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Phase-Field Models for the Failure of Anisotropic Continua

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This study presents a phase-field approach for an anisotropic continuum to model fracture of biological tissues and fiber-reinforced composites. We start with the continuous formulation of the variational principle for the multi-field problem manifested through the deformation map and the crack phase-field at finite strains which leads to the Euler–Lagrange equations of the coupled problem. In particular, the coupled balance equations derived render the evolution of the anisotropic crack phase-field and the balance of linear momentum. In addition, we propose a novel energy-based anisotropic failure criterion which regulates the evolution of the crack phase-field. The coupled problem is solved using a one-pass operator-splitting algorithm composed of a mechanical predictor step and a crack evolution step. Representative numerical examples are devised for crack initiation and propagation in carbon-fiber-reinforced polymerg composites. Model parameters are obtained by fitting the set of novel experimental data to the predicted model response; the finite element results qualitatively capture the effect of anisotropy in stiffness and strength.

1 Introduction

Since the introduction of composite materials in the 1960's such as glass/polyester and carbon/epoxy, great success was achieved in micromechanics estimates of effective elastic properties, homogenization, laminate plate theory, etc. However, theories for treating failure of composite materials did not succeed to the same extent. In fact after numerous efforts extending over approximately five decades many uncertainties and controversies still remain in predicting composite failure [5]. The classical theory of brittle fracture suffers from the shortcomings to determine curvilinear crack paths, crack kinking and branching angles. These problems regarding the Griffith theory can be eliminated through variational principles hinged on energy minimization, as introduced in a phase-field model for quasi-static brittle fracture. The phase-field models of fracture ultimately bypasses the modeling of the discontinuities by providing a diffusive crack topology, where the sharp crack surface smears out over a solid domain because of a length scale parameter [3]. The approach is modular and can be applied to non-standard solids exhibiting complex cracking mechanisms under multiphysics phenomena [4]. This approach was practiced to model the rupture of soft biological tissues with anisotropic texture [1, 2] where several anisotropic failure criteria were thoroughly investigated. In what follows, the fracture of the fiber-reinforced plastics (FRP) composed of a polymer matrix reinforced with fibers will be scrutinized. To this end, a first order anisotropic phase-field theory along with a distinct energy-based failure criteria will be proposed in Section 3 after briefly introducing the multi-field problem and the kinematics in Section 2.

2 Kinematics and the primary field variables

The primary field variables, the deformation map φ and the the crack phase-field d, with the corresponding maps from reference to current configuration are given as

$$\varphi_t(\boldsymbol{X}) : \left\{ \begin{array}{ccc} \mathcal{B}\times\mathcal{T} & \rightarrow & \mathcal{S} \\ (\boldsymbol{X},t) & \mapsto & \boldsymbol{x} = \varphi(\boldsymbol{X},t) \end{array} \right. \qquad d : \left\{ \begin{array}{ccc} \mathcal{B}\times\mathcal{T} & \rightarrow & [0,1] \\ (\boldsymbol{X},t) & \mapsto & d(\boldsymbol{X},t)\,. \end{array} \right.$$

The deformation gradient, and the right and left Cauchy-Green tensors are defined as

$$\boldsymbol{F} = \nabla\varphi, \qquad \boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{g}\boldsymbol{F}, \qquad \text{and} \qquad \boldsymbol{b} = \boldsymbol{F}\boldsymbol{G}^{-1}\boldsymbol{F}^T \qquad \text{where} \qquad \nabla[\bullet] = \nabla_X[\bullet]. \tag{1}$$

The energy stored in a hyperelastic isotropic material is characterized by the invariants

$$I_1 = \mathrm{tr}\boldsymbol{C}, \qquad I_2 = \frac{1}{2}\left[I_1^2 - \mathrm{tr}(\boldsymbol{C}^2)\right], \qquad I_3 = \det\boldsymbol{C}. \tag{2}$$

The anisotropic response of a unidirectional FRP composite requires the description of an additional invariant. To this end, we introduce a reference unit vector $\boldsymbol{f}_0$ for the fiber orientation and its spatial counterpart $\boldsymbol{f} = \boldsymbol{F}\boldsymbol{f}_0$, which idealize the micro-structure of the unidirectional FRP composite. We can express the related Eulerian form of the structure tensor as $\boldsymbol{A_m} = \boldsymbol{f}\otimes\boldsymbol{f}$. Furthermore, the additional invariant $I_4 = \boldsymbol{f}\cdot\boldsymbol{g}\boldsymbol{f}$ accounts for the square of stretches in fibers embedded in the FRP composite.

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3 Coupled balance equations of the multi-field problem

We define the energy storage functional E for a hyperelastic anisotropic solid as

$$E(\boldsymbol{\varphi}, d) := \int_{\mathcal{B}} \Psi(\boldsymbol{F}, \boldsymbol{A}_{\boldsymbol{m}}; d)\mathrm{d}V \quad \text{with} \quad \Psi(\boldsymbol{F}, \boldsymbol{A}_{\boldsymbol{m}}; d) := g(d)\Psi_0(\boldsymbol{F}, \boldsymbol{A}_{\boldsymbol{m}}), \tag{3}$$

where Ψ_0 is the effective free-energy function of the hypothetical intact solid. The monotonically decreasing quadratic degradation function $g(d) := (1-d)^2$ describes the degradation of the solid with the evolving crack phase-field parameter d. The rate of the energy storage functional $\mathcal{E}$ has the form

$$\mathcal{E}(\dot{\boldsymbol{\varphi}}, \dot{d}; \boldsymbol{\varphi}, d) = \int_{\mathcal{B}} (\boldsymbol{P} : \dot{\boldsymbol{F}} - f\dot{d})\mathrm{d}V \quad \text{where} \quad f := -\partial_d \Psi(\boldsymbol{F}, \boldsymbol{A}_{\boldsymbol{m}}; d). \tag{4}$$

Therein, $\boldsymbol{P}$ is the first Piola–Kirchhoff stress tensor and f is the energetic force which is work conjugate to the crack phase-field d. With the help of the external power functional $\mathcal{P}(\dot{\boldsymbol{\varphi}}) = \int_{\mathcal{B}} \rho_0 \bar{\boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\varphi}} \mathrm{d}V + \int_{\partial \mathcal{B}_t} \bar{\boldsymbol{T}} \cdot \dot{\boldsymbol{\varphi}} \mathrm{d}A$, and the crack dissipation functional

$$\mathcal{D}(\dot{d}) = \int_{\mathcal{B}} g_{\mathrm{c}}[\delta_d \gamma(d, \nabla d)]\dot{d}\mathrm{d}V \quad \text{where} \quad \gamma(d, \nabla d) = \frac{1}{2l}(d^2 + l^2|\nabla d|^2) \quad \text{and} \quad \delta_d\gamma = \frac{1}{l}(d - l^2\Delta d), \tag{5}$$

where $\delta_d\gamma$ denotes the variational derivative of the crack surface density γ, the power balance Π for the multi-field problem gives

$$\Pi(\dot{\boldsymbol{\varphi}}, \dot{d}) := \mathcal{E}(\dot{\boldsymbol{\varphi}}, \dot{d}) + \mathcal{D}(\dot{d}) - \mathcal{P}(\dot{\boldsymbol{\varphi}}) = 0. \tag{6}$$

On the basis of (6), a rate-type mixed variational principle can be constructed via a minimization principle for the quasi-static process, i.e.

$$\{\dot{\boldsymbol{\varphi}}, \dot{d}\} = \mathrm{Arg}\left\{ \inf_{\dot{\boldsymbol{\varphi}} \in \mathcal{W}_{\varphi}} \inf_{\dot{d} \in \mathcal{W}_d} \Pi(\dot{\boldsymbol{\varphi}}, \dot{d}) \right\}. \tag{7}$$

The Euler-Lagrange equations of the coupled multi-field problem yields

$$\mathrm{Div}\boldsymbol{P} + \rho_0 \bar{\boldsymbol{\gamma}} = \boldsymbol{0} \qquad \text{and} \qquad (f - g_{\mathrm{c}}\delta_d\gamma)\dot{d} = 0, \tag{8}$$

along with the loading-unloading conditions ensuring the principal of maximum dissipation in case of an evolution of the crack phase-field parameter d, i.e.

$$\dot{d} \geq 0, \qquad f - g_{\mathrm{c}}\delta_d\gamma \leq 0, \qquad (f - g_{\mathrm{c}}\delta_d\gamma)\dot{d} = 0. \tag{9}$$

The first condition ensures the irreversibility of the evolution of the crack phase-field parameter. The second condition is an equality for an evolving crack, and it is negative for a stable crack. The third condition is the balance law for the evolution of the crack phase-field subjected to the former conditions.

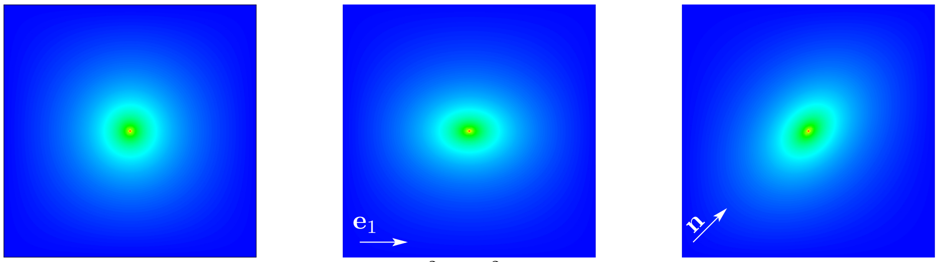
4 Anisotropic phase-field model for fiber-reinforced composites

The constitutive equations describing the nonlinear anisotropic response of a unidirectional FRP composite and the associated energy-based anisotropic failure criterion delineating the state of the material at which the cracking starts and propagates are herein briefly explained. To characterize the local anisotropic mechanical response of an unidirectional FRP composite we specify the free-energy function Ψ_0 and adopt the polyconvex, invariant-based anisotropic free-energy function $\Psi_0(\boldsymbol{F}, \boldsymbol{A}_{\boldsymbol{m}}) := \Psi_0^{\mathrm{iso}}(J, I_1) + \Psi_0^{\mathrm{ani}}(I_4)$, which is additively decomposed into an isotropic compressible neo-Hookean part, responsible for the mechanical behavior of the ground polymer matrix, and an anisotropic free-energy function taking into account the contributions of the unidirectional fibers written in a generic form such that

$$\Psi_0^{\mathrm{iso}}(J, I_1) := \frac{\lambda}{2}(\ln^2 J) + \frac{\mu}{2}(I_1 - 2\ln J - 3), \qquad \Psi_0^{\mathrm{ani}}(I_4) := \frac{\mu_{\mathrm{f}}}{2}(I_4 - 1)^2. \tag{10}$$

Therein, λ denotes the Lamé constant whereas μ is the shear modulus, while in the anisotropic term μ_{f} stands for fiber modulus. Exploiting the Coleman–Noll procedure on the Clausius–Planck inequality, and using the form of the free-energy function Ψ, we retrieve the first Piola–Kirchhoff stress tensor as

$$\boldsymbol{P} := \partial_{\boldsymbol{F}}\Psi = g(d)\boldsymbol{P}_0, \qquad \text{with} \quad \boldsymbol{P}_0 = \partial_{\boldsymbol{F}}\Psi_0. \tag{11}$$



$\boldsymbol{\mathcal{L}} = l^2\mathbf{1}$ $\quad$ $\boldsymbol{\mathcal{L}} = l^2\mathbf{1} + l^2\mathbf{e}_1 \otimes \mathbf{e}_1$ $\quad$ $\boldsymbol{\mathcal{L}}_{\text{ani}} = l^2\mathbf{1} + l^2\mathbf{n} \otimes \mathbf{n}$

Fig. 1: (a) Isotropic damage field; (b) anisotropic damage field with fiber angle $\theta = 0°$; (c) anisotropic damage field with $\theta = 45°$.

Insertion of (10) into the definition $(11)_2$ leads to the stress expression for the intact material, i.e.

$$\boldsymbol{P}_0 = \lambda \ln J \boldsymbol{F}^{-T} + \mu(\boldsymbol{F} - \boldsymbol{F}^{-T}) + 2\psi_4 \boldsymbol{f} \otimes \boldsymbol{f}_0 \quad \text{where} \quad \psi_4 := \partial_{I_4}\Psi_0 = \mu_{\text{f}}(I_4 - 1). \tag{12}$$

In order to describe anisotropic failure, we further elaborate on the equation for the evolution of the crack phase-field and substitute the equations $(4)_2$, $(5)_3$ in $(8)_2$ for $\dot{d} \geq 0$, and then $(3)_2$ and the expression for $g(d)$ in $(4)_2$ to arrive at

$$f - \frac{g_{\text{c}}}{l}(d - l^2\Delta d) = 0, \qquad f = 2(1-d)\Psi_0. \tag{13}$$

We now assume distinct failure processes for the ground matrix and the fibers. Accordingly, the energetic force f can be additively decomposed into an isotropic part f_{iso} and an anisotropic part f_{ani} according to

$$f = f_{\text{iso}} + f_{\text{ani}} \quad \text{where} \quad f_{\text{iso}} = 2(1-d)\Psi_0^{\text{iso}} \quad \text{and} \quad f_{\text{ani}} = 2(1-d)\Psi_0^{\text{ani}}. \tag{14}$$

Next, we introduce the distinct critical fracture energies over distinct length scales $g_{\text{c}}^{\text{iso}}/l_{\text{iso}}$ for the ground matrix and $g_{\text{c}}^{\text{ani}}/l_{\text{ani}}$ for the fibers which are dual to the free-energy functions for the isotropic and the anisotropic parts, respectively. Consequently, (13) can be modified to account for the distinct failure assumption, i.e.

$$f_{\text{iso}} - \frac{g_{\text{c}}^{\text{iso}}}{l_{\text{iso}}}(d - \nabla \cdot [\boldsymbol{\mathcal{L}}_{\text{iso}}\nabla d]) = 0, \qquad f_{\text{ani}} - \frac{g_{\text{c}}^{\text{ani}}}{l_{\text{ani}}}(d - \nabla \cdot [\boldsymbol{\mathcal{L}}_{\text{ani}}\nabla d]) = 0, \tag{15}$$

where $\boldsymbol{\mathcal{L}}_{\text{iso}} = l_{\text{iso}}^2\mathbf{1}$ and $\boldsymbol{\mathcal{L}}_{\text{ani}} = l_{\text{ani}}^2 \boldsymbol{f}_0 \otimes \boldsymbol{f}_0$. After some algebraic manipulations, we obtain

$$2(1-d)\frac{\Psi_0^{\text{iso}}}{g_{\text{c}}^{\text{iso}}/l_{\text{iso}}} = d - \nabla \cdot [\boldsymbol{\mathcal{L}}_{\text{iso}}\nabla d], \qquad 2(1-d)\frac{\Psi_0^{\text{ani}}}{g_{\text{c}}^{\text{ani}}/l_{\text{ani}}} = d - \nabla \cdot [\boldsymbol{\mathcal{L}}_{\text{ani}}\nabla d]. \tag{16}$$

We define dimensionless crack driving functions for the isotropic $\bar{\mathcal{H}}^{\text{iso}}$ and anisotropic $\bar{\mathcal{H}}^{\text{ani}}$ parts in (16), i.e.

$$\bar{\mathcal{H}}^{\text{iso}} = \frac{\Psi_0^{\text{iso}}}{g_{\text{c}}^{\text{iso}}/l_{\text{iso}}}, \qquad \bar{\mathcal{H}}^{\text{ani}} = \frac{\Psi_0^{\text{ani}}}{g_{\text{c}}^{\text{ani}}/l_{\text{ani}}}. \tag{17}$$

With the use of (17), a superposition of the isotropic and anisotropic failure processes (16) engenders

$$d - \nabla \cdot \boldsymbol{\mathcal{L}}\nabla d = (1-d)\bar{\mathcal{H}}, \quad \text{where} \quad \bar{\mathcal{H}} = \bar{\mathcal{H}}^{\text{iso}} + \bar{\mathcal{H}}^{\text{ani}} \quad \text{and} \quad \frac{\boldsymbol{\mathcal{L}}_{\text{iso}} + \boldsymbol{\mathcal{L}}_{\text{ani}}}{2}. \tag{18}$$

The use of distinct length scales for the matrix and the fibers provide us the anisotropic diffusive damage field, see Figure 1. The left-hand side of $(18)_1$ is the geometric resistance to crack growth whereas the right-hand side is the local source term for crack growth. In order to enforce the irreversibility condition and prevent the healing effects, the dimensionless source term $(18)_2$ is modified, i.e. $\mathcal{H}(t) = \max_{s\in[0,t]}\left[\,\langle\, \bar{\mathcal{H}}(s) - 1 \,\rangle\right]$. In the above, the Macaulay brackets $\langle(\bullet)\rangle = [(\bullet) + |(\bullet)|]/2$ filter out the positive values for $\bar{\mathcal{H}}(s)$ and keeps the anisotropic solid intact below a threshold energy density, i.e. until the failure surface is reached. Hence, the crack phase-field does not evolve for a dimensionless crack source term ($\bar{\mathcal{H}}(s) < 1$).

Table 1: Material parameters needed for the constitutive equations.

Parameter	Value	Unit	Parameter	Value	Unit	Parameter	Value	Unit
λ	5.2×10^3	[MPa]	μ	4.04×10^3	[MPa]	μ_{f}	32.3×10^3	[MPa]
$g_{\text{c}}^{\text{iso}}/l_{\text{iso}}$	5.5	[MPa mm]	$g_{\text{c}}^{\text{ani}}/l_{\text{ani}}$	80	[MPa mm]	$\boldsymbol{f}_0$	$[1,0,0]$	[–]

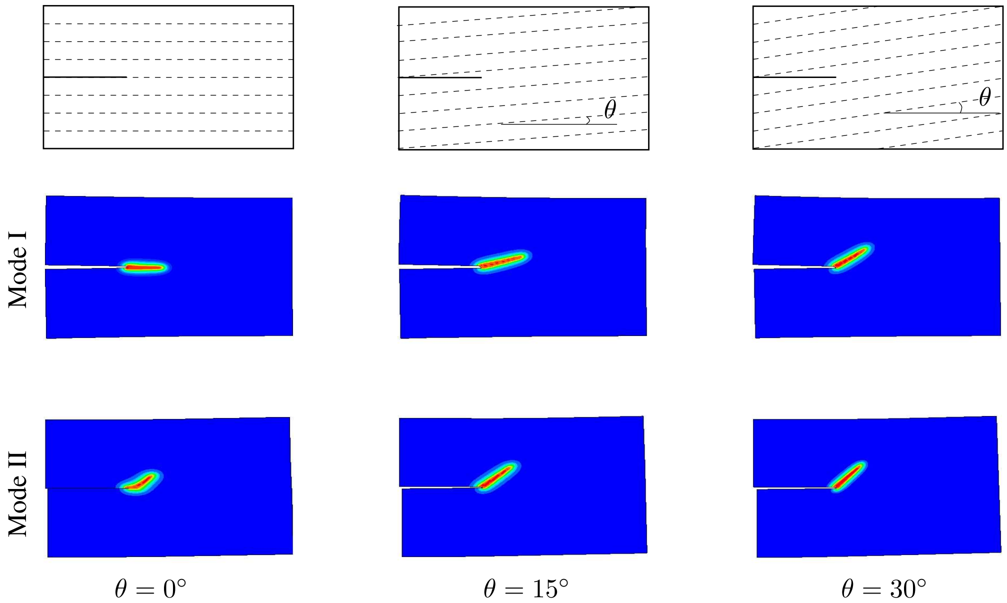


Fig. 2: Single–edge notched tests for three fiber orientations $\theta = 0°$, $15°$ and $30°$.

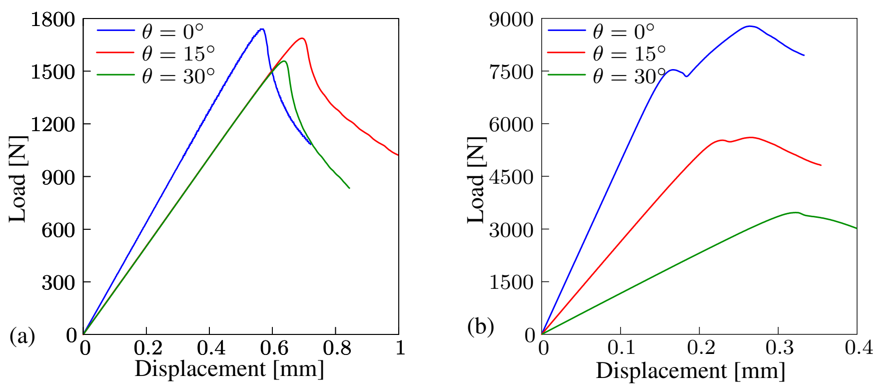


Fig. 3: Load–deflection curves of single–edge notched tests for different fiber orientations: (a) mode-I; (b) mode-II.

5 Representative numerical examples

Single–edge notched specimen is subjected to mode-I and mode-II loads. AS4/3501-6 epoxy lamina is used. The material parameters required for the constitutive equations are retrieved from longitudinal tensile and transverse compression stress–strain test data via the curve fitting technique, see Table 1. The computation of the mode-I and mode-II tests are performed in a displacement driven context. Analysis are done for three different specimens with three different fiber orientations which are $0°$, $15°$ and $30°$, as shown in Figure 2. The crack patterns of the related tests are demonstrated in Figure 2, while the deflection curves obtained are depicted in Figure 3.

The proposed phase-field approach qualitatively captures the dependence of crack onset and crack propagation on the fiber orientation in homogenized anisotropic continuum. Further quantitative examples will be the subject of future work.

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