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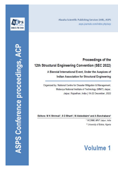

A Review on phase-field modeling of fracture

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Abstract

In cases with complicated crack topologies, the computational modeling of failure processes in materials owing to fracture based on sharp crack discontinuities fails. Diffusive crack modeling based on the insertion of a crack phase-field can overcome this. The phase-field model (PFM) portrays the fracture geometry in a diffusive manner, with no abrupt discontinuities. Unlike discrete fracture descriptions, phase-field descriptions do not need numerical monitoring of discontinuities in the displacement field. This considerably decreases the complexity of implementation. These qualities enable PFM to describe fracture propagation more successfully than numerical approaches based on the discrete crack model, especially for complicated crack patterns. These models have also demonstrated the ability to forecast fracture initiation and propagation in two and three dimensions without the need for any ad hoc criteria. The phase-field model, among numerous options, is promising in the computer modeling of fracture in solids due to its ability to cope with complicated crack patterns such as branching, merging, and even fragmentation. A brief history of the application of the phase-field model in predicting solid fracture has been attempted. An effort has been made to keep the conversation focused on recent research findings on the subject. Finally, some key findings and recommendations for future research areas in this field are discussed.

Keywords: Phase-field model, fracture, diffusive crack modeling

1. Introduction

Fracture is a key mode of failure in engineering materials and structures, and preventing it is a fundamental restriction in engineering designs. The numerical simulation of fracture processes is frequently used in design choices. However, fracturing is a rather complicated process that is difficult to adequately describe in practice. As a result, it is critical to use computer models to simulate and forecast the commencement, propagation, and branching of potential fractures for real engineering applications.

The equilibrium condition of a solid elastic body deformed by specified surface forces, according to the well-known theorem of minimum energy, is such that the potential energy of the entire system is a minimum. The new rupture criteria are obtained by adding to this theory the assertion that the equilibrium position if one exists, must be one in which the solid has ruptured if the system can transition from the unbroken to the broken condition by a process involving a continuous drop in potential energy.

Griffith [1] and Irwin [2] presented the classical theory of brittle fracture in elastic solids, which states that a crack propagates if the energy release rate exceeds a threshold value. They related fracture formation to surface energy, the macroscopic expression of lattice debonding, and crack propagation to the competition between bulk energy away from the crack and surface energy on the crack during an infinitesimal increase in crack length. If the rate of loss of elastic energy per unit surface area of the increment step is equal to some critical energy release rate Gc, crack propagation will occur. If the elastic energy release rate is smaller than Gc, the fracture does not move. On the contrary, if it reaches the critical rate, it becomes unstable. A common notion in Griffith's-type brittle fracture models is that when the critical energy release rate is exceeded, a fully opened crack is nucleated or propagated. As a result, the process zone, or the zone in which the material changes from undamaged to damaged, is consolidated into a single location near the crack tip.

The Griffith theory gives a fracture propagation criterion; however, it is insufficient for determining curved crack routes, crack kinking, and branching angles. Such a hypothesis, in particular, is incapable of predicting crack onset. These shortcomings of the conventional Griffith-type theory of brittle fracture can be circumvented by variational approaches based on energy minimization, as proposed by

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Francfort and Marigo[3], in which the total energy is reduced with regard to both the crack geometry and the displacement field. This formulation overcomes the constraints of conventional Griffith theory by determining the whole development of fractures, including their start and branching, using no additional criteria. However, because the displacement field is discontinuous in the presence of fractures, a straightforward numerical discretization of the model presents significant challenges.

Because of the complexity of fracture processes in engineering applications, numerical approaches are essential in fracture studies. Finite element approaches, in particular, are often utilized in combination with Griffith's-type linear elastic fracture mechanics models. The virtual crack closure approach [4] and, more recently, the extended finite element method proposed by Moes et al. [5] are two of the most widely used finite element models. All of these methods portray fractures as discrete discontinuities, either by introducing discontinuity lines using remeshing strategies or by supplementing the displacement field with discontinuities using Babuka and Melenk's division of unity method [6]. Tracing the growth of complicated fracture surfaces, on the other hand, has proven to be a time-consuming operation, especially in three dimensions.

Alternative approaches for numerical modeling of brittle fracture have recently emerged. Discontinuities are not introduced into the solid in these procedures. Instead, a phase-field is used to mimic the fracture surface, smoothing the crack border across a narrow region. Unlike discrete fracture descriptions, phase-field descriptions do not need numerical monitoring of discontinuities in the displacement field. This considerably decreases the complexity of implementation. Since the late 1990s, phase-field modeling of brittle fracture in elastic materials has been the topic of substantial theoretical and computational research. In general, the phase-field method for modeling systems with sharp interfaces entails including a continuous field variable - the field order parameter - that distinguishes between numerous physical phases within a given system via a smooth transition. In the context of fracture, such an order parameter defines the smooth transition between entirely fractured and intact material phases, so approaching the acute crack discontinuity, and is hence known as the crack field. The ability to skip the time-consuming operation of tracking intricate fracture surfaces in 3D simplifies implementation greatly. In such a method, By accounting for an additional variable, the phase-field parameter, fracture may be approached as an energy minimization issue [7]. As a result, complicated fracture phenomena such as crack branching, break initiation from random locations, and multiple crack coalescence are naturally recorded in the original finite element mesh [8-10]. Not unexpectedly, the strategy is gaining popularity, and the number of applications has increased dramatically. Recent examples include hydrogen embrittlement [11,12], fatigue damage [13,14], lithium-ion battery cracking [15,16], rock fracture [17], composites delamination [18,19], and functionally graded material fracture [20].

Several phase-field methods for brittle fracture have been proposed and researched independently in the physics and mechanics communities. Surprisingly, the philosophical and technical foundations used to derive the constitutive and phase-field evolution equations differ significantly across the two cultures. The dynamic models created within the physics community are generated by extending Landau and Ginzburg's phase transition formalism [21]. In contrast, the models offered within the mechanics community are based on Francfort and Marigo's [3] variational formulation of brittle fracture, regularised by Bourdin et al. [7], which extends the traditional Griffith's theory of fracture.

2. Phase-field approximation of crack topology

Consider an infinitely expanded bar of cross-section Γ occupying the domain $B=\Gamma\times L$ with $L=[-\infty, +\infty]$ and position $x\in L$ of its axis. Assume a crack of the bar at the axial position $x=0$, where Γ represents the fully-broken crack surface.

This sharp crack topology may be described by an auxiliary field variable $d(x) \in[0, 1]$, characterizing for $d=0$ the unbroken state and for $d=1$ the fully broken state of the material. Fig. 1 & 2 gives a visualization.

3. Fundamentals of the PF approach

The PF method for brittle fracture is understood as a regularised variant of the evolutionary issue of crack propagation under quasi-static circumstances. In the spirit of Griffith's theory of fracture, the crack evolution is examined by the minimizing of the functional that characterizes the potential energy of the body under investigation.

Let us consider a homogeneous, isotropic, and linear elastic domain $\Omega \subset R^2$ with a crack Γ and the boundary $\partial\Omega$ as depicted in Fig. 3.

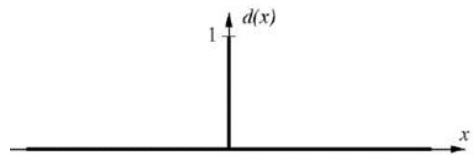

Fig. 1. Sharp crack at x =0

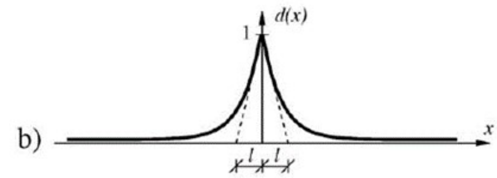

Fig. 2. diffusive crack at x =0 modeled with the length scale l.

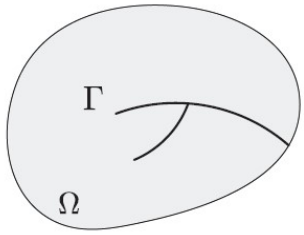

Fig. 3. Sharp interface topology

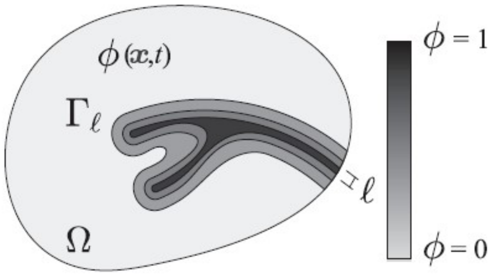

Fig. 4. Phase field model of the interface

In a regularized framework, the crack geometry is a "smeared" representation defined by an auxiliary field variable $\phi(x) \in [0,1], x \in \Omega$, which is denoted as the crack phase-field, as illustrated in Fig. 4. The uncracked and fully cracked states of the considered domain are characterized by $\phi = 0$ and $\phi = 1$, respectively.

4. The phase-field fracture method

Alan Arnold Griffith's energy-based crack analysis in 1920 is regarded as the beginning of the science of fracture mechanics. Griffith's hypothesis [1] predicts that an existing crack will propagate if the energy release rate G linked with the crack extension exceeds a critical value equal to Gc, the material fracture toughness. Griffith's hypothesis, on the other hand, has a flaw in that it cannot account for crack nucleation or anticipate fracture branching. To overcome this limitation, the variational method to fracture mechanics described by Francfort and Marigo [3] offers the following energy functional for the broken body.

$$E(u,\Gamma) = E_d(u,\Gamma) + E_s(\Gamma) + \int_\Omega \psi(\varepsilon(u))d\Omega + G_c H^1(\Gamma)$$

Where $E_d(u,\Gamma)$ is the elastic energy stored in the cracked body, $E_s(\Gamma)$ represents the energy required to create the new crack according to the Griffith theory, ψ is the elastic energy density function, ε is the strain tensor, **u** is the displacement vector, G_c is the critical energy release rate, and H^1 is the Hausdorff surface measure giving the crack length. With the assumption of small deformation, the strain tensor is related to the displacement vector $\varepsilon = (\nabla u + \nabla u^T)/2$. To consider the crack phase field, the energy functional Eq. (1) can be expressed as the following functional

$$E(u,\phi) \approx \int_\Omega \psi((\varepsilon(u),\phi)\ d\Omega + G_c \int_\Omega \gamma(\phi)\ d\Omega$$
$$= \int_\Omega \psi((\varepsilon(u),\phi)\ d\Omega + G_c \int_\Omega \left(\frac{1}{2l}\phi^2 + \frac{l}{2}\nabla\phi \cdot \nabla\phi \right) d\Omega$$

Where $\gamma(\phi, \nabla\phi)$ denotes the crack density function per unit volume l is a regularization parameter describing the width of the smeared crack and recovers for $l \to 0$ the sharp crack topology. It should be noted that if the regularisation value in the standard phase-field model is not properly specified, it might have a substantial impact on the crack propagation route and the accompanying peak load. It is frequently recommended that it be determined in one of two ways: as a pure numerical parameter of a regularised model of brittle fracture or as a real material parameter of a gradient damage model [22]. Furthermore, the element size may have a substantial impact on the numerical convergence of mechanical responses. According to Miehe et al. [23], the criterion must be met. The length-scale insensitive phase-field model proposed by Wu [24], Wu, and Nguyen [25] should be highlighted in this regard.

5. Advances in phase-field modeling

A brief history of the application of the phase-field method for predicting fracture in structural engineering and related applications is given below.

C. Kuhn and R. Muller [26] were the first to reinterpret the crack variable as a phase-field order parameter, addressing cracking as a phase transition problem. In their formulation, the crack formation was driven by an order parameter evolution equation that resembled the Ginzburg-Landau equation, and the numerical treatment was done using finite elements mixed with an implicit Euler scheme for time integration. Later, they used Bourdin's [7] regularised approximation of the variational model, which is better appropriate for numerical treatment. In finite element simulations, they investigated the effects of the regularisation parameter, which governs the interface width between broken and undamaged material, and the mobility constant of the evolution equation. They created a generalized Eshelby tensor to calculate the energy release rate of diffuse phase field fractures.

In a typical time step, Christian Miehe et al. [27] proposed a robust operator split technique that updates the history field, fracture phase field, and finally, displacement field. They added a regularisation based on viscous fracture resistance to the algorithm, which increases its durability. Later [28], the authors provided a thermodynamically consistent framework for phase-field models of fracture propagation in elastic substances. Borden et al. [29] investigated the behavior of the phase-field model in one dimension and demonstrated how it affects material characteristics. They proposed a monolithic and a staggered time integration approach for the temporal discretization of equations of motion. Heike Ulmer et al. [30] offered an extension of fracture's phase-field modeling concepts to Kirchhoff plates and shells. Their use of history fields, which contained the greatest reference energy attained in history, gave a very transparent representation of the coupled balancing equations and enabled the development of a robust operator split approach.

Ambati et al. [31], along with Amor et al. [22], initiated the focus on quasi-static models with a tension-compression split, which inhibits cracking in compression and interpenetration of fracture faces upon closure. They suggested and evaluated the so-called hybrid formulation, which leads to an incrementally linear issue inside a staggered implementation and an adequate ending condition for the staggered scheme.

Borden et al. [32] suggested a fourth-order model for the phase-field approximation of the variational formulation for the brittle fracture to increase the convergence rate of numerical solutions. Their approach produces more regularity in the precise phase-field solution, which may be exploited by the smooth spline function spaces used in the isogeometric analysis, and it has opened the way to higher-order convergence rates for fracture issues. Wheeler et al. [33] presented an enhanced Lagrangian approach for discrete in time and continuous in space phase-field problems to minimize instabilities in the solution process of pressured fractures utilizing phase-field modeling.

A two-dimensional quasi-static phase-field formulation is computationally quite demanding within the finite element framework, owing primarily to the on-convexity of the related free-energy functional, with a robust but slowly converging staggered solution scheme based on algorithmic decoupling typically used. Gerasimov et al. [34] addressed this issue by proposing a faster and equally accurate approach for quasi-static phase-field computing of (brittle) fracture using a monolithic solution scheme accompanied by a novel line search procedure to overcome non-convex minimization iterative convergence issues. Borden et al. [37] expanded the phase-field formulation from brittle to ductile materials, properly representing strains after crack initiation, and included crucial ductile fracture characteristics such as stress triaxiality and plastic deterioration. Ambati et al. [35] followed with a unique phase-field model for ductile fracture of elastoplastic materials. Their formulation covered the complete spectrum of the behavior of a J2-plastic ductile material, including plasticization, fracture initiation, propagation, and failure.

Nguyen et al. [36] proposed a phase-field approach for simulating fracture formation and propagation in very heterogeneous materials using direct microstructure imaging. They explored fracture initiation and propagation in 2D and 3D extremely heterogeneous materials models, such as those acquired by micro-CT images of cementitious materials using the phase-field approach, for the first time. Kiendla et al. [39] proposed a method for phase-field modeling of fracture in thin structures such as plates and shells where the kinematics are dictated by mid-surface variables. As a result, the phase-field is defined as a two-dimensional field on the structure's midpoint. For structural analysis, they used brittle fracture and a Kirchhoff–Love shell model.

Experiments with projectile impacts on pre-notched plates have shown a shift from brittle to ductile failure as strain rate increases. Cracks occur at the notch tip and spread counterclockwise from the loading direction at modest rates. Shear bands develop and spread along a downward curved pattern at high speeds. This happens because the production of shear bands, which happens more easily at greater speeds, precludes the development of the enormous primary stresses required to begin a fracture. McAuliffe and Waisman [40] proposed a linked model that can capture this failure transition.

Miehe and colleagues [41] A novel finite strain theory for chemo-elasticity linked with fracture phase-field modeling that regularises a sharp crack topology is proposed. Later, [42] described a rigorous variational-based framework for phase-field modeling of ductile fracture in elastic-plastic materials subjected to enormous stresses. Two distinct length scales are used in the formulation to regularise both the plastic response and the crack discontinuities. This ensured that the ductile fracture damage zones were contained inside plastic zones. Nguyen et al. [43] explored the effect of various parameters in the model and presented experimental validations of crack initiation and propagation in plaster specimens. They demonstrated, in particular, via theoretical and practical investigations, that the regularisation length should be understood as a material parameter. They showed, through theoretical and experimental investigations, that the regularisation length should be regarded as a material parameter and experimentally detected.

Fracture phase-field modeling is also commonly used in the research of fatigue-related phenomena. In a one-dimensional instance, Alessi et al. [44] introduced a novel variational fatigue phase-field model. The model's primary concept was to have the fracture energy drop as a suitably specified cumulative strain measure increased, which was achieved by introducing a dissipation potential that explicitly relied on the strain history.

Current computational approaches for massive deformations lack the numerical stability required to assure resilience in a variety of loading circumstances. C. Hescha's [45] novel polyconvex fracture formulation ensured numerical stability for the whole spectrum of deformations and for arbitrary hyper elastic materials. The work introduces a new anisotropic split based on the primary invariants of the right Cauchy-Green tensor to give a unique formulation for finite strain polyconvex elasticity. J. Reinoso et al. [46] introduced a novel brittle fracture phase-field model for large deformation analysis of shells based on a mixed enhanced assumed strain (EAS) formulation. The kinematic description of the shell body is built on the solid shell notion.

Although the theoretical explanation of phase-field modeling of fracture was widely accepted, there was no open-source software for its execution. Molnár and Gravouil [47] used the commercial finite element code Abaqus/Standard to create a two- and three-dimensional phase-field technique. The approach is based on the diffuse fracture rate-independent variational concept. The method requires no predetermined fractures and may mimic curved fracture patterns, branching, and even crack coalescence. The elastic displacement and fracture problems were separated and treated independently in a staggered manner. Failure anisotropy, according to Nguyen [48], calls into question the foundations of brittle failure since the equivalence between the principle of local symmetry and the maximum energy release rate criteria is no longer applicable. He suggested a phase-field model that could (energetically) recreate non-free anisotropic crack bifurcation inside a framework that allowed for robust and quick numerical simulations. S. Teichtmeister et al. [50] presented a phase-field fracture model that accounts for anisotropic material behavior at small and large deformations. The majority of extant fracture phase-field models assume that cracks evolve within isotropic materials. He contended that this is an invalid assumption for many natural and artificial materials that display orientation-dependent behavior.

Because of its importance in solid mechanics and physics, the subject of fracture impinging on an interface has been studied throughout the last three decades. New phenomena emerge as the size of the process zone at the interface is increased, or the internal length scale of the phase-field model is varied. Paggia et al. [49] investigated the role of the fracture toughness ratio between the interface and the surrounding bulks, as well as the dissipative models' distinctive fracture length scales. Mandal et al. [64] addressed practical issues such as whether phase-field models should be mesh-bias objective and what value to use for the length scale parameter. They investigated the sensitivity of the solutions to various brittle and quasi-brittle fracture problems with and without singularities and notches to the length scale parameter and mesh alignment.

Wick [51] was able to successfully design and compare modified Newton techniques for completely monolithic quasi-static brittle phase-field fracture propagation. Instead of using line-search or trust-region tactics, he devised a modified Newton scheme in which globalization is based on a dynamic alteration of the Jacobian matrix. Creating a fully monolithic scheme is a difficult endeavor since the underlying issue is non-convex, and Newton's method's Jacobian is indefinite. He used a partitioned strategy to separate the issue and apply alternate minimization.

In a strictly geometric setting, Wu [52] presented the crack phase-field and associated gradient to regularise the acute crack topology. A crack geometric function of the polynomial type and an energetic degradation function of the rational type were used to characterize the energy dissipation functional owing to crack evolution and the stored energy functional of the bulk. Within the context of thermodynamics, he suggested A unified phase-field theory for the mechanics of damage and quasi-brittle failure.

Zhang1 et al. [54] conducted a rigorous numerical evaluation of the accuracy of phase-field modeling of brittle fracture, with a focus on a proposed formula for estimating the length scale. To achieve this purpose, he ran phase-field simulations of a variety of traditional fracture tests for brittle fracture in concretes, with simulated findings qualitatively and quantitatively compared to experimental data. Hansen et al. [55] suggested a phase-field technique for predicting interface failure between potentially different materials. Over a limited width, he regularised the discrete adhesive contact. He also conducted a one-dimensional analytic investigation to assess this impact and recommended a fix. Aditya Kumar et al. [56] provided a macroscopic theory to describe, explain, and forecast fracture and healing in elastomers subjected to arbitrarily large quasi-static deformations. They provided a numerical approach for solving these PDEs in two and three dimensions. This was accomplished through the use of an efficient non-conforming finite-element discretization. The theory entails solving a system of two linked nonlinear PDEs for the deformation field and an order parameter, or phase field.

Tannéa et al. [59] used the problem of an elliptic cavity in an infinite or extended domain to demonstrate how variational phase-field models account for structural and material size effects. Their key claim, which was confirmed by validation and verification across a wide range of materials and geometries, was that crack nucleation may be reliably predicted by the reduction of non-linear energy in variational phase-field models without the need for ad-hoc criteria. Xia et al. [53] created a numerical framework based on the phase-field approach that includes a regularised description of bulk and interface discontinuities in highly heterogeneous fluid-saturated porous media. He demonstrated hydro-mechanical microcracking initiation and propagation in voxel-based models in both 2D and 3D.

Nguyen and Wu [58] provided a dynamic fracture extension of the phase-field cohesive zone model for brittle and quasi-brittle materials. They were in good accord with current findings and experimental outcomes. René de Borst et al. [38] provided a simple overview of phase-field models for the brittle and cohesive approaches to fracture. Later [60], Wu and Nguyen addressed A phase-field regularised cohesive zone model (CZM) with linear softening law and applied it to brittle fracture. Failure strength and the traction–separation law are both independent of the length scale parameter. Classical brittle fracture phase-field models fail to predict length scale-independent global reactions for materials without elastic singularities (e.g., corners, notches, etc.). Their study expanded the quasi-brittle failure model (Wu, 2017, 2018a) and developed a length-scale insensitive phase-field damage model for brittle fracture for the first time. They explicitly addressed and implemented a phase-field regularised cohesive zone model (CZM) with linear softening law to brittle fracture using a set of ideal characteristic functions. In their work, Peng et al. [61] suggested an improved staggered iteration approach in which non-linear subproblems are handled in a one-pass procedure, reducing computational costs and improving iteration stability. They investigated a unified phase-field model that includes numerous coherent interactions. Yanga et al. [68] used the phase-field regularised cohesive zone model (PF-CZM) in conjunction with the X-ray computed tomography (XCT) imaging technology to describe mesoscopic cracking in concrete.

Zhou et al. [62] developed a phase-field model (PFM) to simulate complicated crack patterns in rock, such as crack propagation, branching, and coalescence. Complex fracture patterns for a plate subjected to rising internal pressure were also seen. Bilgen and Weinberg [63] examined several variational formulas for linear and finite elastic materials, as well as ad hoc driving forces driven by generic fracture mechanical concerns. Corominas et al. [66] included a gradient-enhanced damage formulation anchored in the Griffith theory of fracture in their numerical method, which is now expanded for usage in composite laminates applications. Ren et al. [67] suggested a dynamic brittle fracture explicit phase-field model. Christian Miehe et al. [71] proposed an extension of newly established brittle fracture continuum phase-field models to fully linked thermo-mechanical and multi-physics issues at enormous stresses. Paneda et al. [57] established a framework for phase-field modeling of hydrogen-assisted cracking. The model is based on a combined mechanical and hydrogen diffusion response, which is controlled by potential chemical gradients and a hydrogen-dependent fracture energy degradation equation. The linked issue was addressed using an implicit time integration approach, with the major variables being displacements, phase-field order parameters, and hydrogen concentration. They demonstrated that fracture phase field formulations are particularly well suited for capturing material deterioration caused by hydrogen.

Phase-field modeling has also been used in a wide range of smart and novel materials. Hirshikesh et al. [65] provided a fracture phase field formulation in functionally graded materials (FGMs). Based on homogenization theory, the model accounts for the spatial variance of elastic and fracture characteristics. They tackled many paradigmatic case studies to show the modeling framework's capabilities. To simulate fracture initiation and propagation in fiber-reinforced composites, Yina and Zhang [69] developed a three-dimensional phase-field model. They used a staggered technique that was efficient and resilient by decoupling the fracture phase field and displacement field. Peng and colleagues [70] suggested a new phase-field approach for predicting progressive failure in multi-phase materials..

6. Conclusions

Crack propagation modeling in materials has long been a problem in solid-state physics and materials research. The phase-field approach is currently recognized as one of the instruments for describing fracture propagation. The models used are thermodynamically consistent and predict fracture propagation in homogeneous materials under various loading conditions, numerous physical fields, and geometrical nonlinearities. Even dynamic loading mechanisms, including plastic effects, are investigated.

While conventional phase-field models for brittle fracture may represent intricate nucleation, propagation, branching, and merging of fractures in solids within a coherent framework, they fail to predict length scale-independent global reactions for a solid without elastic singularity (e.g., corners, notches, etc.).

Disclosures

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