity-damage theory. *International Journal of Plasticity*, 84:1–32.
- [107] Miehe, C., Hofacker, M., Schänzel, L.-M., and Aldakheel, F. (2015a). Phase field modeling of fracture in multi-physics problems. part ii. coupled brittle-to-ductile failure criteria and crack propagation in thermo-elastic–plastic solids. *Computer Methods in Applied Mechanics and Engineering*, 294:486–522.
- [108] Miehe, C., Hofacker, M., and Welschinger, F. (2010a). A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199(45-48):2765–2778.

- [109] Miehe, C. and Lambrecht, M. (2001). Algorithms for computation of stresses and elasticity moduli in terms of seth–hill’s family of generalized strain tensors. *Communications in numerical methods in engineering*, 17(5):337–353.
- [110] Miehe, C. and Mauthe, S. (2016). Phase field modeling of fracture in multi-physics problems. part iii. crack driving forces in hydro-poro-elasticity and hydraulic fracturing of fluid-saturated porous media. *Computer Methods in Applied Mechanics and Engineering*, 304:619–655.
- [111] Miehe, C., Schaezel, L.-M., and Ulmer, H. (2015b). Phase field modeling of fracture in multi-physics problems. part i. balance of crack surface and failure criteria for brittle crack propagation in thermo-elastic solids. *Computer Methods in Applied Mechanics and Engineering*, 294:449–485.
- [112] Miehe, C., Welschinger, F., and Hofacker, M. (2010b). Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field fe implementations. *International Journal for Numerical Methods in Engineering*, 83(10):1273–1311.
- [113] Mielke, A. (2005). Evolution of rate-independent systems. *Evolutionary equations*, 2:461–559.
- [114] Mielke, A. (2006). A mathematical framework for generalized standard materials in the rate-independent case. In *Multifield Problems in Solid and Fluid Mechanics*, pages 399–428. Springer.
- [115] Moës, N., Stolz, C., Bernard, P.-E., and Chevaugeon, N. (2011). A level set based model for damage growth: the thick level set approach. *International Journal for Numerical Methods in Engineering*, 86(3):358–380.
- [116] Mohammadnejad, T. and Khoei, A. (2013). An extended finite element method for hydraulic fracture propagation in deformable porous media with the cohesive crack model. *Finite Elements in Analysis and Design*, 73:77–95.
- [117] Mühlhaus, H.-B. and Alfantis, E. (1991). A variational principle for gradient plasticity. *International Journal of Solids and Structures*, 28(7):845–857.
- [118] Needleman, A. (1988). Material rate dependence and mesh sensitivity in localization problems. *Computer methods in applied mechanics and engineering*, 67(1):69–85.
- [119] Needleman, A. (1990). An analysis of tensile decohesion along an interface. *Journal of the Mechanics and Physics of Solids*, 38(3):289–324.
- [120] Ngo, T. D., Kashani, A., Imbalzano, G., Nguyen, K. T., and Hui, D. (2018). Additive manufacturing (3d printing): A review of materials, methods, applications and challenges. *Composites Part B: Engineering*, 143:172–196.
- [121] Nguyen, T., Yvonnet, J., Waldmann, D., and He, Q.-C. (2019). Phase field modeling of interfacial damage in heterogeneous media with stiff and soft interphases. *Engineering Fracture Mechanics*, 218:106574.

- [122] Nguyen, T. H., Bui, T. Q., and Hirose, S. (2018). Smoothing gradient damage model with evolving anisotropic nonlocal interactions tailored to low-order finite elements. *Computer Methods in Applied Mechanics and Engineering*, 328:498–541.
- [123] Nguyen, T. T. (2015). *Modeling of complex microcracking in cement based materials by combining numerical simulations based on a phase-field method and experimental 3D imaging*. PhD thesis, Paris Est.
- [124] Nguyen, T. T., Réthoré, J., and Baietto, M.-C. (2017a). Phase field modelling of anisotropic crack propagation. *European Journal of Mechanics-A/Solids*, 65:279–288.
- [125] Nguyen, T.-T., Réthoré, J., Yvonnet, J., and Baietto, M.-C. (2017b). Multi-phase-field modeling of anisotropic crack propagation for polycrystalline materials. *Computational Mechanics*, 60(2):289–314.
- [126] Nguyen, T. T., Yvonnet, J., Bornert, M., and Chateau, C. (2016a). Initiation and propagation of complex 3d networks of cracks in heterogeneous quasi-brittle materials: Direct comparison between in situ testing-microt experiments and phase field simulations. *Journal of the Mechanics and Physics of Solids*, 95:320–350.
- [127] Nguyen, T. T., Yvonnet, J., Bornert, M., Chateau, C., Bilteryst, F., and Steib, E. (2017c). Large-scale simulations of quasi-brittle microcracking in realistic highly heterogeneous microstructures obtained from micro ct imaging. *Extreme mechanics letters*, 17:50–55.
- [128] Nguyen, T. T., Yvonnet, J., Bornert, M., Chateau, C., Sab, K., Romani, R., and Le Roy, R. (2016b). On the choice of parameters in the phase field method for simulating crack initiation with experimental validation. *International Journal of Fracture*, 197(2):213–226.
- [129] Nguyen, T. T., Yvonnet, J., Zhu, Q.-Z., Bornert, M., and Chateau, C. (2015). A phase field method to simulate crack nucleation and propagation in strongly heterogeneous materials from direct imaging of their microstructure. *Engineering Fracture Mechanics*, 139:18–39.
- [130] Nguyen, T. T., Yvonnet, J., Zhu, Q.-Z., Bornert, M., and Chateau, C. (2016c). A phase-field method for computational modeling of interfacial damage interacting with crack propagation in realistic microstructures obtained by microtomography. *Computer Methods in Applied Mechanics and Engineering*, 312:567–595.
- [131] Nguyen, V. P. (2014). Discontinuous galerkin/extrinsic cohesive zone modeling: Implementation caveats and applications in computational fracture mechanics. *Engineering fracture mechanics*, 128:37–68.
- [132] Nguyen-Vinh, H., Bakar, I., Msekh, M., Song, J.-H., Muthu, J., Zi, G., Le, P., Bordas, S. P. A., Simpson, R., Natarajan, S., et al. (2012). Extended finite element method for dynamic fracture of piezo-electric materials. *Engineering Fracture Mechanics*, 92:19–31.
- [133] Ni, T., Pesavento, F., Zaccariotto, M., Galvanetto, U., Zhu, Q.-Z., and Schrefler, B. A. (2020). Hybrid fem and peridynamic simulation of hydraulic fracture propagation in saturated porous media. *Computer Methods in Applied Mechanics and Engineering*, 366:113101.

- [134] Ni, T., Zhu, Q.-z., Zhao, L.-Y., and Li, P.-F. (2018). Peridynamic simulation of fracture in quasi brittle solids using irregular finite element mesh. *Engineering Fracture Mechanics*, 188:320–343.
- [135] Oliver, J., Huespe, A. E., and Sánchez, P. J. (2006). A comparative study on finite elements for capturing strong discontinuities: E-fem vs x-fem. *Computer methods in applied mechanics and engineering*, 195(37-40):4732–4752.
- [136] Ortiz, M. and Pandolfi, A. (1999). Finite-deformation irreversible cohesive elements for three-dimensional crack-propagation analysis. *International journal for numerical methods in engineering*, 44(9):1267–1282.
- [137] Papoulia, K. D., Sam, C.-H., and Vavasis, S. A. (2003). Time continuity in cohesive finite element modeling. *International Journal for Numerical Methods in Engineering*, 58(5):679–701.
- [138] Park, K. and Paulino, G. H. (2011). Cohesive zone models: a critical review of traction-separation relationships across fracture surfaces. *Applied Mechanics Reviews*, 64(6).
- [139] Park, K., Paulino, G. H., and Roesler, J. R. (2008). Determination of the kink point in the bilinear softening model for concrete. *Engineering Fracture Mechanics*, 75(13):3806–3818.
- [140] Peerlings, R. H., de Borst, R., Brekelmans, W., and Geers, M. G. (1998). Gradient-enhanced damage modelling of concrete fracture. *Mechanics of Cohesive-frictional Materials: An International Journal on Experiments, Modelling and Computation of Materials and Structures*, 3(4):323–342.
- [141] Peerlings, R. H., de Borst, R., Brekelmans, W. M., and De Vree, J. (1996). Gradient enhanced damage for quasi-brittle materials. *International Journal for numerical methods in engineering*, 39(19):3391–3403.
- [142] Perdikaris, P. C. and Romeo, A. (1995). Size effect on fracture energy of concrete and stability issues in three-point bending fracture toughness testing. *Materials Journal*, 92(5):483–496.
- [143] Pham, K., Marigo, J.-J., and Maurini, C. (2011). The issues of the uniqueness and the stability of the homogeneous response in uniaxial tests with gradient damage models. *Journal of the Mechanics and Physics of Solids*, 59(6):1163–1190.
- [144] Rabczuk, T. (2013). Computational methods for fracture in brittle and quasi-brittle solids: state-of-the-art review and future perspectives. *ISRN Applied Mathematics*, 2013.
- [145] Rodriguez, P., Ulloa, J., Samaniego, C., and Samaniego, E. (2018). A variational approach to the phase field modeling of brittle and ductile fracture. *International Journal of Mechanical Sciences*, 144:502–517.
- [146] Roux, S., Réthoré, J., and Hild, F. (2009). Digital image correlation and fracture: an advanced technique for estimating stress intensity factors of 2d and 3d cracks. *Journal of Physics D: Applied Physics*, 42(21):214004.

- [147] Roy, P., Deepu, S., Pathrikar, A., Roy, D., and Reddy, J. (2017). Phase field based peridynamics damage model for delamination of composite structures. *Composite Structures*, 180:972–993.
- [148] Russ, J. B. and Waisman, H. (2019). Topology optimization for brittle fracture resistance. *Computer Methods in Applied Mechanics and Engineering*, 347:238–263.
- [149] Russ, J. B. and Waisman, H. (2020). A novel topology optimization formulation for enhancing fracture resistance with a single quasi-brittle material. *International Journal for Numerical Methods in Engineering*, 121(13):2827–2856.
- [150] Saad, Y. (2003). *Iterative methods for sparse linear systems*. SIAM.
- [151] Salzman, A., Moës, N., and Chevaugeon, N. (2016). On use of the thick level set method in 3d quasi-static crack simulation of quasi-brittle material. *International Journal of Fracture*, 202(1):21–49.
- [152] San, B. and Waisman, H. (2016). Optimization of carbon black polymer composite microstructure for rupture resistance. *Journal of Applied Mechanics*, 84(2):021005.
- [153] San, B. and Waisman, H. (2017). Optimization of carbon black polymer composite microstructure for rupture resistance. *Journal of Applied Mechanics*, 84(2).
- [154] Seleš, K., Jurčević, A., Tonković, Z., and Sorić, J. (2019). Crack propagation prediction in heterogeneous microstructure using an efficient phase-field algorithm. *Theoretical and Applied Fracture Mechanics*, 100:289–297.
- [155] Shakoar, M., Buljac, A., Neggers, J., Hild, F., Morgeneyer, T. F., Helfen, L., Bernacki, M., and Bouchard, P.-O. (2017). On the choice of boundary conditions for micromechanical simulations based on 3d imaging. *International Journal of Solids and Structures*, 112:83–96.
- [156] Sigmund, O. (2001). A 99 line topology optimization code written in matlab. *Structural and multidisciplinary optimization*, 21(2):120–127.
- [157] Sigmund, O. and Maute, K. (2013). Topology optimization approaches. *Structural and Multidisciplinary Optimization*, 48(6):1031–1055.
- [158] Silling, S. A. (2000). Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48(1):175–209.
- [159] Simo, J. and Hughes, T. (1998). *Computational Inelasticity*. Springer-Verlag.
- [160] Simo, J. C., Oliver, J., and Armero, F. (1993). An analysis of strong discontinuities induced by strain-softening in rate-independent inelastic solids. *Computational mechanics*, 12(5):277–296.
- [161] Simone, A., Askes, H., and Sluys, L. J. (2004). Incorrect initiation and propagation of failure in non-local and gradient-enhanced media. *International journal of solids and structures*, 41(2):351–363.

- [162] Stock, S., Guvenilir, A., Breunig, T., Kinney, J., and Nichols, M. (1995). Computed tomography part iii: Volumetric, high-resolution x-ray analysis of fatigue crack closure. *JOM*, 47(1):19–23.
- [163] Strouboulis, T., Babuška, I., and Copps, K. (2000a). The design and analysis of the generalized finite element method. *Computer methods in applied mechanics and engineering*, 181(1-3):43–69.
- [164] Strouboulis, T., Copps, K., and Babuška, I. (2000b). The generalized finite element method: an example of its implementation and illustration of its performance. *International Journal for Numerical Methods in Engineering*, 47(8):1401–1417.
- [165] Suéry, M., Adrien, J., Landron, C., Terzi, S., Maire, E., Salvo, L., and Blandin, J.-J. (2010). Fast in-situ x-ray micro tomography characterisation of microstructural evolution and strain-induced damage in alloys at various temperatures: Dedicated to professor dr. h.-p. degischer on the occasion of his 65th birthday. *International journal of materials research*, 101(9):1080–1088.
- [166] Svanberg, K. (1987). The method of moving asymptotes a new method for structural optimization. *International journal for numerical methods in engineering*, 24(2):359–373.
- [167] Tanné, E., Li, T., Bourdin, B., Marigo, J.-J., and Maurini, C. (2018). Crack nucleation in variational phase-field models of brittle fracture. *Journal of the Mechanics and Physics of Solids*, 110:80–99.
- [168] Teichtmeister, S., Kienle, D., Aldakheel, F., and Keip, M.-A. (2017). Phase field modeling of fracture in anisotropic brittle solids. *International Journal of Non-Linear Mechanics*, 97:1–21.
- [169] Van den Bosch, M., Schreurs, P., and Geers, M. (2006). An improved description of the exponential xu and needleman cohesive zone law for mixed-mode decohesion. *Engineering Fracture Mechanics*, 73(9):1220–1234.
- [170] Wang, X., Jiang, M., Zhou, Z., Gou, J., and Hui, D. (2017). 3d printing of polymer matrix composites: A review and prospective. *Composites Part B: Engineering*, 110:442–458.
- [171] Wilson, Z. A. and Landis, C. M. (2016). Phase-field modeling of hydraulic fracture. *Journal of the Mechanics and Physics of Solids*, 96:264–290.
- [172] Wu, C., Fang, J., Zhou, S., Zhang, Z., Sun, G., Steven, G. P., and Li, Q. (2020). Level-set topology optimization for maximizing fracture resistance of brittle materials using phase-field fracture model. *International Journal for Numerical Methods in Engineering*, 121(13):2929–2945.
- [173] Wu, J.-Y. and Huang, Y. (2020). Comprehensive implementations of phase-field damage models in abaqus. *Theoretical and Applied Fracture Mechanics*, 106:102440.
- [174] Wu, J.-Y., Li, F.-B., and Xu, S.-L. (2015). Extended embedded finite elements with continuous displacement jumps for the modeling of localized failure in solids. *Computer Methods in Applied Mechanics and Engineering*, 285:346–378.

- [175] Wu, J.-Y. and Nguyen, V. P. (2018). A length scale insensitive phase-field damage model for brittle fracture. *Journal of the Mechanics and Physics of Solids*, 119:20–42.
- [176] Xia, L., Da, D., and Yvonnet, J. (2018a). Topology optimization for maximizing the fracture resistance of quasi-brittle composites. *Computer Methods in Applied Mechanics and Engineering*, 332:234–254.
- [177] Xia, L., Fritzen, F., and Breitkopf, P. (2017a). Evolutionary topology optimization of elastoplastic structures. *Structural and Multidisciplinary Optimization*, 55(2):569–581.
- [178] Xia, L., Xia, Q., Huang, X., and Xie, Y. M. (2018b). Bi-directional evolutionary structural optimization on advanced structures and materials: a comprehensive review. *Archives of Computational Methods in Engineering*, 25(2):437–478.
- [179] Xia, L., Yvonnet, J., and Ghabezloo, S. (2017b). Phase field modeling of hydraulic fracturing with interfacial damage in highly heterogeneous fluid-saturated porous media. *Engineering Fracture Mechanics*, 186:158–180.
- [180] Xu, X.-P. and Needleman, A. (1994). Numerical simulations of fast crack growth in brittle solids. *Journal of the Mechanics and Physics of Solids*, 42(9):1397–1434.
- [181] Xu, X.-P. and Needleman, A. (1996). Numerical simulations of dynamic crack growth along an interface. *International journal of fracture*, 74(4):289–324.
- [182] Yang, U. M. et al. (2002). Boomeramg: a parallel algebraic multigrid solver and preconditioner. *Applied Numerical Mathematics*, 41(1):155–177.
- [183] Yang, Z.-J., Li, B.-B., and Wu, J.-Y. (2019). X-ray computed tomography images based phase-field modeling of mesoscopic failure in concrete. *Engineering Fracture Mechanics*, 208:151–170.
- [184] Yin, B. and Kaliske, M. (2020). A ductile phase-field model based on degrading the fracture toughness: Theory and implementation at small strain. *Computer Methods in Applied Mechanics and Engineering*, 366:113068.
- [185] You, T., Zhu, Q.-Z., Li, P.-F., and Shao, J.-F. (2019). Incorporation of tension-compression asymmetry into plastic damage phase-field modeling of quasi brittle geomaterials. *International Journal of Plasticity*.
- [186] Yvonnet, J. (2019). *Computational Homogenization of Heterogeneous Materials with Finite Elements*. Springer.
- [187] Zhang, P., Hu, X., Bui, T. Q., and Yao, W. (2019a). Phase field modeling of fracture in fiber reinforced composite laminate. *International Journal of Mechanical Sciences*, 161:105008.
- [188] Zhang, P., Hu, X., Yang, S., and Yao, W. (2019b). Modelling progressive failure in multi-phase materials using a phase field method. *Engineering Fracture Mechanics*, 209:105–124.
- [189] Zhang, X., Sloan, S. W., Vignes, C., and Sheng, D. (2017a). A modification of the phase-field model for mixed mode crack propagation in rock-like materials. *Computer Methods in Applied Mechanics and Engineering*, 322:123–136.

- [190] Zhang, X., Vignes, C., Sloan, S. W., and Sheng, D. (2017b). Numerical evaluation of the phase-field model for brittle fracture with emphasis on the length scale. *Computational Mechanics*, 59(5):737–752.
- [191] Zhang, Z., Chen, J., Li, E., Li, W., Swain, M., and Li, Q. (2016). Topological design of all-ceramic dental bridges for enhancing fracture resistance. *International journal for numerical methods in biomedical engineering*, 32(6):e02749.
- [192] Zhou, S., Zhuang, X., Zhu, H., and Rabczuk, T. (2018). Phase field modelling of crack propagation, branching and coalescence in rocks. *Theoretical and Applied Fracture Mechanics*, 96:174–192.
- [193] Zhu, Q.-z. and Ni, T. (2017). Peridynamic formulations enriched with bond rotation effects. *International Journal of Engineering Science*, 121:118–129.
- [194] Zou, R., Xia, Y., Liu, S., Hu, P., Hou, W., Hu, Q., and Shan, C. (2016). Isotropic and anisotropic elasticity and yielding of 3d printed material. *Composites Part B: Engineering*, 99:506–513.

