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A rate-dependent and unconstrained phase-field model for brittle fracture

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Abstract. This work deals with the formulation and numerical implementation of a rate-dependent model for brittle fracture that allows for damage healing. The model formulation, which is carried out within the framework of continuum mechanics, relies on the introduction of an extra independent kinematical descriptor, the phase field, along with the corresponding force system, the microforce system. The governing equations of theory are obtained by supplementing the standard and extra force balances with a constitutive theory consistent with a mechanical version of the second law of thermodynamics. A particular version of the theory is singled out to provided a regularization of a standard theory constrained by the assumption of damage irreversibility. The model shows a derivation of an "optimal" kinetic modulus function from an "optimal" penalization of rate-independent model in the literature, which made it capable to avoid healing at a level previously unknown for rate-dependent models of that type. A few simulation results are shown for different problem parameters previously explored by other works. To solve the equations of the model, we use the finite-element method, for spatial discretization, and a backward Euler scheme, for the time integration, in a Python implementation aided by an open-source computing platform *FEniCS*.

Keywords: Phase-field, Fracture, Crack propagation, Residual stress, Finite elements.

1 Introduction

An elastic body $\mathcal{B}$ is considered under residual stress — achieved by prescribing a stress-free strain field —, which is capable of experiencing brittle fracture. The target was the formulation of a theory for the behaviour of $\mathcal{B}$ to provide a systematic way of describing the interaction between elastic deformation, residual stress and fracture. A theory was selected to numerically study crack nucleation and growth in a residually-stressed elastic solid from an undamaged initial condition at the damage field. This work builds upon Duda et al. [1] where the general description of fracture is made by means of phase field and considering stress-free strains, differing to the mentioned work on the fact that the damage irreversibility conditions are not treated as a contraint, but rather as a penalization to the damage healing. Further, the stress-free strain is given rather than calculated. Some references for approaching brittle fracture in the repsence of residual stress with Phase-Field Method are Salvati [2], da Silva et al. [3], Aranson et al. [4].

2 Phase-field model for brittle fracture

From the point of view of kinematics, $\mathcal{B}$ is considered as described by two independent fields: the displacement field $\mathbf{u}$ and the phase, or damage, field φ, which may be interpreted as the fraction of broken bonds and takes values on the interval $[0; 1]$. Then, by the principle of virtual power one can derive the local forms of the basic balances of the theory, namely the standard force balance and the micro-force balance:

$$\operatorname{Div}\mathbf{S} + \mathbf{b} = 0; \quad \operatorname{Div}\xi + \pi + \gamma_e = 0, \tag{1}$$

where "Div" is the divergence operator, $\mathbf{S}$, the stress tensor, $\mathbf{b}$ the body force density, ξ the microstress vector, and π and γ_e the internal and external microforces densities. In addition to these balances, a free-energy imbalance is used in order to enforce the first and second laws of thermodynamics:

$$\dot{\psi} - \mathbf{S} \cdot \dot{\mathbf{E}} + \pi\dot{\varphi} - \xi \cdot \nabla\dot{\varphi} \leq 0, \tag{2}$$

where ψ is the free-energy density, $\mathbf{E} = \frac{1}{2}\left[\nabla\mathbf{u} + \nabla\mathbf{u}^\top\right]$ the infinitesimal strain tensor, and ∇ the gradient operator.

In order to derive the constitutive equations, response functions for ψ, $\mathbf{S}$, ξ, and π are considered in terms of $(\mathbf{E}, \varphi, \nabla\varphi, \dot{\varphi})$, which for obeying Eq. (2) in every admissible process. One can show that the free-energy can not depend on $\dot{\varphi}$ and the following relations must hold:

$$\mathbf{S} = \frac{\partial\psi(\mathbf{E}, \varphi, \nabla\varphi)}{\partial\mathbf{E}}; \quad \xi = \frac{\partial\psi(\mathbf{E}, \varphi, \nabla\varphi)}{\partial\nabla\varphi}; \quad \pi = -\frac{\partial\psi(\mathbf{E}, \varphi, \nabla\varphi)}{\partial\varphi} - \beta(\mathbf{E}, \varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}, \tag{3}$$

with $\beta(\mathbf{E}, \varphi, \nabla\varphi, \dot{\varphi}) \geq 0$. Therefore, from the constitutive standpoint the theory is determined by the scalar response functions for the free energy ψ and for the kinetic modulus β. For the free energy, it can be shown the following response function is admissible:

$$\psi(\mathbf{E}, \varphi, \nabla\varphi) = \frac{(1-\varphi)^2}{2}\left(\lambda(\mathrm{tr}(\mathbf{E} - \mathbf{E}_0))^2 + 2\mathrm{G}|\mathbf{E} - \mathbf{E}_0|^2\right) + \frac{g_f}{2\ell}\left(\varphi^2 + \ell^2(\nabla\varphi)^2\right). \tag{4}$$

Here, λ and G are the Lamé moduli, $\mathbf{E}_0$ the stress-free strain, g_f the fracture energy, and ℓ a characteristic length.

In order to provide a non-healing feature to the model so that the damage is irreversible the kinetic modulus is assumed to have different values on the negative and positive sides of the domain as shown in Eq.(5).

$$\hat{\beta}(\dot{\varphi}) \begin{cases} \beta^- & \dot{\varphi} < 0 \\ \beta^+ & \dot{\varphi} \geq 0 \end{cases} \tag{5}$$

where β^- represents a value, not necessarily constant in space and time, that β will assume so that when β^- goes to infinity, the reversibility towards healing direction becomes impossible. Meanwhile β^+ works as a type of a "cushioning" coefficient that will work limiting the speed of damage.

At the right side of Fig. 1 the negative part of the domain is shown in a schematic way such that β^- is a much higher value than β^+. At the left side of Fig. 1 a schematic graph of the response function for the kinetic modulus β multiplied by the damage rate $\dot{\varphi}$ is shown for different values of $\dot{\varphi}$, which shows that due to the response function chosen, the absolute value of $\beta\dot{\varphi}$ will grow much faster towards the negative direction from the origin than towards the positive direction, making it really difficult for a point to reverse its damage condition.

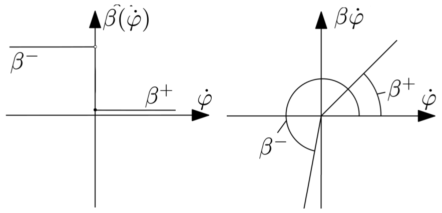


Figure 1. Penalization of the kinetic coefficient β for irreversibility hypothesis.

3 Numerical application and results

In order to verify the numerical behaviour of the exposed phase field model, residual stresses were applied under a plane-strain state formulation. For this, consider the scheme shown in Fig. 2 where it demonstrates a two-dimensional body governed by Eqs.(1), whose constitutive equations follow the Eqs.(3), (4) and (5). Some considerations are important to be defined to solve this problem: the first one is the term ϵ_0^{2d} which indicates a residual stress modelling that will be imposed on the model, equivalent to a problem of drying gel specimen being constrained whose deformation follows the additive decomposition of an elastic and a chemical part, in which $\bar{\epsilon}$ will be the only parameter: $\mathbf{E} = \mathbf{E}_e + \mathbf{E}_0$; $\mathbf{E}_0 = \epsilon_0^{2d} = \bar{\epsilon}\sqrt{\frac{G_c}{ER}}\mathbf{I}_2$.

The second consideration of the problem is the Dirichlet boundary condition that characterizes a numerical model of a constrained boundary fully attached to the external environment at the edges of the specimen, therefore, not allowed to damage, as defined in Eq. $(6)_1$. The third consideration refers to the initial condition of the problem, which was set for no damage at the whole domain in time 0, as shown in Eq. $(6)_2$, in order to observe the concentration of stress in the specimen through out the simulation and allow repeatability of the simulations for a given set of parameters.

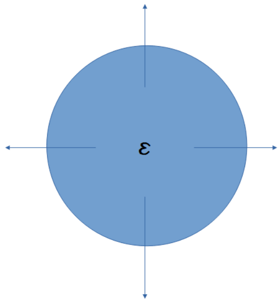


Figure 2. Body under residual stresses.

$$\begin{cases} \varphi(x,y,t)=0;\ \mathbf{u}(x,y,t)=0 & \text{at} \quad \{(x,y)\in\partial\mathcal{B}\}, \\ \varphi(x,y,0)=0 & \text{at} \quad t=0s \end{cases} \tag{6}$$

In Eq. (6). The parameters used, inspired by the simulations of Maurini et al. [5] , follow Tab. 1, the generated mesh is unstructured and has $0.025/R$ to $0.05/R$ triangular elements, necessary refinement to have numerical convergence in the propagation interface described by the characteristic parameter ℓ respectively $0.05/R$ to $0.2/R$.

For the spatial discretization of the elements, we consider for the calculation of the variable of the displacement vector $\mathbf{u}$ triangular quadratic elements and for the calculation of the damage φ triangular linear. For the temporal discretization, for reasons of simplicity and stability, the implicit Euler method was used.

Regarding the response function $\hat{\beta}(\dot{\varphi})$ a continuous formulation one could consider β^- to be infinitely high, but for numerical applications, it can be shown that instabilities will appear for very high values of β^- and this limit will vary depending on the time step used at each step of the simulation. This work used a previous work of a rate-independent formulation as a guide to choose a proper value for $\beta -$ as shown in Eq.(7).

Also β^+ could be adjusted depending on the crack growth speed desired, which can also be treated as a parameter of the material. In this application, since there is no aim to produce a specific crack growth speed, β^+ was set as 1. Eq. (7) shows the discretized form of $\hat{\beta}$.

$$\hat{\beta}(\dot{\varphi}) \begin{cases} \gamma \cdot \mathrm{d}t & \dot{\varphi} \leq 0 \\ 1 & \dot{\varphi} \geq 0 \end{cases} \tag{7}$$

Here, γ is a parameter-based value defined by Gerasimov and De Lorenzis [6] as explained later and dt is the time step used to calculate $\dot{\varphi}$. See Fig. 1.

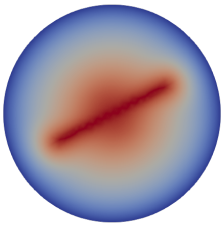
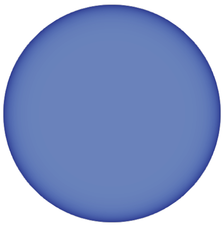
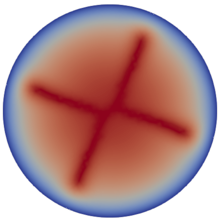
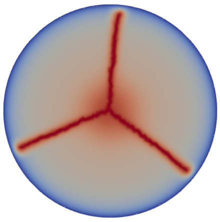
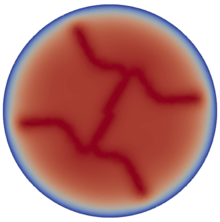
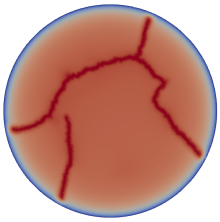
As per Gerasimov and De Lorenzis [6], γ is intended to be an estimation of an optimal value that is high enough to allow very little reversibility and, at the same time, provides a stable simulation. γ definition is based on the analogous constant defined based on an analytical study of the similar one-dimensional problem. The formula used for γ is shown in Tab. 1.

In our interpretation dt has to enter multiplying γ in order to keep the stability and irreversibility regardless of the time step used — which is variable throughout our simulation —, since γ was calculated based on a tolerance for dφ rather than based on a tolerance for $\dot{\varphi}$.

The computational simulation code was all developed in Python using the *FEniCS* finite element library for solving partial differential equations. The jobs were run using four cores with an intel i7 computer with 16GB of RAM taking from 30 minutes to 5 five hours to reach the final equilibrium state in which the cracks stop propagating. The results were post-processed through the open-platform Paraview tool.

Table 1. Elastic, fracture and numerical parameters of the computational simulation.

E (kN/mm^2)	ν	g_f (kN/mm)	Δt (s)	ℓ (mm)	γ	$\bar{\epsilon}$
1.0	0.3	1.0	variable	0.05 to 0.2	$\frac{g_f}{\ell\left[\left(\frac{1}{0.01}\right)^2-1\right]}$	1.2 to 4.0

$\bar{l}$ / $\bar{e}$	0.2	0.05
1.2		
2.2		
4.0		

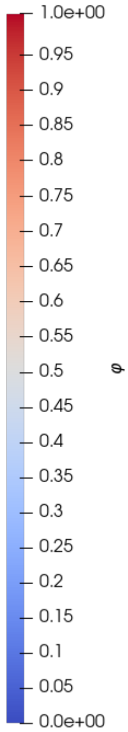


Table 2. Results at steady state equilibrium.

The results show that, as expected, the residual stress changes the crack patterns, what is predictable since more surface area needs to be created in order to balance with the all the free energy coming from a higher residual stress level.

A not so obvious result, but still predictable, is that the characteristic length will have influence on the crack nucleation and propagation. That is explained because a smaller characteristic length will allow the damage to occur closer to the boundaries, what will result in a less concentrated damage at the center.

4 Conclusions

The paper presented a phase-field model for brittle fracture accounting for the presence of residual stresses, wherein damage irreversibility was imposed by penalizing damage healing. A solver suitable to linear and isotropic elastic solids was developed using the finite element method and implemented in Python with the aid of *FEniCS* library. As an illustrative example, we considered the nucleation and propagation of crack patterns due to dehydration-induced residual stresses. When considering undamaged initial conditions, we observed the expected invariability of the crack patterns given the same parameters.

As a subsequent step, we aim to compare the time to achieve the steady state and compare the crack patterns for benchmark problems, as well as check at which level randomness in the initial condition may influence the crack patterns.

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