

Abstract of “A Variational Mechanics Theory for Modeling the Evolution of Crack Networks in Composite Materials with Brittle Interfaces” by Kaushik Vijaykumar, Ph.D., Brown University, October, 2019.

Predicting crack patterns and toughness of structural biomaterials (SBs) is a complex problem due to their complicated microstructures. Most SBs are heterogeneous in nature and consist of a ceramic (stiff) phase and an organic (compliant) phase. The organic phase serves as a weak interface between the ceramic phases of the SBs. For example, spicules, which are needle-like structures found in most sponges, are one type of such SBs, where the ceramic phase occupies a volume fraction $> 95\%$ of the material. The stiff phase of spicules is arranged in concentric layers that are separated by nanometer-thin layers of compliant phase, which forms the interface. Toughness enhancement in SBs is attributed to various fracture mechanisms such as crack deflection and arrest at the weak interface. Modeling the fracture behavior of such SBs requires a computational fracture technique that can handle intricate crack topological changes without a priori information of the crack path. Regularized variational fracture theory (RVFT) provides a straight forward methodology to simulate the evolution of complex crack patterns. In RVFT, cracks are modeled using a continuous scalar field, termed the damage field, which takes values between zero (intact solid) and unity (fully broken solid). I modified the traditional RVFT to introduce interfaces by varying the fracture toughness of the solid spatially. I studied fracture of two-dimensional (2D) lamellar composites with weak interfaces under three-point bending and found the underlying mechanism for toughness enhancement to be crack deflection, arrest, and re-nucleation. I also performed three-dimensional (3D) simulations of concentric lamellar composites, which mimics the structure of spicules. I revealed that concentric lamellar architecture does not show significant toughness enhancement as compared to planar lamellar architecture. To experimentally study the role of weak interface in toughness enhancement of composites, I designed an architected composite composed of Polymethyl methacrylate (PMMA) with a complex network of interfaces (composed of weak adhesive) that mimics SBs. I observed crack arrests and deflections during the fracture tests of architected composites under three-point bending loading conditions. I found that the architected composites are almost an order of magnitude tougher than monolithic PMMA.

A Variational Mechanics Theory for Modeling the Evolution of Crack Networks in Composite Materials with Brittle Interfaces

by

Kaushik Vijaykumar

B.E, Birla Institute of Technology and Science, Pilani, 2009

MSc(Engg), Indian Institute of Science, 2013

Sc. M., Brown University, 2017

Submitted in partial fulfillment of the requirements
for the Degree of Doctor of Philosophy in
Solid Mechanics at Brown University

Providence, Rhode Island

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This dissertation by Kaushik Vijaykumar is accepted in its present form by
the School of Engineering as satisfying the dissertation requirement
for the degree of Doctor of Philosophy.

Date _____

Haneesh Kesari, Ph.D., Advisor

Recommended to the Graduate Council

Date _____

Allan Bower, Ph.D., Reader

Date _____

Vikas Srivastava, Ph.D., Reader

Approved by the Graduate Council

Date _____

Andrew G. Campbell, Ph.D.
Dean of the Graduate School

Curriculum Vitæ

Kaushik Vijaykumar received his bachelors degree in Mechanical Engineering in 2009 from Birla Institute of Technology and Science, Pilani. He received his MSc(Engg) in Mechanical Engineering from Indian Institute of Science in 2009. He also received his Master of Science degree in Solid Mechanics in the fall of 2017.

Conference Presentations

Vijaykumar K and Kesari H, “A variational model for simulating fracture in solids containing weak interfaces”. Society of Engineering Science 52th annual technical meeting, October 2015.

Vijaykumar K and Kesari H, “Stability analysis of regularized variational fracture model”. Society of Engineering Science 53rd annual technical meeting, October 2016.

Vijaykumar K and Kesari H, “Effective toughness of interfaces”. Society of Engineering Science 54th annual technical meeting, July 2017.

Vijaykumar K and Kesari H, “Effective toughness in materials with interfaces”. International Mechanical Engineering Congress & Exposition, The American Society of Mechanical Engineers, November 2018.

Teaching Experience at Brown

Graduate

Continuum Mechanics, TA (Fall '14)

Undergraduate

Advanced Engineering Mechanics, TA (Spring '15)

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DEDICATED TO MY GRANDMOTHER

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Chapter 1

Introduction

Designing materials that have both strength and toughness is desirable for many industries and purposes, including structural, automotive, and aerospace technology. However, in most structural materials, such as steels and aluminum alloys, it is found that as strength increases, toughness decreases [1]. Naturally occurring composites, or *structural biomaterials* (SBs), such as nacre, conch shells, and bone, are predominantly comprised of brittle materials such as calcium carbonate and silica but show both superior strength and toughness when compared to their brittle constituents [1,2,11,19–21]. This class of materials can serve as a template to guide the engineering of materials with superior mechanical properties. Understanding the fundamental mechanisms that enhance strength and toughness in SBs is key to achieving this goal.

1.1 Structural biomaterials are model materials to design for high toughness

Most SBs are heterogeneous in nature and consist of a mineral (stiff) phase and an organic (compliant) phase. Nacre is one such SB, in which the mineral phase occupies more than 95% of the volume fraction of the material [20]. The bulk properties of nacre, which can be described by measurements of tensile strength, Young's modulus, and Poisson's ratio, are almost identical to

aragonite (CaCO_3). This is because over 95% of the volume fraction of nacre is comprised of aragonite. Although similar in strength, however, the two materials differ in toughness. The work of fracture of nacre is about 1500 J/m^2 , while in aragonite it measures 10 J/m^2 [19]. The area under the load-displacement response divided by two times the nominal crack area is called the *work of fracture* [22]. The nominal crack area is determined by subtracting the notch length from the width of the sample and multiplying the result by the thickness of the sample. This disparity in toughness makes SBs an ideal template to engineer materials with high toughness and strength. This can be achieved by understanding the operating fracture mechanisms in SBs that lead to high toughness.

The micro-architectural arrangement of phases vary in different SBs, although the organic phase is predominantly present at the interfaces. An example of such an SB is nacre. The micro-architecture of nacre resembles a brick-and-mortar type architecture as seen in Figure 1.1(A), in which the brick and mortar represent the mineral phase and organic phase, respectively. However, in other SBs, such as spicules, some of the organic phase is also mixed with the mineral phase [23–25]. The micro-architecture of spicules resemble that of a lamellar structure, as seen in Figure 1.1(B), where the mineral phase is arranged concentrically and is separated by a nanometer-thin layer ($\approx 35 \text{ nm}$ [26]) of the organic phase. Attempts to replicate these micro-architectural designs have been quite promising. As shown in Figure 1.1(C), an alumina-based composite mimicking the micro-architecture of nacre shows higher peak stress and a greater area under the stress-strain curve when subjected to notched three point bending experiments. The work of fracture is a measure of fracture toughness in materials. It can be clearly seen from Figure 1.1(C) that the alumina-based composite has greater strength and toughness than nacre. The superior toughness properties of SBs, such as bone and nacre, are summarized in Figure 1.1(D). From the figure, we see that bone and nacre display higher toughness than their respective mineral and organic phases alone. Furthermore, the alumina-based composite has higher fracture toughness than the SBs. Therefore, a comprehensive understanding of fracture mechanisms in SBs can help to optimize the micro-architecture for maximum toughness.

It has been postulated that higher toughness in SBs can be attributed to fracture mechanisms such as crack deflection and crack arrest, which are seen in Figure 1.1(B) [2, 20]. However, insights

into the underlying toughening mechanisms are not adequately studied. These include the interactions between fracture mechanisms at different length scales and the operating extrinsic toughening mechanisms, such as crack deflection and crack arrest (see Figure 1.1(B)). Furthermore, the effect of parameters such as the thickness of the interface, the toughness of the phases, and the arrangement of the phases and how they impact the overall toughness of the SBs is still unexplored. Thus, I believe that computational models capable of modeling such complex architectural designs can be used to conduct virtual experiments which can aid in engineering synthetic materials with both high strength and toughness.

1.2 Fracture studies in heterogeneous materials

In recent years, researchers have performed experimental and analytic studies to explore mechanisms that increase toughness in ceramic composites [9, 27, 28]. Enhancing toughness through crack trapping and crack bridging has been studied [29–32], as well as enhancing toughness by varying the elastic moduli in heterogeneous materials through perturbation methods [33]. Studies in semi-infinite geometries, predominantly using semi-analytic methods, have investigated the toughness of interfaces in bi-materials [7, 34–37]. Many of the existing mechanics models used to explain toughness in SBs rely on the set of toughening mechanisms originally presented by Evans [38]. These mechanisms, such as micro cracking, fiber bridging, and fiber pull-out, were first used to understand the origins of toughness in early generations of fiber-reinforced composites. Similarly, the shear-lag model originally developed to describe the mechanism of force transmission in fiber reinforced composites [39] has also been used to explain the mechanical behavior of SBs [40, 41]. However, models based on these mechanisms fail to quantitatively capture the enhanced toughness observed in SBs [20, 42–44]. This is because these models do not consider the evolution of complex crack networks and the interaction of the cracks with the 3D interfaces.

Numerical methods such as cohesive zone models (CZM) have been used to study how toughness can be enhanced in materials with interfaces [45, 46]. These studies are limited by the fact that cracks can only extend in pre-defined paths, and thus crack jumps cannot occur. Therefore, instabilities such as crack jumps from the interface to the bulk material cannot be simulated. Begley

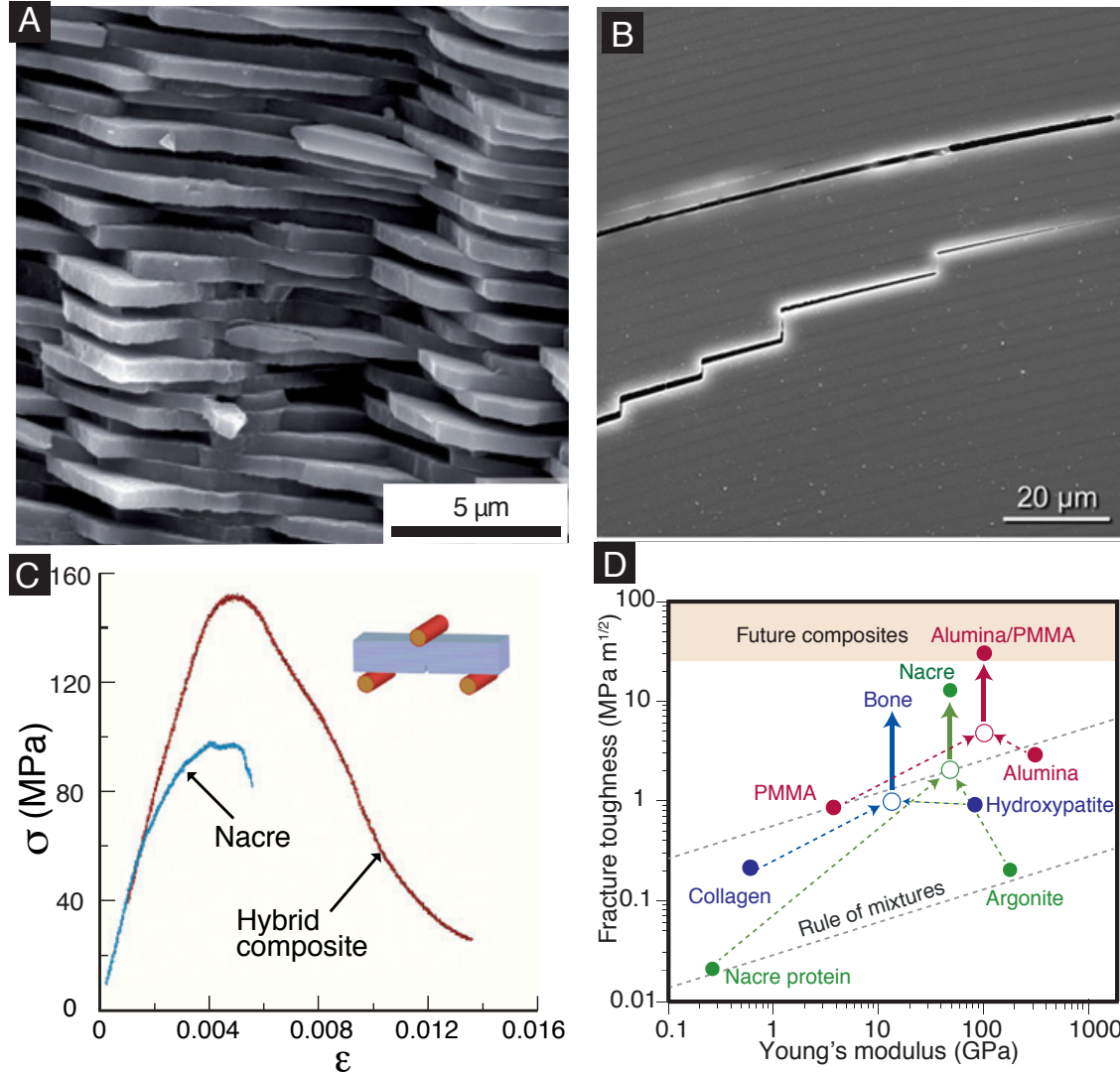


Figure 1.1: (A) SEM micrograph of nacre showing the brick-and-mortar micro-architecture [1]. (B) SEM micrograph of *Monorhaphis chuni* (*M.chuni*) specimen subjected to a three-point bending test. It can be seen that the specimen fails through crack deflection at the interfaces [2]. (C) The stress-strain response of nacre and a synthetic composite made of 75% alumina. The synthetic composites have both higher peak stress and a greater area under the stress-strain curve as compared to nacre. This indicates that the synthetic composite has both higher strength and toughness as compared to nacre [1]. (D) A comparison between the toughness of structural biomaterials and their respective constituents [3].

et al. [47, 48] were able to develop a large-scale simulation of brick-and-mortar micro-architecture using rigid bricks and cohesive interfaces. The problem was solved using Monte Carlo methods by prescribing displacements to the bricks and iteratively solving it until a configuration with minimum energy was achieved. The most promising approach lately has been that of Hossain et al. [49], where

simulations based on regularized variational fracture theory (RVFT) were performed to define the effective toughness of the material in the presence of elastic heterogeneities (i.e. heterogeneity in toughness and heterogeneity in the elastic properties). The focus of Hossain et al.'s study pertained to evaluating effective toughness in multi-layered solids, with an alternating arrangement of stiff and compliant materials subjected to Mode-I loading. However, the study does not present a perspective on how the effective toughness changes when the thickness of the interface (compliant material) is orders of magnitude smaller than that of the bulk material (stiff material), akin to that seen in SBs.

1.3 Overview of potential computational fracture methods to model SBs

A robust and accurate computational tool is necessary to model the evolution of complex crack patterns in SBs. The crack patterns are quite complicated for traditional fracture mechanics methods to evaluate, such as cohesive zone models [50, 51], extended finite element methods (XFEM) [52], and the singularity element method [53, 54]. Some of these methods use a stress-based approach of fracture, where the singular stress field given by Williams is incorporated to model cracks. These approaches run into numerical difficulties due to singularities in the stress field. Additional concerns about the efficacy of traditional methods are mesh sensitivity [55, 56], ill-conditioning [57, 58], apriori knowledge of crack paths [56], and complex crack topologies (such as crack branching, merging, or jumping across the interface). In the last few years, models based on RVFT have been used to study brittle fracture, and in this method, cracks are allowed to evolve such that the total energy of the system is minimized. Cracks are modeled using a scalar valued damage field, and, unlike the standard fracture methods, this theory is devoid of stress singularities. The ability to model and track complex crack topologies, such as crack branching or crack jumping across heterogeneities, has been demonstrated [49, 59, 60]. Therefore, these advantages make RVFT-based numerical simulations the most suitable to model SBs.

Even with state-of-the-art computational fracture mechanics techniques, it is challenging to accurately simulate the evolution of complex crack patterns in SBs and SB-inspired composites. I have reviewed the most widely used computational fracture mechanics techniques to determine

the advantages and disadvantages of each technique. The different techniques are evaluated using five criteria that are critical to accurately model SB's (see Table 1.1). It can be seen that none of the computational techniques satisfy all the criteria. The generalized CZM, XFEM and the RVFT came closest to satisfying the criteria, but none satisfy all five. For example, the generalized CZM cannot accurately reproduce experimentally observed crack paths [61–63]. Furthermore, the crack paths predicted by CZM are highly sensitive to the mesh. The XFEM cannot independently handle topology changes during the evolution of crack patterns. That is, it cannot capture phenomena such as the merging of two (or more) cracks to form a single crack (Figure 1.2(B)), the splitting of a crack into two (or more) daughter branches (Figure 1.2(A)), or the nucleation of new cracks (Figure 1.2(C)). Computational expense is the main drawback of RVFT because to accurately simulate crack growth, the mesh size in the calculations must be very small compared to the dimensions of the geometry.

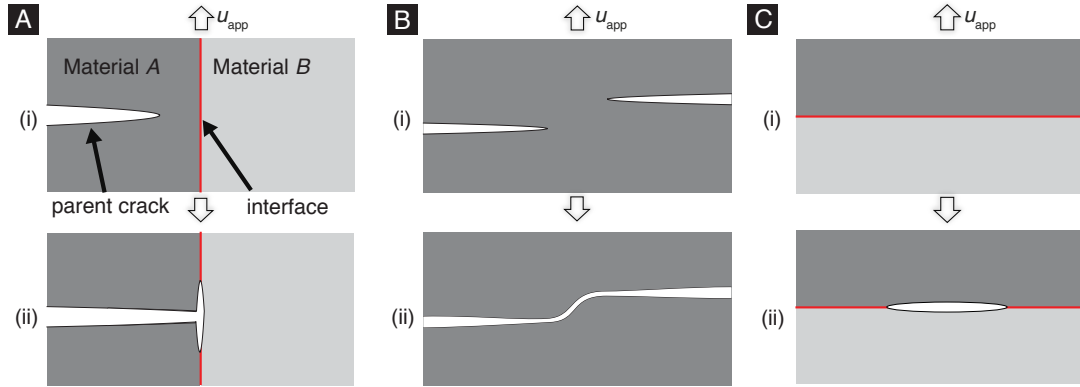


Figure 1.2: Examples of crack topology changes. (A) A single crack impinging on an interface (red) and branching into two cracks. (B) Two cracks propagating and merging to form a single crack. (C) The nucleation or formation of a new crack at an interface (red).

1.4 Objectives and organization of the dissertation

In this dissertation, I have developed a computational fracture mechanics tool based on RVFT to predict crack patterns and understand the underlying fracture mechanisms in SBs. Chapter 2 of this thesis provides an overview of the regularized variational fracture theory for brittle fracture. The finite element implementation of RVFT is benchmarked against analytical solutions and experiments.

Table 1.1: A comparison of different computational fracture mechanics methods.

CZ method (Hillerborg <i>et al.</i>)	Generalized CZ method (Xu and Needleman)	Damage mechanics	Element Deletion	XFEM	RVFT
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1. Capable of capturing topology changes independently, i.e., without a priori knowledge of crack path(s), user input, or resorting to ad-hoc or heuristic techniques.

No [64]	Yes [50, 61]	Yes [65]	Yes	No [66, 67]	Yes [68]
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2. Good accuracy. Able to quantitatively reproduce experimental observations of crack growth and the evolution of a crack network as long as there are no topology changes in the network.

does not apply	No [61–63]	No	No [56]	competitive	competitive
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3. Well conditioned, i.e., no problems with numerical stability.

Yes	Yes	No	Yes	No [69]	Yes [65]
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4. Mesh independence.

No	No [61, 62]	No [70]	No [71]	Yes [72]	Yes [68, 73, 74]
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5. Computationally affordable.

Yes	Yes	No	Yes	Yes	No
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In Chapter 3, RVFT is modified to introduce interfaces by spatially varying the fracture toughness such that it is g_I in the interface region and g_b in the bulk solid. The width of the interface region scales with the regularization parameter ℓ of RVFT such that as $\ell \rightarrow 0$, the width of the interface goes to 0. The interface toughness g_{int} is derived in the limit of $\ell \rightarrow 0$. The modified RVFT model for interfaces is applied to study two dimensional and three dimensional analogues of SBs in Chapter 4. The simulations shed light into the toughness enhancement mechanisms in SBs. In Chapter 5, SB-like composites are designed using polymethyl methacrylate (PMMA) as the base material with glue occupying the interface region. The work of fracture of the composites are found to be an order of magnitude higher than monolithic PMMA under three-point bending loading conditions. The salient conclusions from the thesis work and future directions are detailed in Chapter 6.

Chapter 2

Variational fracture model for brittle materials

2.1 Introduction

The concept of fracture toughness in elastic, brittle materials stems from the seminal work of Griffith [75], which is based on the minimization of total free energy with respect to an infinitesimal increase in crack length. This led to the postulate of crack growth by Griffith, where the crack is assumed to advance when the energy release rate at the crack tip is greater than or equal to the fracture toughness of the material. In Griffith's theory, crack growth is proposed in the form of an energy-based concept, and it is devoid of singularities (unlike the stress-based approach to fracture mechanics). Thus, a computational tool based on the Griffith theory would be ideal to study crack growth.

A computational tool based on Griffith theory would necessitate modeling a discontinuous crack surface and tracking the evolution of the crack surface based on a crack growth criterion. Several techniques such as XFEM ([66,76]), virtual crack closure technique [77], and partition of unity [78] have been proposed. However, tracking the evolution of complex crack surfaces is a difficult task. In the last few years, numerical models that approximate crack surfaces using damage or phase-field parameters have been developed. The evolution of the damage variable comes from the solution of a

coupled pde. Therefore, individually tracking crack paths is not necessary as the spatial distribution of the damage variable will represent the crack path. Additionally, phenomena such as the branching of cracks or merging of cracks can be conveniently dealt with, since the evolution of cracks in these models is a part of the solution from the coupled pde. A class of models based on Ginzburg-Landau phase-field equations have been used to study dynamic fracture and crack kinking [79,80]. Another class of models developed by Francfort, Marigo and Bourdin [74,81] are based on a generalization of Griffith criterion and are called the variational fracture models. In this thesis, we adopt the latter methodology because a model based on Griffith theory is relevant for engineering and structural applications.

2.2 Variational fracture theory

To predict crack patterns, a robust theoretical framework is required that combines Griffith's theory with a criterion for crack growth direction. Variational fracture theory (VFT), introduced by Francfort and Marigo [82], is a generalization of Griffith's theory that is utilized to predict crack patterns. VFT postulates that on the application of a load, crack growth occurs when the energy release rate is greater than or equal to the fracture toughness of the material, and crack patterns evolve such that the total energy of the system is minimized. In the absence of body forces, the total energy E is written as the sum of the elastic strain energy and surface energy,

$$E[\mathbf{u}, \Gamma] = \int_{\mathcal{B} \setminus \Gamma} \Psi_0(\mathbf{X}, \mathbf{u}) \, d\Omega + \int_{\Gamma} g_c \, d\Gamma. \quad (2.1)$$

In this equation, the surface energy is $\int_{\Gamma} g_c \, d\Gamma$, Γ is the crack set, and g_c is the fracture toughness. The elastic strain energy is given by $\int_{\mathcal{B} \setminus \Gamma} \Psi_0(\mathbf{X}, \mathbf{u}) \, d\Omega$, where Ψ_0 is the strain energy density, $\mathbf{X}$ is the material point in the solid $\mathcal{B}$, and $\mathbf{u}$ is the displacement field. The crack set Γ and the displacement fields $\mathbf{u}$ evolve such that E is minimized. It should be noted that the surface integral is 2D (resp. 1D) and the strain energy functional is 3D (resp. 2D), thus, making it difficult to solve the variational problem numerically. To circumvent this issue, Bourdin et al. [83] introduced the regularized variational fracture theory (RVFT) and a version of RVFT given by [59] is given here,

where the regularized energy functional

$$E_\ell[\mathbf{u}, d] = \int_{\mathcal{B}} \Psi_d(\mathbf{X}, \mathbf{u}, d) d\Omega + \int_{\mathcal{B}} \frac{g_c}{2} \left(\frac{d(\mathbf{X})^2}{\ell} + \ell \|\nabla d(\mathbf{X})\|^2 \right) d\Omega. \quad (2.2)$$

The symbol $\|\cdot\|$ is the Euclidean 2-norm, $\nabla(\cdot)$ is the gradient operator with respect to $\mathbf{X}$, ℓ is the regularization parameter, $d(\mathbf{X})$ is the damage field which takes values between zero and one, and $\Psi_d(\mathbf{X}, \mathbf{u}, d) = (g(d) + k) \Psi_0(\mathbf{X}, \mathbf{u})$ is the degraded strain energy density. The function $g(d)$ is the degradation function defined as $g(d) := (1 - d)^2$. The symbol k is the residual stiffness in the system and is added to the energy functional to prevent numerical difficulties when $g(d) = 0$. The damage field $d(\mathbf{X})$ indicates the extent of damage in the material such that, at $d = 1$, the material is fully damaged (i.e., $\Psi_d = 0$ at $d = 1$) and at $d = 0$ it is undamaged. The governing pdes are obtained from the energy functional E_ℓ by minimizing it with respect to $(\mathbf{u}, d)$, and is given as

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \quad \text{in } \mathcal{B}, \quad (2.3a)$$

$$g_c \ell \nabla \cdot (\nabla d) - \frac{g_c d}{\ell} = \frac{\partial \Psi_d}{\partial d} \quad \text{in } \mathcal{B} \quad (2.3b)$$

where, $\boldsymbol{\sigma}$ is the Cauchy stress tensor that is given by $\partial \Psi_d / \partial \boldsymbol{\epsilon} = ((1 - d)^2 + k) \boldsymbol{\sigma}^0$. The symbol $\boldsymbol{\sigma}^0$ is the undamaged stress tensor. The symbol $\boldsymbol{\epsilon}$ is the elastic small strain tensor given by $1/2(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$. The boundary conditions (BCs) for the pdes given by Eqns. 2.3a and 2.3b are

$$\mathbf{u} = \hat{\mathbf{u}} \quad \text{in } \partial \mathcal{B}_u, \quad (2.4a)$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \hat{\mathbf{t}} \quad \text{in } \partial \mathcal{B}_t, \quad (2.4b)$$

$$\nabla d \cdot \mathbf{n} = 0 \quad \text{in } \partial \mathcal{B}, \quad (2.4c)$$

where $\partial \mathcal{B}$ is the boundary of the solid, $\partial \mathcal{B}_u$ is the part of the boundary $\partial \mathcal{B}$ on which displacement boundary conditions are prescribed, and $\partial \mathcal{B}_t$ is the rest of the boundary on which traction $\hat{\mathbf{t}}$ is prescribed. The symbol $\mathbf{n}$ is the outward normal vector on the boundary $\partial \mathcal{B}$. A schematic of VFT is depicted in Figure. 2.1(A), where the solid $\mathcal{B}$ is shown in blue and the crack set/surface Γ is denoted by a black curve. The solid is subjected to traction and displacement boundary conditions $\partial \mathcal{B}_t$ and $\partial \mathcal{B}_u$, respectively. The regularized version of VFT, i.e. RVFT, is shown in Figure. 2.1(B),

where the solid $\mathcal{B}$ is subjected to identical boundary conditions to that shown in Figure. 2.1(A). The scalar parameter d represents the diffused crack surface. In the limit of $\ell \rightarrow 0$ the diffused crack surface in Figure. 2.1(B) converges to the zero-thickness crack surface Γ shown in Figure. 2.1(A). (See Γ –convergence results in [81, 84, 85] for the proof.)

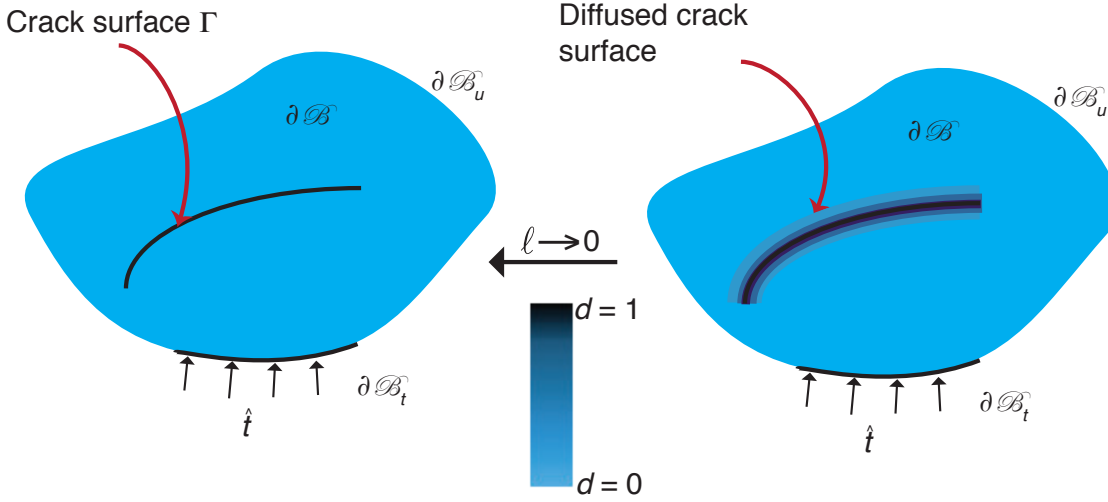


Figure 2.1: (A) A schematic of a solid, denoted by $\mathcal{B}$, with a zero thickness crack surface Γ . The solid is subjected to traction boundary conditions $\hat{t}$ on the boundary $\partial \mathcal{B}_t$ and displacement boundary conditions on the boundary $\partial \mathcal{B}_u$. (B) The solid $\mathcal{B}$ is subjected to identical boundary conditions as those shown in (A). However, the zero-thickness crack surface is approximated by a diffused crack surface represented by the scalar variable d . The scalar variable $d = 1$ and $d = 0$ indicates that the solid is fully damaged and completely intact, respectively. Additionally, as the regularization parameter $\ell \rightarrow 0$, the diffused crack surface converges to the crack surface Γ .

2.3 Analytical solutions to RVFT in one dimension

The governing pdes given in Eq. 2.3a-2.3b for RVFT are very difficult to solve analytically in two dimensions (2D) and three dimensions (3D). However, analytical solutions in one dimension (1D) can give insights into several important features of the pdes, such as the functional form of d and the theoretical strength of the solid.

2.3.1 1D solution to the damage field

The functional form for the damage field d can be solved analytically in a 1D setting. The functional form of the damage field that approximates a sharp crack can be useful in quantifying the role of the regularization parameter ℓ in the decay of d away from the crack surface. Consider a 1D domain $\mathcal{B} = \{L : L \in (-\infty, \infty)\}$, in which x is a spatial point in $\mathcal{B}$. Let us introduce a crack at $x = 0$, assuming that the elastic fields are absent. The governing differential equation (Eq. 2.3b) reduces to

$$\ell \frac{\partial^2 d(x)}{\partial x^2} - \frac{d(x)}{\ell} = 0, \quad (2.5)$$

where $d(0) = 1$. The solution to the differential equation is

$$d(x) = e^{-|x|/\ell}, \quad (2.6)$$

where the symbol $|\cdot|$ denotes the absolute value or the positive value. The solution $d(x)$ is plotted w.r.t to x in Figure 2.2. It can be seen from the figure that $d(0) = 1$, indicating the presence of a crack. The damage function decays exponentially and as the value of regularization parameter ℓ reduces, the diffused crack region is confined to a small zone. The width of the diffused crack region can be estimated to be roughly of the order of ℓ .

2.3.2 Theoretical strength of the solid from RVFT

In linear elastic fracture mechanics theory, there are several models that give an estimate of the theoretical strength of the solid based on the atomic view of fracture [86]. For example, in one such model, the force-displacement relationship between atoms is assumed to vary sinusoidally and the theoretical strength σ_{th} is estimated to be $0.707(Eg_c/x_0)$ [86]. The symbol E is the Young's modulus of the solid and x_0 is the equilibrium distance between the atoms. Is it possible to quantify the theoretical strength of a solid from RVFT?

Consider a straight bar of length a and Young's modulus E with fracture toughness g_c lying along the $\hat{e}_x$ direction. The end $x = 0$ is fixed and the right end of the bar is subject to an tensile

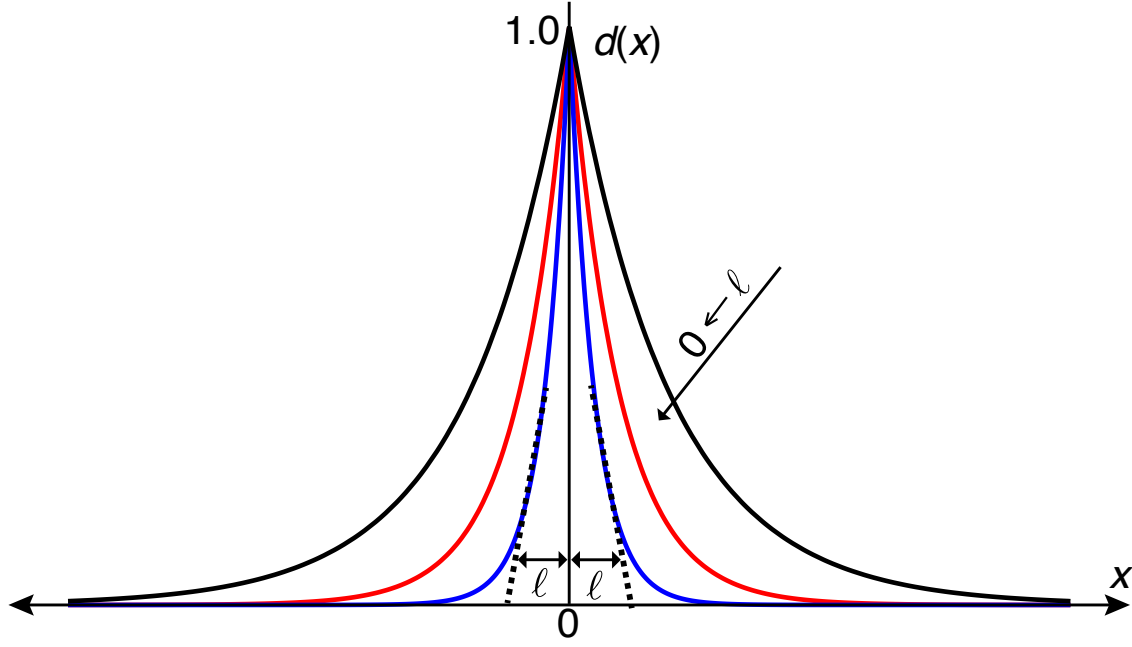


Figure 2.2: The 1D solution to the damage variable d for different values of ℓ is plotted in an infinite bar with the crack located at $x = 0$.

axial force $\sigma_{\text{app}}A$, where $\sigma_{\text{app}} \in \mathbb{R}^+$, and A is the cross-sectional area of the bar. The bar's cross-sections are normal to the direction $\hat{e}_x$ and only axial deformation of the bar is considered. The axial displacement of the bar is represented by the field $u : [0, a] \rightarrow \mathbb{R}$. The axial component of the stress $e_x \cdot \sigma e_x$, where σ is the Cauchy stress tensor, is denoted as σ_{xx} . For this 1D case, the governing equations of RVFT are

$$\frac{d\sigma_{xx}}{dx} = 0, \quad (2.7)$$

$$g_c \ell d_{,xx} - \frac{g_c d}{\ell} + 2(1-d)\Psi_0(u) = 0, \quad \forall x \in \mathcal{B}, \quad (2.8)$$

where $\sigma_{xx} = (1-d)^2 E u_{,x}$, the domain $\mathcal{B} = (0, a)$ is the undeformed configuration of the bar, and $\Psi_0(u) = E u_{,x}^2 / 2$ is the strain energy density. The boundary conditions are $u = 0$ at $x = 0$, $d_{,x} = 0$ at $x = 0$ and a , and $\sigma_{xx} = \sigma_{\text{app}}$ at $x = a$. The symbols $(\cdot)_{,xx} = d^2(\cdot)/dx^2$ and $(\cdot)_{,x} = d(\cdot)/dx$. Solving Eq. 2.7 along with the boundary conditions on σ_{xx} , we find that σ_{xx} in the bar is a constant and is equal to σ_{app} ,

$$u_{,x} = \frac{\sigma_{\text{app}}}{E(1-d)^2}, \quad (2.9)$$

and

$$\Psi_0(u) = \frac{\sigma_{\text{app}}^2}{2E(1-d)^4}. \quad (2.10)$$

Substituting Eq. 2.9–2.10 into Eq. 2.8 we find that

$$g_c \ell d_{,xx} - \frac{g_c d}{\ell} + \frac{\sigma_{\text{app}}^2}{E(1-d)^3} = 0, \quad \forall x \in \mathcal{B}. \quad (2.11)$$

Introducing non-dimensional variables $\xi = x/a$, $\alpha = a/\ell$, and $\beta = \sigma_{\text{app}}/\sigma_0$, where $\sigma_0 = (Eg_c/\ell)^{1/2}$.

Therefore, Eq. 2.11 can be rewritten as

$$\varphi_{,\xi\xi} - \alpha^2 \varphi + \frac{\beta^2 \alpha^2}{(1-\varphi)^3} = 0, \quad \forall \xi \in \Omega, \quad (2.12)$$

where $\Omega = (0, 1)$, $\varphi(\xi) = d \circ x(\xi)$, and $x(\xi) = a\xi$. The boundary conditions on φ are $\varphi_{,\xi} = 0$ at $\xi = 0, 1$. The parameter β is the measure of the loading in comparison to the theoretical strength of the solid.

It is difficult to solve for the closed form solution to the non-linear ordinary differential equation (ODE) in Eq. 2.12. Let us consider the homogeneous case, i.e. when $\varphi(\xi)$ is a constant over Ω . In this case, the ODE reduces to

$$\varphi(1-\varphi)^3 = \beta^2. \quad (2.13)$$

The maximum value for the function $\varphi(1-\varphi)^3$ is 27/256 and it occurs when $\varphi = 1/4$. Therefore, the maximum value of β is denoted by $\beta_c = 3\sqrt{3}/16$. From the definition of β , the theoretical strength of the solid $\sigma_{th} = 0.324(Eg_c/\ell)^{1/2}$. For the homogeneous solution, a non-dimensional stress-strain relation can be established by non-dimensionalizing Eq. 2.9 as

$$\tilde{\varepsilon} = \frac{\beta}{(1-\varphi)^2}, \quad (2.14)$$

where $\tilde{\varepsilon} = u_{,x}/\varepsilon_0$. The parameter $\varepsilon_0 = \sigma_0/E$ is the intrinsic strain parameter. Using Eqns. 2.14 and

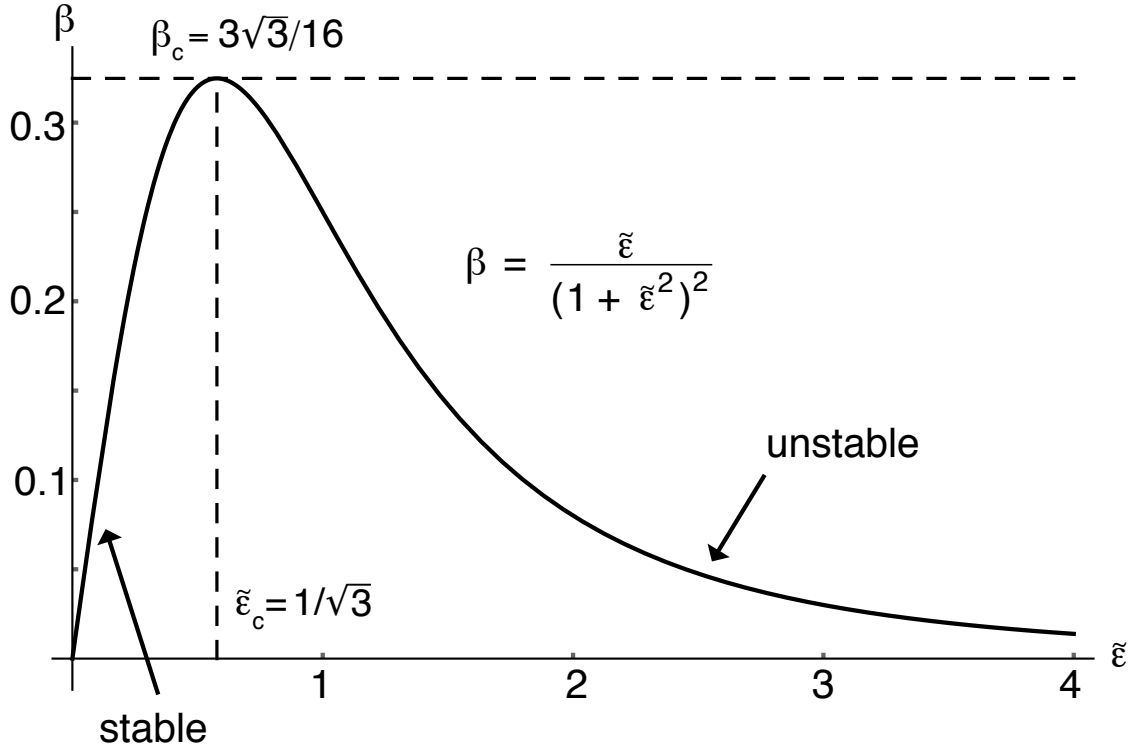


Figure 2.3: The non-dimensional force, β , as a function of the strain $\tilde{\epsilon}$. The horizontal and the vertical dashed lines mark the critical stress and strain β_c and $\tilde{\epsilon}_c$, respectively. The solid black line is the stress-strain response, Eq. 2.15, when it is assumed that the plausible damaged state is always homogeneous.

2.12, φ is eliminated to obtain a relationship between β and $\tilde{\epsilon}$ to be

$$\beta = \frac{\tilde{\epsilon}}{(1 + \tilde{\epsilon}^2)^2}. \quad (2.15)$$

The dimensional form of 2.15 is derived in [60]. The homogeneous response for the non-dimensional stress β vs. strain $\tilde{\epsilon}$ is shown in Figure 2.3. The critical strain $\tilde{\epsilon}_c = 1/\sqrt{3}$ is the strain at which the theoretical strength is achieved. It has been shown by Bourdin et al. [81] that the unloading branch, i.e., the stress-strain response $\tilde{\epsilon} > \tilde{\epsilon}_c$, is unstable. Therefore, once the solid reaches the theoretical strength it will form a localized damage and fail.

2.4 Modification to RVFT for predictive fracture modeling

There are two important characteristics of RVFT that need to be modified so that it is a good predictive tool for fracture mechanics problems:

1. *Irreversibility*: The damage field should be constrained such that $d_{n+1} \geq d_n$, where n denotes the load step, because crack growth is an irreversible process; and
2. *Preventing damage under compressive loads*: The damage field can evolve under both tensile or compressive states of stress, since its evolution is governed by $\Psi_0(\mathbf{u})$ (see Eq. 2.3b). Therefore, the governing equations should be suitably modified to ensure that damage occurs only in the state of tension.

2.4.1 Irreversibility constraint

Crack growth is an irreversible process. Cracks that form as a result of external loading cannot vanish once the applied loads are removed. From the governing equations of the damage variable d (see Eq. 2.3b), the evolution of d depends on $\partial\Psi_d/\partial d = -2(1-d)\Psi_0$. Therefore, when Ψ_0 reduces locally in the geometry, then d also reduces, leading to crack healing. One strategy proposed by Bourdin et al. is to enforce the constraint that $d_{n+1} > d_n$ while numerically solving the governing equations, where n is the load step number. Another strategy proposed by Miehe et al. (see [87]) is to introduce a history variable $\mathcal{H}(\mathbf{X}, n)$, defined as

$$\mathcal{H}(\mathbf{X}, n) := \max_{s \in [0, n]} \Psi_0(\epsilon(\mathbf{X}, s)), \quad (2.16)$$

where n indicates the load step number. On replacing the strain energy density with $\mathcal{H}$ in Eq. 2.3b, we get

$$g_c \ell \nabla \cdot (\nabla d) - \frac{g_c d}{\ell} = -2(1-d)\mathcal{H} \quad \text{in } \mathcal{B}. \quad (2.17)$$

An alternative strategy to enforce the irreversibility constraint is to obtain the values of the damage variable at every node from the finite element calculations. The value of the damage variable

at load step $n + 1$ is compared to the corresponding value of the damage variable at load step n . If $d_{n+1} < d_n$ at a node, then that nodal value is replaced with d_n . The solution for d is then iterated until convergence is achieved. This will be explained further in the numerical procedure of the thesis (see section 2.7).

2.4.2 Tension-compression split

It is well understood from fundamental fracture mechanics theory that only local tensile stresses acting on the crack faces can lead to crack opening and crack growth. Conversely, local compressive stresses that act on the crack faces lead to crack closure. However, according to VFT or RVFT, crack growth can occur when the crack faces are subjected to local compressive stress, which is nonphysical. In RVFT, the evolution of the damage variable d is dependent on the strain energy density Ψ_0 or the history variable $\mathcal{H}$. Therefore, d will evolve to form cracks even if the stress state is entirely compressive in the material. Several strategies have been proposed in literature to tackle this problem (see [87–90]). Some of the strategies are explained in the following subsections.

Amor et al.'s strategy to prevent crack growth under compression

The strategy proposed by Amor et al. [88] comprises of splitting the strain energy density such that the tensile volumetric and the deviatoric elements of the strain energy density are subjected to damage while the compressive element of the volumetric strain energy density remains undamaged. The modified form of the degraded strain energy density Ψ_d is

$$\Psi_d = g(d) \left(\frac{\kappa}{2} \langle \text{tr}(\epsilon) \rangle^2 + \mu \epsilon^{dev} : \epsilon^{dev} \right) + \frac{\kappa}{2} ((\text{tr}(\epsilon) - \langle \text{tr}(\epsilon) \rangle))^2, \quad (2.18)$$

where $\langle \cdot \rangle$ is defined as

$$\langle x \rangle = \begin{cases} 0, & x < 0, \\ x, & x \geq 0. \end{cases} \quad (2.19)$$

The symbols κ and μ are the bulk and shear modulus, respectively. The symbol $\text{tr}(\cdot)$ is the trace operator defined as $\text{tr}(\epsilon) := \epsilon_{11} + \epsilon_{22} + \epsilon_{33}$. The symbol ϵ^{dev} is the deviatoric part of the strain energy defined as $\epsilon^{dev} := \epsilon - (1/3)\text{tr}(\epsilon)\mathbf{I}$, where $\mathbf{I}$ is the identity tensor (see [91]). The primary drawback

of this strategy is that it fails to predict the crack path in single edge notched geometries subjected to three-point bending loading conditions.

Miehe et al.'s tension-compression split

Similar to Amor et al., Miehe et al. [87] proposed a strategy to split the strain energy into two parts, one constructed using the positive eigenvalues of the strain tensor ϵ and the other using the negative eigenvalues of ϵ . The degradation function $g(d)$ only degrades the strain energy composed of positive eigenvalues of ϵ , while the negative strain energy remains unaffected. The modified form of the degraded strain energy density Ψ_d is

$$\Psi_d(\epsilon, d) = g(d)\Psi_0^+(\epsilon) + \Psi_0^-(\epsilon), \quad (2.20)$$

where

$$\Psi_0^+(\epsilon) = \frac{1}{2}\lambda \langle \text{tr}(\epsilon) \rangle^2 + \mu \epsilon^+ : \epsilon^+ \quad \text{and}, \quad (2.21a)$$

$$\Psi_0^-(\epsilon) = \frac{1}{2}\lambda (\text{tr}(\epsilon) - \langle \text{tr}(\epsilon) \rangle)^2 + \mu \epsilon^- : \epsilon^-, \quad (2.21b)$$

respectively. The symbol λ is the Lamé parameter and is equal to $\kappa - (2/3)\mu$. The strain ϵ is split into ϵ^+ and ϵ^- , which can be defined as:

$$\epsilon^+ = P\Lambda^+P^T \quad (2.22a)$$

$$\epsilon^- = P\Lambda^-P^T \quad (2.22b)$$

where Λ^+ is a diagonal square matrix with the positive eigenvalues of ϵ (i.e., $(\langle \Lambda_1 \rangle, \langle \Lambda_2 \rangle, \langle \Lambda_3 \rangle)$). The symbol P is a matrix of the corresponding eigenvectors arranged column wise. I have incorporated this strategy in the 2D version of the finite element implementation of RVFT. The primary drawback of this strategy is that the strain energy density becomes non-linear under certain loading conditions due to the introduction of the energy density split, which leads to convergence problems.

Gershgorin circle theorem based strategy

In this work, I have implemented a new strategy to prevent crack growth under compression. I have implemented this strategy for 3D simulations for geometries subjected to three-point bending loading. We obtain the bounds on the eigenvalues of the undamaged stress tensor $\boldsymbol{\sigma}^0$ ($\partial\Psi_0/\partial\epsilon$) using the Gershgorin circle theorem [92]. The theorem is applied to the stress tensor $\boldsymbol{\sigma}^0$ (a 3-by-3 square matrix) which can be used to construct the Gershgorin discs $D_i(\sigma_{ii}^0, R_i)$, where $R_i = \sum_{j \neq i} |\sigma_{ij}^0|$. The indices $i = \{1, 2, 3\}$ and $j = \{1, 2, 3\}$. The theorem states that every eigenvalue of $\boldsymbol{\sigma}^0$ lies within at least one of these discs. Therefore, we use this information to compute a lower bound on the eigenvalues of $\boldsymbol{\sigma}^0$. The lower bound on the eigenvalues denoted as $\lambda_{\min}$ is given as

$$\lambda_{\min} = \min (\sigma_{ii}^0 - R_i). \quad (2.23)$$

We modify the damage part of the pde, i.e. Eq. 2.3b as follows:

$$g_c \ell \nabla \cdot (\nabla d) - \frac{g_c d}{\ell} = -2(1-d)\Psi_0 H(\lambda_{\min}) \quad \text{in } \mathcal{B}, \quad (2.24)$$

where $H(\cdot)$ is the Heaviside function. Introducing the Heaviside function on $\lambda_{\min}$ in the above equation ensures that the damage field d does not evolve in the region where the smallest eigenvalue of $\boldsymbol{\sigma}^0$ is negative. This strategy is conservative because damage evolution should be governed by the local stress state resolved with respect to the orientation of the crack tip. Furthermore, only local traction vectors normal to the crack faces drive the crack growth process. The principal stress vectors may or may not be aligned with the orientation of the crack tip. Therefore, crack growth can occur in scenarios where some of the stress components are negative, which are precluded from using this strategy.

2.5 Artificial viscosity for numerical convergence

Crack growth in RVFT occurs when the damage variable $d = 1$ and is sometimes accompanied by a large spatial region in the domain simultaneously reaching the value of $d = 1$. This process

destabilizes the system of equations while solving the governing equations given in Eqns. 2.3a-2.3b. A simple strategy to overcome the convergence problem is provided by Gao and Bower [93], where they introduced a viscosity parameter to stabilize the system of equations. As long as the viscosity parameter is sufficiently small, the solution to the pde remains almost unaffected. A similar formulation is incorporated by Miehe et al. [87], where artificial viscosity $\bar{\eta}$ is introduced into Eq. 2.24 as follows:

$$g_c \ell \nabla \cdot (\nabla d) - \frac{g_c d}{\ell} + \bar{\eta} \dot{d} = -2(1-d)\Psi_0 \quad \text{in } \mathcal{B}, \quad (2.25)$$

where $\dot{d} = (d_{n+1} - d_n)/\Delta t$. The symbol n is the load step number and Δt is the fictitious time increment for the load step to go from n to $n+1$.

2.6 Finite element implementation

The energy functional given in Eq. 2.2 is discretized using the finite element method [94, 95]. The weak form for the functional is obtained by multiplying the governing equations given by Eq. 2.3a and Eq. 2.3b with test functions $\boldsymbol{\eta}(\mathbf{X})$ and $\beta(\mathbf{X})$, respectively. The test functions $\boldsymbol{\eta}(\mathbf{X})$ and $\beta(\mathbf{X})$ are zero on $\partial\mathcal{B}_u$ and $\partial\mathcal{B}$, respectively. The weak form of the governing equations is given as

$$\int_{\mathcal{B}} \boldsymbol{\sigma} : \nabla \boldsymbol{\eta} \, d\Omega = \int_{\partial\mathcal{B}_t} \hat{\mathbf{t}} \cdot \boldsymbol{\eta} \, d\partial\Omega, \quad \text{and}, \quad (2.26a)$$

$$\int_{\mathcal{B}} g_c \ell \nabla d \cdot \nabla \beta \, d\Omega + \int_{\mathcal{B}} \left(\frac{g_c d}{\ell} - 2(1-d)\Psi_0 \right) \beta \, d\Omega = 0. \quad (2.26b)$$

These equations can be discretized using global shape functions [91, 95]. The displacement field $\mathbf{u}$ and damage field d can be approximated as

$$\begin{aligned} u_i(\mathbf{X}) &= \sum_{a=1}^n N^a(\mathbf{X}) u_i^a, \\ d(\mathbf{X}) &= \sum_{a=1}^n N^a(\mathbf{X}) d^a, \\ \eta_i(\mathbf{X}) &= \sum_{a=1}^n N^a(\mathbf{X}) \eta_i^a, \quad \text{and,} \\ \beta(\mathbf{X}) &= \sum_{a=1}^n N^a(\mathbf{X}) \beta^a, \end{aligned} \quad (2.27)$$

where n is the total number of nodes in the domain. The symbol $i = \{1, 2, \dots, \text{ndim}\}$, where $\text{ndim} = 2$ for 2D and $\text{ndim} = 3$ for 3D. The symbols u_i^a , d^a , η_i^a and β^a are the nodal variables. The symbol N^a denotes the interpolation function, which is a function of the spatial variable $\mathbf{X}$ in the domain $\mathcal{B}$. The interpolation function N^a must satisfy

$$u_i^b = \sum_{a=1}^n N^a(\mathbf{X}^b) u_i^a \quad (2.28)$$

for all $b \in \{1, n\}$. Additionally, the interpolation functions have partition of unity property, i.e. $\sum_{a=1}^n N^a(\mathbf{X}) = 1$ and must satisfy

$$N^a(\mathbf{X}^b) = \begin{cases} 1, & a = b, \\ 0, & a \neq b. \end{cases} \quad (2.29)$$

After substituting the nodal approximations for $\boldsymbol{\eta}$ and $\boldsymbol{\beta}$ given in Eq. 2.27 into the weak form Eq. 2.26, we obtain the following set of equations:

$$\sum_{a=1}^n \int_{\mathcal{B}} ((1-d)^2 + k) \sigma_{ij}^0 \frac{\partial N^a}{\partial X_j} \eta_i^a d\Omega = \sum_{a=1}^n \int_{\partial \mathcal{B}_t} \hat{t}_i N^a \eta_i^a d\partial\Omega \quad \text{and,} \quad (2.30)$$

$$\sum_{a=1}^n \int_{\mathcal{B}} g_c \ell \frac{\partial d}{\partial X_i} \frac{\partial N^a}{\partial X_i} \beta^a d\Omega + \int_{\mathcal{B}} \left(\frac{g_c d}{\ell} - (1-d) \mathbb{C}_{ijkl} \epsilon_{ij} \epsilon_{kl} \right) N^a \beta^a d\Omega = 0, \quad (2.31)$$

where the summation of indices i, j, k, l is implied, $\mathbb{C}_{ijkl}$ is the linear elasticity stiffness tensor [91] and $\sigma_{ij}^0 = \sigma_{ij}/((1-d)^2 + k)$. These equations are satisfied for arbitrary values of the nodal coefficients η_i^a and β^a which can be dropped from the equations. The residual vector is obtained by employing Voigt-notation [94, 96] which is denoted by an under bar:

$$\{R^a\} = \int_{\mathcal{B}} \begin{bmatrix} ((1-d)^2 + k) [B_u^a]^T \underline{\sigma}^0 \\ g_c \ell [B_d^a]^T \underline{\nabla} d + \left[\frac{g_c}{\ell} + \underline{\varepsilon}^T \mathbb{C} \underline{\varepsilon} \right] N^a d - N^a \underline{\varepsilon}^T \mathbb{C} \underline{\varepsilon} \end{bmatrix} d\Omega \quad (2.32)$$

where the matrices $[B_u^a]$ and $[B_d^a]$ for a general 3D setting are given as

$$[B_u^a] = \begin{bmatrix} N_{,1}^a & 0 & 0 \\ 0 & N_{,2}^a & 0 \\ 0 & 0 & N_{,3}^a \\ N_{,2}^a & N_{,1}^a & 0 \\ 0 & N_{,3}^a & N_{,2}^a \\ N_{,3}^a & 0 & N_{,1}^a \end{bmatrix},$$

$$[B_d^a] = \begin{bmatrix} N_{,1}^a \\ N_{,2}^a \\ N_{,3}^a \end{bmatrix}.$$

The notation $N_{,i}^a$ denotes $\partial N^a / \partial X_i$ for $i = 1, 2, 3$. The stress tensor and the gradient of d in Voigt notation are $\underline{\sigma}^0 = \{\sigma_{11}^0, \sigma_{22}^0, \sigma_{33}^0, \sigma_{12}^0, \sigma_{32}^0, \sigma_{31}^0\}$, $\underline{\varepsilon}^0 = \{\varepsilon_{11}^0, \varepsilon_{22}^0, \varepsilon_{33}^0, \varepsilon_{12}^0, \varepsilon_{32}^0, \varepsilon_{31}^0\}$ and $\underline{\nabla} d = \sum_{a=1}^n [B_d^a] d^a$, respectively. The strain $\underline{\varepsilon}$ is given by, $\underline{\varepsilon} = \sum_{a=1}^n [B_u^a] u^a$. After substituting the approximation for the displacement and damage fields from Eq. 2.27 into the residual form, we can evaluate the global stiffness matrix to be

$$[K^{ab}] = \int_{\mathcal{B}} \begin{bmatrix} ((1-d)^2 + k) [B_u^a]^T [D] [B_u^b] & -2(1-d) [B_u^a]^T \underline{\sigma}^0 N^b \\ -2(1-d) [B_u^a]^T \underline{\sigma}^0 N^b & g_c \ell [B_d^a]^T [B_d^b] + \left[\frac{g_c}{\ell} + \underline{\varepsilon}^T \mathbb{C} \underline{\varepsilon} \right] N^a N^b \end{bmatrix} d\Omega,$$

where summation over b is implied and $\underline{D}$ is the elasticity tensor in Voigt notation. The global traction vector is given as

$$\{T^a\} = \int_{\partial\mathcal{B}_t} \begin{Bmatrix} N^a \hat{\mathbf{t}} \\ 0 \end{Bmatrix} d\partial\Omega. \quad (2.33)$$

The global degree of freedom vector is

$$\{U^b\} = \begin{Bmatrix} \mathbf{u}^b \\ d^b \end{Bmatrix}. \quad (2.34)$$

The global equilibrium equations can be expressed as

$$[K^{ab}]\{U^b\} = \{R^a\} + \{T^a\}, \quad (2.35)$$

where summation over a, b is implied. The global stiffness matrix K^{ab} is inverted to solve for U^b at all the nodes. From U^b , one can obtain the equilibrium displacement and damage field as given in Eq. 2.34.

2.6.1 Modification of the global stiffness matrix and residual vector to introduce tension-compression split, irreversibility, and artificial viscosity

In Sections 2.4 and 2.5, I have detailed modifications to RVFT that will ensure that this method is a predictive computational method to study fracture mechanics problems. The tension-compression split summarized in section 2.4.2 can be introduced into the formulation by first defining the Cauchy stress tensor $\boldsymbol{\sigma}$ as

$$\boldsymbol{\sigma} := [(1-d)^2 + k] \boldsymbol{\sigma}^+ + \boldsymbol{\sigma}^-, \quad (2.36)$$

where

$$\boldsymbol{\sigma}^+ = (\lambda \langle \text{tr} \boldsymbol{\epsilon} \rangle \mathbf{I} + 2\mu \boldsymbol{\epsilon}^+) \quad \text{and} \quad (2.37)$$

$$\boldsymbol{\sigma}^- = \lambda (\text{tr} \boldsymbol{\epsilon} - \langle \text{tr} \boldsymbol{\epsilon} \rangle) \mathbf{I} + \mu \boldsymbol{\epsilon}^-. \quad (2.38)$$

The symbol $\mathbf{I}$ is the identity tensor. Irreversibility is enforced by defining a history variable which is defined for tension-compression split as:

$$\mathcal{H}(\mathbf{X}, n) := \max_{s \in [0, n]} \Psi_0^+(\epsilon(\mathbf{X}, s)). \quad (2.39)$$

Artificial viscosity for numerical convergence is implemented by introducing the $\eta \dot{d}$ in the global stiffness matrix and $\eta \dot{d}^2/2$ in the residual vector. The residual vector is modified appropriately as

$$\{R^a\} = \int_{\mathcal{B}} \begin{bmatrix} [B_u^a]^T ((1-d)^2 + k) \underline{\sigma}^+ + \underline{\sigma}^- \\ g_c \ell [B_d^a]^T \underline{\nabla} d + \left[\frac{g_c}{\ell} + 2\mathcal{H} \right] N^a d - 2N^a \mathcal{H} + \frac{\eta}{2} \dot{d}^2 \end{bmatrix} d\Omega. \quad (2.40)$$

Similarly, the global stiffness matrix is

$$[K^{ab}] = \int_{\mathcal{B}} \begin{bmatrix} [B_u^a]^T [\underline{D}_{\text{eff}}] [B_u^a] & -2(1-d) [B_u^a]^T \underline{\sigma}^+ N^b \\ -2(1-d) [B_u^a]^T \underline{\sigma}^+ N^b & g_c \ell [B_d^a]^T [B_d^a] + \left[\frac{g_c}{\ell} + \mathcal{H} \right] N^a N^b + \eta \dot{d} \end{bmatrix} d\Omega,$$

in which $\underline{D}_{\text{eff}}$ is the effective elasticity matrix. Its derivation is given in Appendix A.

2.7 Summary of the solution procedure

In the previous section, the expression for the global stiffness matrix and the residual vector are given, for which the domain is discretized into standard isoparametric elements. Element stiffness matrices K_e^{ab} and residual vectors R_e^a are computed using standard isoparametric shape functions and Gauss integration procedures [94]. The 2D element for the coupled elasticity-damage problem is implemented using user element subroutine in Abaqus and the Newton-Raphson solver of Abaqus is used to solve the global equilibrium equations [97].

Solution procedure for the fully coupled problem

1. *Initialization:* The displacement $\mathbf{u}_n$, damage d_n and history field $\mathcal{H}_{n-1}$ are known at the time step t_n . Update boundary conditions $\hat{\mathbf{t}}_{n+1}$ and $\hat{\mathbf{u}}_{n+1}$.
2. *History field:* Compute the quantity $\Psi_0^+(\mathbf{u}_n)$ and compare that with history field $\mathcal{H}_{n-1}$ to set the history variable $\mathcal{H}_n$.

3. *Assembly*: Assemble the global stiffness matrix K^{ab} , global residual vector R^a , and global traction vector T^a .
4. *Newton-Raphson*: Solve for $\mathbf{u}_{n+1}$ and d_{n+1} using the Abaqus standard Newton-Raphson non-linear solver [94, 97]

Numerical calculations for RVFT are computationally expensive and usually take 24 – 80 hours to solve for a 2D problem. Additionally, the user element subroutine in Abaqus is not parallelizable. Thus, solving a three dimensional (3D) fracture problem using RVFT in Abaqus is challenging. Therefore, I developed a finite element (FE) formulation in Mathematica [98] to study RVFT-based fracture problems in 3D. The advantage to Mathematica is that it is highly parallelizable, which would enable a person to run calculations on 192 cores. Thus, solving 3D problems is computationally feasible. In the FE formulation that I developed for 3D, I employed a staggered solution procedure. In a staggered procedure, the displacement field $\mathbf{u}$ is solved assuming the damage variable d is constant during the solution step. Similarly, during the solution for d , the displacement is taken as a constant. Therefore, the global stiffness matrix K_u^{ab} , the residual vector R_u^a and traction vector T_u^a for the elasticity problem is:

$$[K_u^{ab}] = \int_{\mathcal{B}} ((1-d)^2 + k) [B_u^a]^T [D] [B_u^b] d\Omega, \quad (2.41)$$

$$\{R_u^a\} = \int_{\mathcal{B}} ((1-d)^2 + k) [B_u^a]^T \underline{\sigma}^0 d\Omega, \quad (2.42)$$

$$\{T_u^a\} = \int_{\partial\mathcal{B}_t} N^a \hat{\mathbf{t}} d\partial\Omega. \quad (2.43)$$

Similarly, the global stiffness matrix K_d^{ab} and the residual vector R_d^a for the damage problem is:

$$[K_d^{ab}] = \int_{\mathcal{B}} g_c \ell [B_d^a]^T [B_d^b] + \left[\frac{g_c}{\ell} + \underline{\epsilon}^T \mathbb{C} \underline{\epsilon} \right] N^a N^b d\Omega, \quad (2.44)$$

$$\{R_d^a\} = \int_{\mathcal{B}} g_c \ell [B_d^a]^T \underline{\nabla} d + \left[\frac{g_c}{\ell} + \underline{\epsilon}^T \mathbb{C} \underline{\epsilon} H(\lambda_{\min}) \right] N^a d - N^a \underline{\epsilon}^T \mathbb{C} \underline{\epsilon} H(\lambda_{\min}) d\Omega. \quad (2.45)$$

It is important to note that the history variable $\mathcal{H}$ is replaced by a Heaviside function $H(\lambda_{\min})$ and there is no longer any artificial viscosity. Similar procedure has been adopted in [74].


```

1 Initialization: The displacement  $u_n$  and damage  $d_n$  are known at the time step  $t_n$ . Update
  boundary conditions  $\hat{t}_{n+1}$  and  $\hat{u}_{n+1}$  for time  $t_{n+1}$ .
2 Let  $i = 1$ ,  $d_{i-1} = d_n$ , and  $d = d_{i-1}$ 
3 while  $i < 2$  or  $\|d_i - d_{i-1}\|_\infty \geq tol$  do
4   Solve for  $u_i$ 
5   Compute  $\Psi_0(u_i)$  and solve for the damage field  $d_i$ .
6   Replace  $d_i$  with  $\max(d_i, d_{i-1})$  to ensure irreversibility.
7   Update  $d = d_i$ 
8    $i = i + 1$ 
9 end
10  $u_{n+1} = u_i$  and  $d_{n+1} = d_i$ .

```

Algorithm 1: Staggered solution procedure

2.8 Mesh sensitivity

As previously mentioned, one of the advantages of RVFT is that simulation results obtained from this technique do not depend on the mesh size. This is only true when the mesh size $h < \ell/2$. However, this advantage comes at the cost of increased computational expense. To model accurate crack paths using RVFT, ℓ should be smaller than the geometric dimensions being considered and the mesh size should be smaller than $\ell/2$. This leads to very fine discretization of geometries, thus increasing the computational cost.

I have carried out systematic calculations for crack paths in single edge notched geometries subjected to mode-I loading conditions. The geometry and loading conditions are shown in Figure 2.4(A). The regularization parameter for these calculations is 0.01 mm. The Young's modulus $E = 210$ GPa, Poissons ratio $\nu = 0.3$, and $g_c = 2.7$ N/mm. The geometry is discretized using linear quadrilateral finite elements. Three different meshes of sizes $h = \ell/2$, $h = \ell/4$ and $h = \ell/8$, are shown in Figure 2.4(B). The contour plot of the damage variable d indicates the crack path for the three different mesh sizes in Figure. 2.4(D.i), (D.ii) and (D.iii), respectively, with the cracked region shown in red ($d \approx 1$). The crack initiates at the notch tip and grows straight along y-axis.

This is the typical fracture mechanism in brittle solids under mode-I loading. It can be seen that the crack path does not change with mesh size. The load-displacement response for the three cases $h = \ell/2$, $h = \ell/4$ and $h = \ell/8$ is shown in Figure 2.4(C). It can be seen that in the three cases, the peak load is almost identical (≈ 570 N). Beyond the peak load, there is little difference in the load-displacement response. Therefore, it can be concluded that the results are independent of mesh size as long $h < \ell/2$.

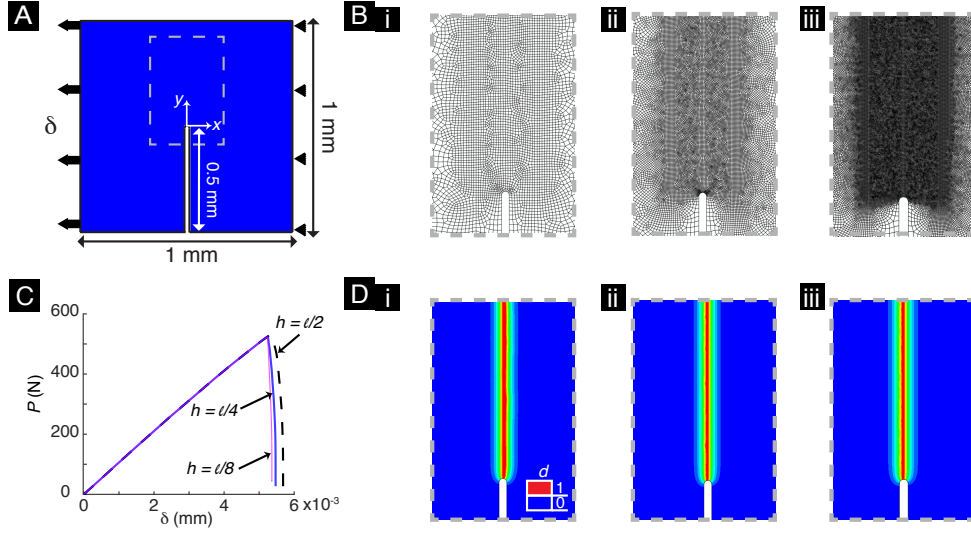


Figure 2.4: (A) A single edge notched geometry subjected to mode-I loading conditions. (B) The discretized region of the geometry corresponding to dashed box in subfigure (A) is shown. The mesh sizes in subfigures (B.i), (B.ii) and (B.iii) are $h = \ell/2$, $h = \ell/4$ and $h = \ell/8$, respectively. (C) The load-displacement response when $h = \ell/2$ is represented by a dashed black curve while the case of $h = \ell/4$ is represented by a red curve. (D) The crack paths for $h = \ell/2$, $h = \ell/4$ and $h = \ell/8$ are shown in subfigures (i), (ii) and (iii), respectively. As can be seen, they are almost identical.

2.9 Benchmark problems

The finite element implementation of RVFT is benchmarked to validate its predictive capability and accuracy to model classical problems in fracture mechanics. The benchmark problems are:

1. Verification of the Griffith postulate.
2. Crack growth under mode-II loading conditions and comparison of crack initiation angle with theory and experiments.

3. Crack path in a glass plate with three vertically aligned holes and an off-centered notch.
4. Mixed-mode failure mechanism in double-edge notched concrete samples subjected to mixed-mode loading.

2.9.1 Verification of the Griffith postulate using analytical fracture mechanics

The variational fracture model is based on the Griffith theory of fracture where crack growth occurs when the energy release rate at the crack tip g is greater than or equal to the fracture toughness g_c . A straightforward method to verify that crack growth in RVFT indeed occurs when $g \geq g_c$ is to compute g numerically using the J -integral contour methodology and compare it against the prescribed value of g_c . An alternative approach is to compute the far-field stress at crack initiation and obtain a numerical value of g using the analytical solution for stress intensity factors in known geometries.

For the case of a semi-infinite geometry with a finite length edge crack, the analytical solution for the mode-I stress intensity factor is given in [99]. The geometry is shown Figure 2.5(A), where the width is denoted by b and the notch length by a . The far field stress is σ^∞ . The mode-I stress intensity factor denoted by K_I is

$$K_I = \sigma^\infty \sqrt{2b \tan \frac{\pi a}{2b}} C\left(\frac{a}{b}\right), \quad (2.46)$$

where the function $C(a/b)$ is,

$$C\left(\frac{a}{b}\right) = \frac{0.752 + 2.02(a/b) + 0.37(1 - \sin((\pi/2)(a/b)))^3}{\cos((\pi/2)(a/b))}. \quad (2.47)$$

The energy release rate g under plane strain conditions is related to K_I as $g = K_I^2/E^*$ ([86]). In this equation, $E^* = E/(1 - \nu^2)$, E is the Young's modulus and ν is the Poisson's ratio of the solid. Therefore, the analytical solution for g is

$$g = \frac{1}{E^*} \left(\sigma^\infty C\left(\frac{a}{b}\right) \right)^2 \left(2b \tan \frac{\pi a}{2b} \right). \quad (2.48)$$

When we apply the Griffith criterion with the equality condition, we get

$$g_c = \frac{1}{E^*} \left(\sigma_{cr}^\infty C \left(\frac{a}{b} \right) \right)^2 \left(2b \tan \frac{\pi a}{2b} \right), \quad (2.49)$$

where σ_{cr}^∞ is the critical stress at which the Griffith criterion is satisfied and crack growth occurs. After rearranging Eq. 2.49, the non-dimensional quantity σ_{cr}^∞/E^* can be as expressed in terms of non-dimensional quantities $g_c/(E^*2b)$ and a/b as

$$\frac{\sigma_{cr}^\infty}{E^*} = \left(\sqrt{\frac{g_c}{E^*2b}} \right) \left(\sqrt{\frac{1}{(\tan \pi a/(2b)) C(a/b)}} \frac{1}{C(a/b)} \right). \quad (2.50)$$

The semi-infinite geometry is approximated by choosing a height h to be significantly larger than the width ($h \approx 10b$) so that the notch tip fields do not interact with the boundary at $y = h/2$ and $y = -h/2$. The boundary value problem is further simplified by using the symmetry of mode-I crack growth, so that the crack will begin from the notch tip and extend along positive x direction. Therefore, half of the geometry is modeled, i.e. $0 \leq y \leq h/2$, and the symmetry boundary conditions are imposed at $y = 0$. The symmetry boundary conditions are the displacement field $u_x = 0$ at $x \geq 0, y = 0$. The traction boundary conditions $t = \{0, \sigma^\infty\}$ is applied at the boundary $y = h/2$. The applied traction is incremented over a number of steps. The critical stress σ_{cr}^∞ is computed when the value of d at the node immediately in front of the notch tip reaches a value of 0.99. The results for these calculations are shown in Figure 2.5(B), where the solid curves correspond to the analytical solution given in Eq. 2.50 for different values of the quantity $g_c/(E^*2b)$. The results from RVFT calculations for various values of the non-dimensional quantities a/b and $g_c/(E^*2b)$ are shown using markers. It can be seen that the numerical solutions are very close to the analytical solutions. From this analysis, we can conclude that RVFT is indeed consistent with the Griffith postulate.

2.9.2 Mode-II shear validation against theory and experiments

Griffith's postulate gives the necessary condition for crack growth in brittle materials, i.e. that the energy release rate should be greater than or equal to the fracture toughness of the material for the crack to grow. However, the direction of the crack path cannot be predicted by Griffith's

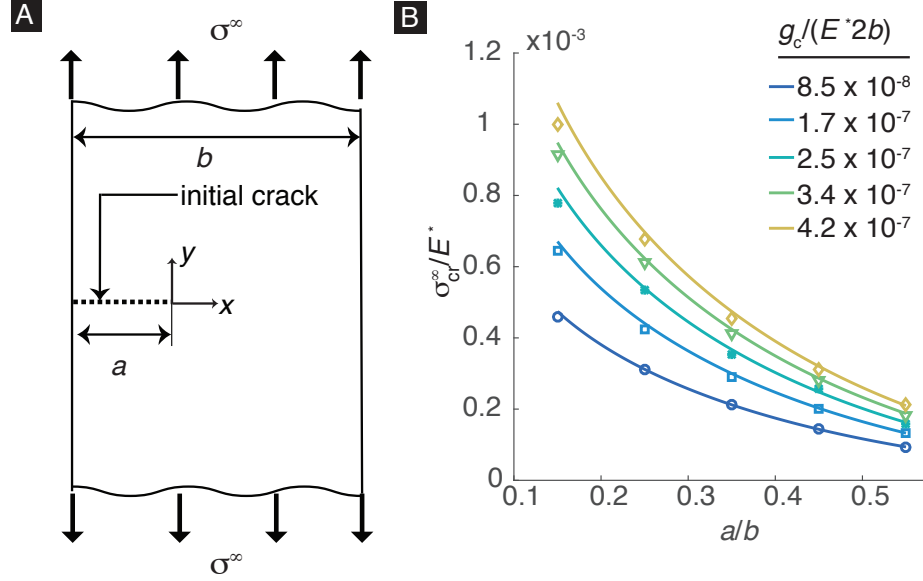


Figure 2.5: (A) This subfigure illustrates a semi-infinite geometry of width b with single edge notch of length a , subjected to far-field stress σ^∞ . (B) This comparison of numerical solution of σ_{cr}^∞/E^* from RVFT with the analytical solution from Eq. 2.50 for different values of a/b and $g_c/(E^*2b)$ is shown.

postulate. Several crack growth criteria have been postulated, such as maximum tangential stress criterion [100], maximum energy release rate criterion [101], the mode-II stress intensity factor equal to zero [102]. It is difficult to comment on which one of the criteria is most accurate for crack growth analysis. Crack growth under mode-II loading is a classical fracture mechanics problem and is well studied. For the case of pure mode-II loading, maximum tangential stress criterion predicts the crack initiation angle to be 70.5° [100]. Mode-II shear experiments on plexiglass under quasi-static loading showed crack initiation angles varying between $67.5^\circ - 72.5^\circ$ which compares well with what is predicted by maximum tangential stress criterion.

It is difficult to ascribe the crack path predicted by RVFT to any of the criteria mentioned above. However, for RVFT to be considered a good predictive fracture mechanics tool, it is important to validate its predictions against standard fracture mechanics problems such as mode-II shear. An illustration of the boundary value problem along with boundary conditions is shown in Figure 2.6(A). On the boundary $x = 1$, the displacements $u_x = u_y = 0$ and on the boundary $x = -1$ the displacements $u_x = 0$ and $u_y = \delta$ is prescribed. The material properties and the crack path for this simulation are shown in Figure 2.6(B). The red region in the contour plot indicates the crack with the value

of the damage parameter $d \approx 1$. The crack initiation angle is measured as the angle between the y -axis and the tangent to the crack path. The angle is computed to be 69.2° . The crack initiation angle measured from experiments [100] is between $67.5^\circ - 72.5^\circ$, and therefore compares well with RVFT calculations.

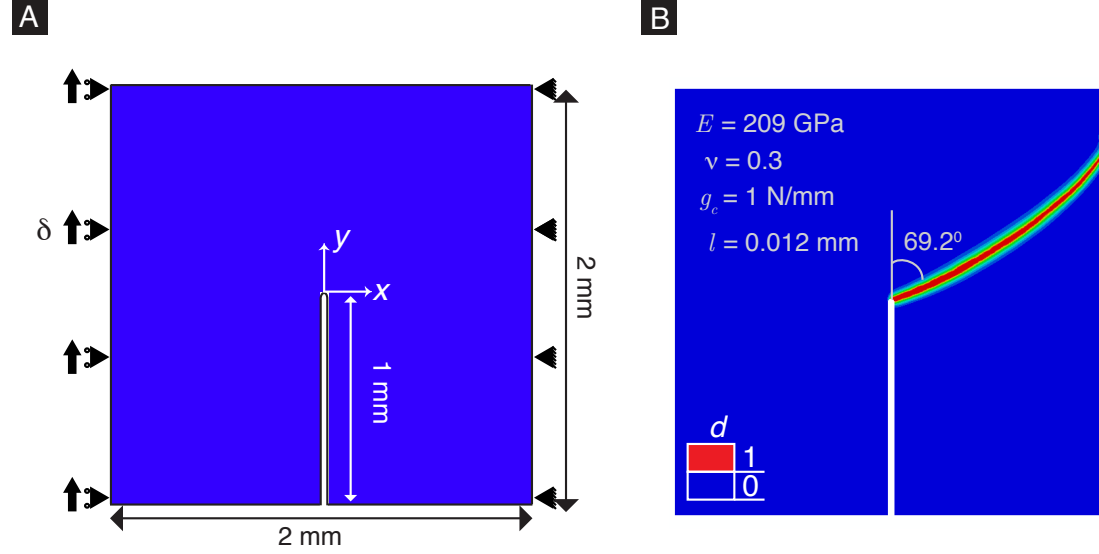


Figure 2.6: (A) A solid with an edge notch subjected to mode-II shear loading is shown here. The boundary conditions are $u_x = u_y = 0$ at $x = 1$ and $u_x = 0, u_y = \delta$ at $x = -1$. (B) RVFT simulation of the crack path is shown here, with the cracked region indicated in red, where $d \approx 1$. The crack initiation angle is measured to be 69.2° . The simulation parameters are shown on the top left corner.

2.9.3 Crack path in plate with three holes

In this section, the predictive capability of RVFT is validated against experimentally observed crack paths in brittle materials. To do this, I considered a more complex boundary value problem where the crack path has a curvilinear trajectory and interacts with features such as holes. This validation would truly test the RVFT's ability to handle cracks terminating at free surfaces (i.e. holes). Therefore, I conducted three-point bending experiments on a glass plate with three vertically aligned holes and an off-centered notch [4]. The boundary value problem is illustrated in Figure 2.7(A). The crack path from the experiment is adapted from [4] and the region enclosed by the dashed lines in subfigure (A) is shown in Figure 2.7(B). The data points of the crack path are extracted in terms of the angle θ , which is defined as the angle between the tangent to the crack path and the

x -axis. The experimental crack path is shown in Figure 2.7(D) using a solid blue line and is plotted against the distance measured along x -axis from the notch tip. RVFT calculations are carried out for the geometry and material properties shown in subfigure (A). The crack path determined by the RVFT calculations is shown in Figure 2.7(C), and it can be seen that it is almost identical to the experimentally observed crack shown in subfigure (B). A comparison of the crack path between the experiment and RVFT in subfigure (D) shows close alignment. Thus, RVFT's ability to predict experimentally observed crack path is complete.

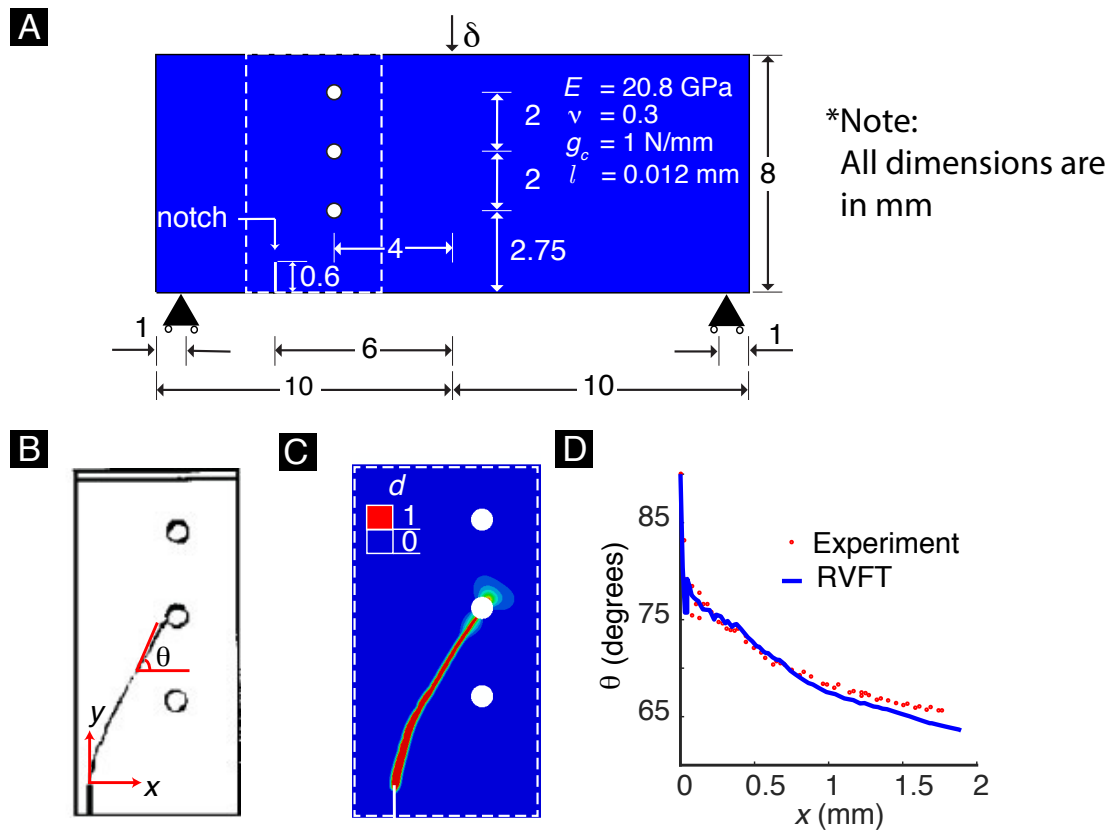


Figure 2.7: (A) A schematic of a glass plate with three vertically aligned holes and an off-centered notch, subjected to three-point bending loading conditions is shown. The region corresponding to the dashed lines are shown in subfigures (B) and (C). (B) The experimentally observed crack path adapted from [4] for the plate in subfigure (A) is shown here. (C) The RVFT simulation of the crack path, where the crack emanates from the notch tip and eventually terminates at the second hole is shown here. (D) A comparison of the experimental and RVFT crack paths show good agreement.

2.9.4 Mixed-mode cracks in concrete samples

In this benchmark problem, I have applied RVFT to study mixed-mode crack propagation and failure mechanisms in concrete samples. Fracture experiments on double edge, notched concrete specimens was conducted by Galvez et al. [103], and an illustration of the loading conditions is shown in Figure 2.8(A). The concrete sample is subjected to displacements $u_x = \delta$ and $u_x = -\delta$ on the boundary $x = -2, y > 0$ and $x = 2, y > 0$, respectively. The crack path from the experiment at an intermediate stage of loading is shown in Figure 2.8(B.i). The cracks growing from the notch tip in the negative y -direction are marked using blue circles. The compressive loading in the upper half of the geometry induces local tensile stress at the notch tip that drives the crack into the lower half of the geometry. Further, cracks nucleate in the compressive half of the geometry, i.e. in the region of $y > 0$. These cracks are marked using red circles. The mechanism that leads to the eventual failure of the concrete sample is shown in Figure 2.8(B.ii). It can be seen that the tensile cracks in the region $y < 0$ stop growing and the compressive crack in the region $y > 0$ becomes a dominant crack, extending in either direction of the notch tips, leading to failure.

RVFT simulations are conducted for the geometric dimensions and the material properties shown in Figure. 2.8(A) [103]. The crack paths from the simulations are shown in Figure 2.8(C). It can be seen that short cracks emanate from the notch tip and a long crack forms in the compressive region. RVFT simulations do not predict the coalescence of the long crack with the notch as seen in the experiments. However, RVFT does predict failure mechanisms in this loading condition qualitatively.

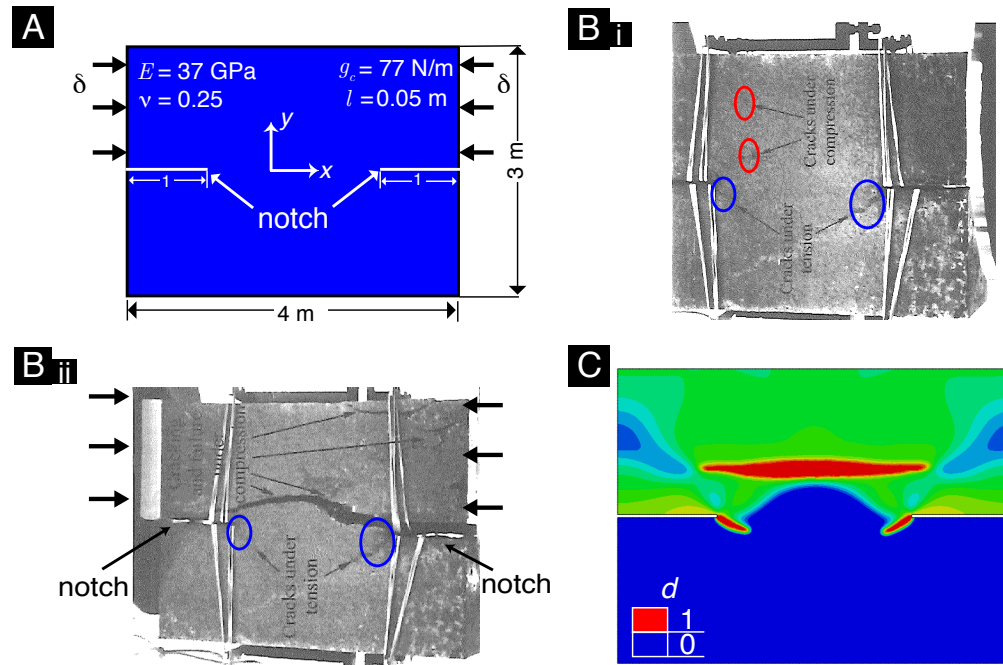


Figure 2.8: (A) The geometry and the loading conditions of a double edge notched concrete sample. The geometry is subjected to compressive displacements on the boundaries $x = -2, y > 0$ and $x = 2, y = 0$. (B.i) Crack patterns from the experiments at an intermediate loading stage. The regions marked by a blue circle indicate the occurrence of tensile cracks emanating from the notch tip. The regions marked by red circles indicate the occurrence of cracks in the compressive region. (B.ii) The failure mechanism of the concrete sample, where the crack in the compressive region grows, leading to failure. (D) RVFT simulation contours of the damage field show the formation of a dominant crack in the compressive region along with the occurrence of short cracks at the notch tip.

Chapter 3

Regularized variational fracture model for interfaces

3.1 Introduction

The micro-architecture of *structural biomaterials* (SBs) (see Chapter 1) shows that the building blocks of the architecture comprises of a brittle material, such as silica or aragonite, and a network of interfaces made of an organic phase. One such example of a SB is nacre, and the arrangement of the brittle phase and interfaces in nacre is shown in Figure 3.1(a) (adapted from [5]). The arrangement mimics that of a brick-and-mortar architecture where the brick is the brittle phase and the mortar is the organic phase. It can be seen from the figure that the brittle phase occupies a large volume fraction of nacre ($> 95\%$ [19]) as compared to the organic phase (or interface). The crack path in nacre shows crack deflection at the interfaces followed by crack arrest and crack re-nucleation. This then leads to a convoluted crack path. Figure 3.1(b) shows a scanning electron microscope image of the cross-section of a spicule (from a marine sponge *Euplectella Aspergillum* (Ea)) adapted from [6]. The geometry of EA spicules resembles that of a cylindrical shape and is predominantly composed of silica. From the cross-section image of the spicule it can be seen that there is a solid inner core of silica which is surrounded by concentric layers of silica. A nanometer thin organic phase lies in between the silica layers. The fracture sample of one such spicule is shown in Figure. 3.1(c)

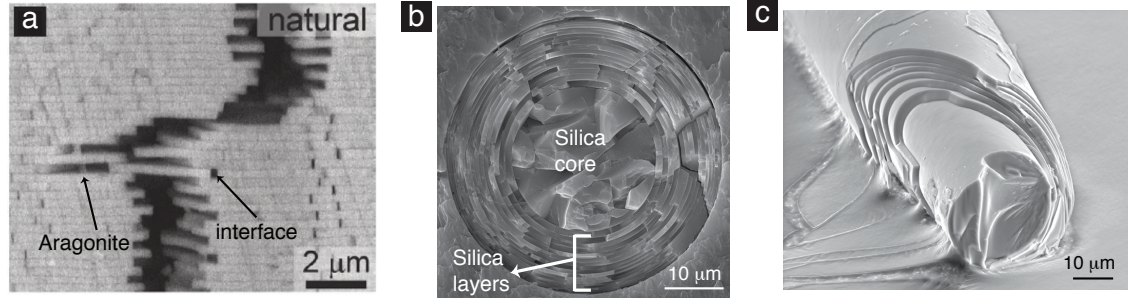


Figure 3.1: (a) The micro-architecture of nacre adapted from [5] shows the brittle material and the interface. (b) The cross section of a spicule from *Euplectella Aspergillum* (adapted from [6]) with a solid inner core made of silica surrounded by concentric silica layers. (c) A fractured sample of a spicule. The failure mechanism of the sample indicates crack arrest and crack deflection, which is a typical interfacial fracture mechanism. (Image courtesy of Michael Monn.)

(Image courtesy of Michael Monn). The failure mechanism in the sample can be described as crack deflection followed by crack re-nucleation at the concentric layers of silica. These fracture mechanisms are typically interfacial fracture mechanisms ([9, 38, 104]). Thus, to simulate fracture patterns in SBs, RVFT needs to be modified to model interfaces.

To model SBs accurately, the micro-architecture should be modeled accurately. Additionally, the material properties of the brittle phase and organic phase must be characterized. Therefore, the phases have to be extracted from the SBs in order to characterize the properties. However, due to the micrometer dimensions of these SBs, the process of characterizing the material properties is not straightforward. From the failure mechanism of the SBs, it can be seen that interfacial fracture is the operating mechanism. Interfacial fracture is a well-studied phenomenon and several theoretical and numerical models have been proposed to understand the crack-tip fields of a crack at the interface ([7, 37, 105]). Most of these models assume the thickness of the interface to be zero. Taking these assumptions into account, RVFT is suitably modified to introduce interfaces which in the limit of $\ell \rightarrow 0$ also goes to zero. The elastic properties in the modified RVFT correspond to that of the brittle phase. The fracture toughness g_c is spatially varied such that the toughness of the brittle phase is g_b and the toughness at the interface is g_I .

3.2 Interface model for heterogeneous materials

The goal of this work is to study crack patterns in SBs and gain insights into fracture mechanisms that enhance toughness. To this end, the traditional RVFT is modified by spatially varying g_c such that $g_c = g_c(\mathbf{X})$, where $\mathbf{X}$ is the material point in the solid $\mathcal{B}$. In order to accurately represent SBs, g_c is varied as a piecewise continuous function in the solid where $g_c = g_I$ in the interface region of thickness $m\ell$ and $g_c = g_b$ in the rest of the solid. The symbol m is a modeling parameter and belongs to the set of positive real numbers. Therefore, as $\ell \rightarrow 0$ the interface thickness goes to zero. In traditional RVFT (brittle fracture model), as $\ell \rightarrow 0$ the diffused crack patterns converge to sharp crack patterns and the toughness of the solid is $g_c = \text{constant}$ [81]. Therefore, for the modified RVFT model, what is the effective interface toughness as $\ell \rightarrow 0$?

It would seem straightforward to assume that the effective interface toughness is g_I , but the effective interface toughness g_{int} is found to depend on g_I , g_b , and the parameter m . To determine this relationship, an infinite solid is considered and the solid is cleaved such that the initial and final states are stress-free, as shown in Figure 3.2(a.i) and (a.ii), respectively. In this process, two new surfaces are created which are denoted by Γ at $Y = 0$. For simplicity, consider a homogeneous solid with a fracture toughness of g_b as shown in Figure 3.2(a.iii). From RVFT, toughness is defined as the least work per unit length of Γ required to cleave a material in the vanishing limit of ℓ . It is given as

$$g_{int} = \frac{2}{\text{Per}(\Gamma)} \lim_{\ell \rightarrow 0} \int_{\mathcal{B}} \frac{g_c}{2} \left(\frac{d(\mathbf{X})^2}{\ell} + \ell \|\nabla d(\mathbf{X})\|^2 \right) d\Omega, \quad (3.1)$$

where $\text{Per}(\cdot)$ is the perimeter. The solution to the damage field d can be obtained using the governing Eq. 2.3b with BC of $d = 1$ at the cleaved surface ($Y = 0$). After substituting the solution to d in Eq. 3.1 and taking the limit $\ell \rightarrow 0$, g_{int} is evaluated to be equal to g_b [81, 84]. Let us consider an identical boundary value problem (BVP) as mentioned above and introduce a vanishingly thin or sharp interface, which is marked as red thin line in Figure 3.2(b.i). The sharp interface is prescribed with a fracture toughness of g_I while the fracture toughness in the rest of the solid is g_b , as shown in green in Figure 3.2(b.i). I propose to approximate this BVP by replacing the sharp interface with a diffused one of thickness $m\ell$ as shown in Figure 3.2(b.ii), such that on considering the vanishing

limit of ℓ , the thickness of the interface goes to 0. After cleaving the solid at the interface and solving for d in a manner similar to that of the homogeneous BVP, the effective interface toughness is evaluated to be

$$g_{int} = g_I \left(\frac{e^{\hat{\alpha}} + \tanh(m)}{e^{\hat{\alpha}} \tanh(m) + 1} \right), \quad (3.2)$$

where $\hat{\alpha} = \ln(g_b/g_I)$ and m is the parameter that dictates how the diffused interface approaches the sharp interface as $\ell \rightarrow 0$. The solution for g_{int} in 1D is derived in Section 3.3.1. The result is generalized for arbitrary 2D solid geometries in section 3.3.2. A numerical verification of g_{int} is presented in section 3.4.

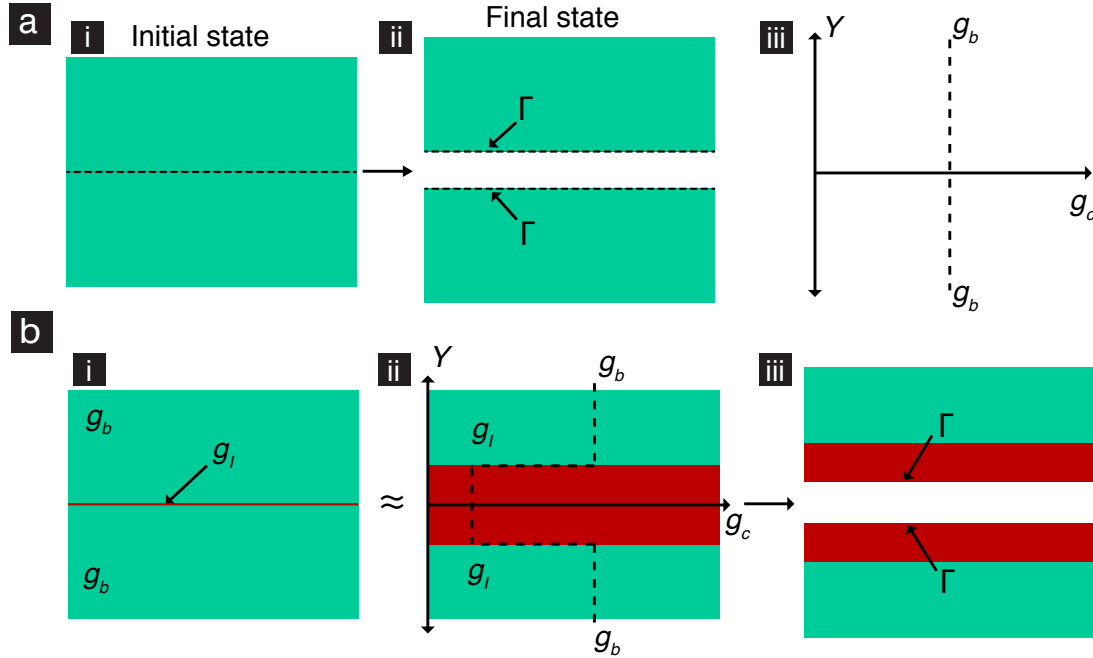


Figure 3.2: In subfigure (a.i), a stress-free homogeneous material of fracture toughness g_b is shown. Subfigure (a.ii) shows the material cleaved to create two surfaces, such that the final state is also stress free. Subfigure (a.iii) shows the variation of fracture toughness along Y axis and the fracture toughness is equal to g_b (which is a constant). In subfigure (b.i), a material with spatially varying fracture toughness $g_c(Y)$ is shown such that $g_c = g_I$ at the interface of zero thickness (sharp interface) and $g_c = g_b$ in the remainder of the solid. The sharp interface is approximated by a diffused interface of thickness $m\ell$ as shown in the subfigure (b.ii), where the fracture toughness is g_I for $-m\ell \leq Y \leq m\ell$ and g_b elsewhere. In subfigure (b.iii) the material is cleaved at $Y = 0$ to create two new surfaces such that both the initial and final states are stress-free.

3.3 Regularized variational fracture theory for elastic solids with interfaces

3.3.1 Effective interface toughness in 1D

To better understand the 2D BVP described in Figure 3.2(b), a 1D bar of length a subjected to BCs of $d = 1$ at $Y = 0$ and $d = 0$ at $Y = a$ is considered. The BVP can be expressed in terms of non-dimensional variables $\xi = Y/a$, $\varepsilon = \ell/a$, $\hat{\alpha} = \ln(g_b/g_I)$ and the BCs read as $d = 1$ at $\xi = 0$ and $d = 0$ at $\xi = 1$. We solve for the surface energy by first considering the functional

$$I_\varepsilon[d] := \int_0^1 \frac{g_\varepsilon(\xi; m)}{2} \left(\varepsilon d'^2 + \frac{d^2}{\varepsilon} \right) d\xi, \quad (3.3)$$

where, $g_\varepsilon(\xi; m)$ is chosen to be

$$g_\varepsilon(\xi; m) = \begin{cases} g_I, & 0 \leq \xi \leq m\varepsilon, \\ g_b, & \text{otherwise.} \end{cases} \quad (3.4)$$

The minimization problem (M) for the functional I_ε is

$$(M) \quad I_\varepsilon^* := \inf \{ I_\varepsilon[d] : d \in \mathcal{V} \}, \quad (3.5)$$

where the space of admissible functions $\mathcal{V}$ is

$$\mathcal{V} = \{ d \in W^{1,2}(0, 1), d(0) = 1, d(1) = 0 \}. \quad (3.6)$$

Therefore, one can solve for the unique minimizer d_ε^* for (M) by deriving the Euler-Lagrange (E-L) equations for the variational problem M . The functional I_ε given in Eq. 3.3 is rewritten using the definition of g_ε given in Eq. 3.4 as

$$I_\varepsilon[d] = \int_0^{m\varepsilon} \frac{g_I}{2} \left(\varepsilon d'^2 + \frac{d^2}{\varepsilon} \right) d\xi + \int_{m\varepsilon}^1 \frac{g_b}{2} \left(\varepsilon d'^2 + \frac{d^2}{\varepsilon} \right) d\xi. \quad (3.7)$$

The unique minimizer (d_ε^*) to the above problem (Eq. 3.7) can be determined using the E-L equations, which are given as

$$\begin{aligned}\varepsilon (d_\varepsilon^*)'' - \frac{d_\varepsilon^*}{\varepsilon} &= 0, & 0 \leq \xi \leq m\varepsilon, \\ d_\varepsilon^*(0) &= 1,\end{aligned}\tag{3.8a}$$

and

$$\begin{aligned}\varepsilon (d_\varepsilon^*)'' - \frac{d_\varepsilon^*}{\varepsilon} &= 0, & m\varepsilon \leq \xi \leq 1, \\ d_\varepsilon^*(1) &= 0,\end{aligned}\tag{3.8b}$$

along with the Weierstrass-Erdmann corner condition

$$\lim_{\xi \rightarrow (m\varepsilon)^-} g_I (d_\varepsilon^*(\xi))' = \lim_{\xi \rightarrow (m\varepsilon)^+} g_b (d_\varepsilon^*(\xi))' .\tag{3.9}$$

After solving for d_ε^* from the E-L equations, we get

$$d_\varepsilon^* = \begin{cases} \frac{\sinh\left(\frac{1-\xi}{\varepsilon}\right) - \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(\frac{\xi-2m\varepsilon+1}{\varepsilon}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(2m - \frac{1}{\varepsilon}\right)}, & 0 \leq \xi \leq m\varepsilon, \\ \frac{e^{-\hat{\alpha}/2} \operatorname{sech}\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(\frac{1-\xi}{\varepsilon}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(2m - \frac{1}{\varepsilon}\right)}, & m\varepsilon \leq \xi \leq 1. \end{cases}\tag{3.10}$$

After substituting d_ε^* in the Eq. 3.7 and taking $\lim_{\varepsilon \rightarrow 0} I_\varepsilon^*$, we get

$$\lim_{\varepsilon \rightarrow 0} I_\varepsilon^* = \frac{g_I}{2} \left(\frac{e^{\hat{\alpha}} + \tanh(m)}{e^{\hat{\alpha}} \tanh(m) + 1} \right).\tag{3.11}$$

Hence, the measure of toughness in 1D is $g_I (e^{\hat{\alpha}} + \tanh(m)) / (e^{\hat{\alpha}} \tanh(m) + 1)$. In the next section, we generalize this result for a 2D solid.

3.3.2 Effective interface toughness in 2D

The result derived for the 1D variational problem in Section 3.3.1 is extended for a 2D solid. The regularized functional I_ε in 2D is

$$I_\varepsilon[d] := \int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} \left(\varepsilon \|\nabla d\|^2 + \frac{d^2}{\varepsilon} \right) d\Omega, \quad (3.12)$$

where $\mathcal{B} \subset \mathbb{R}^2$ is a bounded, simply-connected domain and $\hat{r}$ is the distance function with respect to a local coordinate system along the arc-length and the arc-length normal. (Refer to B.1 for details.)

The minimization problem for the functional I_ε (Eq. 3.12) is

$$(M) \quad I_\varepsilon^* := \inf \{ I_\varepsilon[d] : d \in \mathcal{V} \}, \quad (3.13)$$

where the space of admissible functions $\mathcal{V}$ is

$$\mathcal{V} = \{ d \in W^{1,2}(\mathcal{B}; \mathbb{R}^2), d = 1, \text{ on } \Gamma \}, \quad (3.14)$$

where Γ is the crack boundary. The function $g_\varepsilon(\hat{r}; m)$ for the 2D BVP is defined as

$$g_\varepsilon(\hat{r}; m) = \begin{cases} g_I, & 0 \leq \hat{r} \leq m\varepsilon, \\ g_b, & \text{otherwise.} \end{cases} \quad (3.15)$$

Unlike 1D cases, it is not straightforward to find the minimizer d_ε^* for the functional I_ε in 2D. Therefore, in Sections 3.3.2 and 3.3.2, the upper and lower bound for I_ε is derived and it is shown that the bounds converge to $\lim_{\varepsilon \rightarrow 0} I_\varepsilon^*$.

Upper bound solution

To derive the upper bound for the regularized functional given by Eq. 3.12, a trial solution d^g is chosen. From variational principles, it is known that for such a solution

$$I_\varepsilon^* \leq I_\varepsilon[d^g]. \quad (3.16)$$

The trial function $d^g(\hat{r}, m)$ is given as

$$d^g = \begin{cases} \frac{\sinh\left(\frac{1-\hat{r}}{\varepsilon}\right) - \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(\frac{\hat{r}-2m\varepsilon+1}{\varepsilon}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(2m - \frac{1}{\varepsilon}\right)}, & 0 \leq \hat{r} \leq m\varepsilon, \\ \frac{e^{-\hat{\alpha}/2} \operatorname{sech}\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(\frac{1-\hat{r}}{\varepsilon}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \tanh\left(\frac{\hat{\alpha}}{2}\right) \sinh\left(2m - \frac{1}{\varepsilon}\right)}, & m\varepsilon \leq \hat{r} \leq 1, \\ 0, & \text{otherwise.} \end{cases} \quad (3.17)$$

After substituting the d^g in Eq. 3.12 and using the spatial variation of g_ε given in Eq. 3.15, it can be shown that

$$\frac{1}{\operatorname{Per}(\Gamma)} I_\varepsilon^* \leq \frac{g_I}{2} \frac{\cosh\left(\frac{1}{\varepsilon}\right) + \cosh\left(\frac{2m\varepsilon-1}{\varepsilon}\right) \tanh\left(\frac{\hat{\alpha}}{2}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \sinh\left(\frac{2m\varepsilon-1}{\varepsilon}\right) \tanh\left(\frac{\hat{\alpha}}{2}\right)} L. \quad (3.18)$$

The full derivation can be found in the B.2. When considering the functional I_ε^* as $\varepsilon \rightarrow 0$, we get

$$\frac{1}{\operatorname{Per}(\Gamma)} \lim_{\varepsilon \rightarrow 0} I_\varepsilon^* \leq \frac{g_I}{2} \frac{e^{\hat{\alpha}} + \tanh(m)}{e^{\hat{\alpha}} \tanh(m) + 1}. \quad (3.19)$$

Lower bound solution

The lower bound for I_ε can be derived using the duality principle of convex functionals by introducing two conjugate variables $\mathbf{P}$ and q , such that

$$\int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} \left(\varepsilon \|\nabla d - \mathbf{P}\|^2 + \frac{(d - q)^2}{\varepsilon} \right) d\Omega \geq 0. \quad (3.20)$$

After further simplification, it can be shown that

$$I_\varepsilon[d] \geq \int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} \left(2\varepsilon \nabla d \cdot \mathbf{P} - \varepsilon \mathbf{P} \cdot \mathbf{P} + \frac{2qd - q^2}{\varepsilon} \right) d\Omega. \quad (3.21)$$

Without any loss in generality, a constraint on $\mathbf{P}$ and q is imposed, so that they satisfy

$$q - \varepsilon^2 \nabla \cdot \mathbf{P} = 0 \quad \text{on } \mathcal{B}. \quad (3.22)$$

On substituting the constraint and simplifying Eq. 3.21 further, it is found that

$$I_\varepsilon[d] \geq \int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} (2\varepsilon \nabla d \cdot \mathbf{P} - \varepsilon \mathbf{P} \cdot \mathbf{P} + 2\varepsilon \nabla \cdot \mathbf{P} d - \varepsilon^3 \nabla \cdot \mathbf{P}^2) d\Omega. \quad (3.23)$$

Therefore, the variational problem statement can be formulated as

$$I_\varepsilon^* = \min_{d \in \mathcal{V}} \max_{\mathbf{P} \in \mathcal{A}} \int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} (2\varepsilon \nabla d \cdot \mathbf{P} - \varepsilon \mathbf{P} \cdot \mathbf{P} + 2\varepsilon \nabla \cdot \mathbf{P} d - \varepsilon^3 \nabla \cdot \mathbf{P}^2) d\Omega, \quad (3.24)$$

where the space of admissible functions $\mathcal{A}$ is given as

$$\mathcal{A} = \{ \mathbf{P} \in W^{1,2}(\mathcal{B}; \mathbb{R}^2) \}. \quad (3.25)$$

Additionally, $\mathbf{P}$ also satisfies the natural boundary conditions at the interface

$$\left(\lim_{\hat{r} \rightarrow m\varepsilon^-} g_I \mathbf{P} - \lim_{\hat{r} \rightarrow m\varepsilon^+} g_b \mathbf{P} \right) \cdot \mathbf{n} = 0, \quad (3.26)$$

where $\mathbf{n}$ is the outward boundary normal to the interface. The lower bound for the functional I_ε^* is calculated to be

$$I_\varepsilon^* \geq \max_{\mathbf{P} \in \mathcal{A}} \min_{d \in \mathcal{V}} \int_{\mathcal{B}} \frac{g_\varepsilon(\hat{r}; m)}{2} (2\varepsilon \nabla d \cdot \mathbf{P} - \varepsilon \mathbf{P} \cdot \mathbf{P} + 2\varepsilon \nabla \cdot \mathbf{P} d - \varepsilon^3 \nabla \cdot \mathbf{P}^2) d\Omega. \quad (3.27)$$

After simplifying Eq. 3.27 using the definition of g_ε given in Eq. 3.15, the details of which can be found in the B.2.1, it is shown that

$$\frac{1}{\text{Per}(\Gamma)} I_\varepsilon^* \geq \frac{g_I}{2} \frac{e^{\hat{\alpha}} + \tanh(m)}{e^{\hat{\alpha}} \tanh(m) + 1}. \quad (3.28)$$

Therefore, from Eqns. 3.19 and 3.28 it is seen that both the upper and lower bounds converge to $g_{int}/2$ as $\varepsilon \rightarrow 0$. Therefore, it can be concluded that for a 2D geometry with a sharp interface, the effective interface toughness is given by g_{int} .

3.4 Numerical verification of the variational fracture model for interfaces

In this section, a numerical verification of g_{int} , derived in Section 3.3.2, is provided. The modified RVFT model given in Section 3.2 is implemented using finite element analysis (FEA). The verification provided in this section is as follows:

1. In the absence of any elastic energy, the upper and lower bound formulations given in Sections 3.3.2 and 3.3.2 are verified by numerically solving the functional I_ε over an arbitrary 2D domain. The optimal solution I_ε^* , which is obtained by minimizing I_ε for non-zero values of ε , is shown to be sandwiched between the upper bound and lower bound for all values of ε . Furthermore, as ε approaches 0, I_ε^* is shown to approach $g_{int}/2$.
2. In the RVFT model for brittle fracture, it has been shown that crack initiation occurs when the energy release rate is equal to the constant fracture toughness g_c [96]. In the modified RVFT for interfaces, we show that crack initiation occurs when the energy release rate is equal to g_{int} . The BVP is numerically solved for a single edge crack (SEC) geometry with an interface of thickness $m\ell$, subjected to far field mode-I loading, using the modified RVFT formulation. The energy release rate at which the crack initiates is evaluated and compared against the analytically derived effective toughness.
3. The RVFT for interfaces is developed on the theoretical foundation of zero-thickness interfaces proposed in classical interfacial mechanics theory [7, 35, 37, 104]. To ascertain the accuracy of the modified RVFT based model, results from this RVFT model are compared against semi-analytical analysis of an interface crack at the bi-material interface, subjected to far-field loading, given by He and Hutchinson [7]. In this semi-analytical analysis, He and Hutchinson predict the angle at which the interface crack kinks into material-1 or material-2, given the far-field loading conditions. The elastic properties of material-1 and material-2 are characterized by Dundur's parameters (refer to [106]) on either side of the interface. For the numerical verification conducted here in this section, the fracture toughness of both material-1 and material-2 is chosen to be identical to g_b , so that the interface toughness can be compared

to g_{int} . Based on the analysis given in [7], for a given loading condition and for certain ratios of g_b/g_{int} , the interface crack won't kink into either material-1 or material-2. The crack will remain trapped in the interface and this phenomenon is termed *crack trapping*. Simulations based on the modified RVFT are conducted to investigate this phenomenon and qualitatively similar trends are observed to that predicted in [7].

3.4.1 Verification of upper and lower bound formulations

In this section, we verify the upper and lower bound formulations given in Sections 3.3.2 and 3.3.2 by numerically solving the functional I_ε (refer to Eq. 3.12) using finite element analysis (FEA) in Mathematica [98]. A schematic of the 2D domain is presented in Figure 3.3(a), where the green outer region is prescribed with a fracture toughness of g_I and the blue inner region with a fracture toughness of g_b . The green region is the diffused interface of thickness $m\varepsilon$, which is measured along the inward normal to the outer boundary Γ . We prescribe $d = 1$ on Γ as the boundary condition and numerically solve for the minimizer (d_ε^*) of the functional I_ε . Upon substituting d_ε^* into Eq. 3.12, we obtain the optimal solution (I_ε^*), which is the minimum for the functional I_ε . Similarly, using the trial solution d^g given by Eq. 3.17, we evaluate the upper and lower bound values. (Refer to B.2-B.2.1.) From the results in Section 3.3.2, we know that the upper and lower bounds converge to $g_{int}/2$ as $\varepsilon \rightarrow 0$. Furthermore, the bounds should also converge to the optimal solution as $\varepsilon \rightarrow 0$. I verify both these claims by studying the behavior of the bounds and the optimal solution with decreasing values of ε in Figure 3.3(b). The upper bound, lower bound, $g_{int}/2$ and the optimal solution are represented by thick red, cyan, black and dashed black curves, respectively, for $\varepsilon \in [0.03, 0.1]$. The parameters chosen for the verification are $g_I=1$, $m=7$, and $\hat{\alpha} = \ln(5)$. The upper and lower bound enclose the optimal solution and approach the optimal solution with decreasing values of ε . Furthermore, all three curves approach $g_{int}/2$ as $\varepsilon \rightarrow 0$, thus substantiating both our claims.

3.4.2 Crack initiation toughness for the interface model

In the previous section, elastic energy is neglected, assuming that the cleavage process for creating two surfaces is stress-free. However, in practical problems, crack initiation and growth occur at finite values of stress. In this numerical verification, a single edge crack (SEC) solid of a uniform

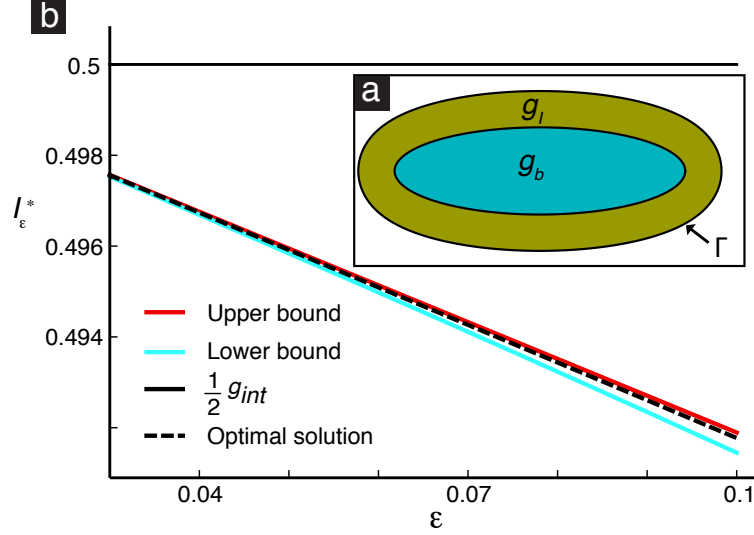


Figure 3.3: (a) A schematic of the 2D domain, where the green region is the interface prescribed with fracture toughness of g_I and the cyan region with g_b . The outer boundary is denoted as Γ . (b) A comparison of the optimal solution for the 2D domain subjected to a boundary condition (BC) of $d = 1$ on Γ , which is the minimum value of I_ϵ denoted by I_ϵ^* , against the analytical expressions for upper and lower bounds given in Section 3.3.2. It can be seen that the upper and lower bounds converge to the optimal solution as $\epsilon \rightarrow 0$. More importantly, all the three curves approach $g_{int}/2$ as $\epsilon \rightarrow 0$.

elastic modulus with a toughness of g_I at the interface and g_b in the rest of the solid is studied. The solid is subjected to a far field stress σ^∞ as shown in Figure 3.4(a). The solid has a crack length of a , width of b and an interface thickness of $m\ell$. The initial crack is modeled by setting $d = 1$ at $0 \leq x \leq a$ and $y = 0$. Crack initiation in these simulations is defined when the first node in front of the crack tip ($x = a$) attains a value of $d = 0.99$. The analytical solution to the mode-I stress intensity factor for this geometry is given in [99]. The mode-I stress intensity factor denoted by K_I is

$$K_I = \sigma^\infty \sqrt{2b \tan \frac{\pi a}{2b} C\left(\frac{a}{b}\right)}, \quad (3.29)$$

where the function $C(a/b)$ is

$$C(a/b) = \frac{0.752 + 2.02(a/b) + 0.37(1 - \sin((\pi/2)(a/b)))^3}{\cos((\pi/2)(a/b))}. \quad (3.30)$$

The energy release rate g under plane strain conditions is related to K_I as $g = K_I^2/E^*$ ([86]). In the equation $E^* = E/(1 - \nu^2)$, E is the Youngs modulus and ν is the Poissons ratio of the solid.

Therefore, the analytical solution for g is

$$g = \frac{1}{E^*} (\sigma^\infty C(a/b))^2 (2b \tan \pi a / (2b)). \quad (3.31)$$

Griffith postulates that for crack growth to occur, the energy release rate at the crack tip should be greater than the toughness of the material. The postulate for the SEC geometry with an interface that is considered here can be summarized as $g \geq g_{int}$. The energy release rate computed using RVFT is denoted by g_{int}^n and can be described as

$$g_{int}^n = \frac{1}{E^*} (\sigma_{cr}^\infty C(a/b))^2 2b \tan(\pi a / 2b), \quad (3.32)$$

where σ_{cr}^∞ is the far-field stress at which the crack initiates. The computations are performed for $m = \{0.1, 0.2, 0.3, 0.4, 0.5\}$, $\ell = 0.02$, $g_I = \{1, 5\}$ and $\hat{\alpha} = \{\ln(2), \ln(5), \ln(20)\}$ by numerically solving the energy functional using FEA in the commercial FEA package Abaqus 6.12 [97]. The interface toughness g_{int}^n is computed by substituting σ_{cr}^∞ obtained from the simulations into Eq. 3.32. The results from the computations are plotted in Figure 3.4(b), where the y-axis corresponds to the numerical non-dimensional toughness g_{int}^n / g_I and the x-axis corresponds to the analytical non-dimensional toughness g_{int} / g_I . The thick dashed line of slope 1 corresponds to the analytical solution. It can be seen that the numerically obtained data does not deviate substantially from the analytical solution (displayed as a thick dashed line). Furthermore, the error in numerical data is within 8% of the analytical value. Hence, it is concluded that the numerically obtained values for interface toughness are largely consistent with their analytical counterparts.

3.4.3 Interface crack at the bi-material interface

The modified RVFT model for interfaces is built on the theoretical model by He and Hutchinson [7]. Therefore, the simulation results from modified RVFT are compared against the analysis of a semi-infinite crack present at the bi-material interface, subjected to far-field loading, given by He and Hutchinson [7]. An illustration of the geometry is shown in Figure 3.5, where a semi-infinite crack is present along the interface of material-1 and material-2. The shear modulus and Poisson's ratio of material-1 and material-2 are μ_1, ν_1 and μ_2, ν_2 , respectively. For a given applied far-field loading,

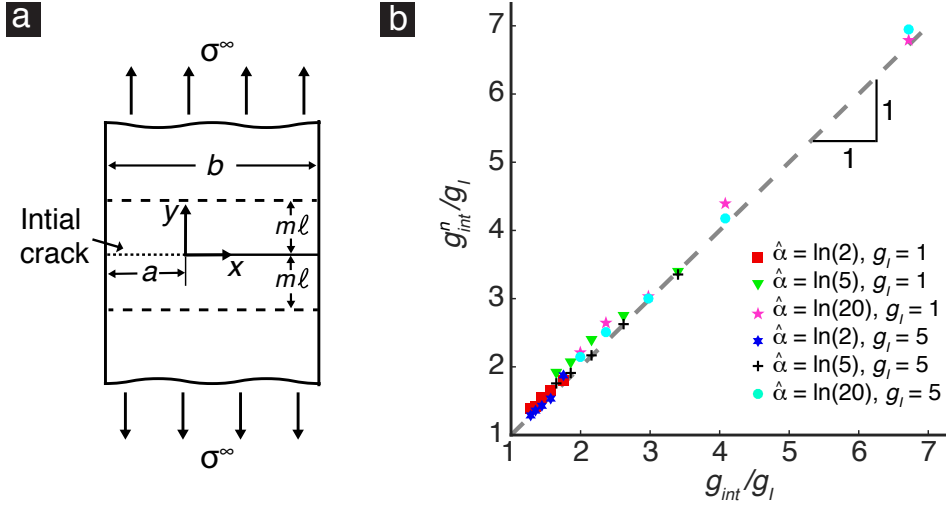


Figure 3.4: (a) A schematic of edge-crack geometry subjected to far-field stress σ^∞ . The initial crack length is a , the width of the geometry is b , and the interface thickness is $m\ell$. The initial crack length is $a = b/4$. (b) The non-dimensional interface toughness (g_{int}^n/g_I) is computed from finite element simulations for the edge crack geometry given in subfigure (a) is plotted against the non-dimensional effective interface toughness (g_{int}/g_I) for $m = \{0.1, 0.2, 0.3, 0.4, 0.5\}$, $\ell = 0.02$, $g_I = \{1, 5\}$ and $\hat{\alpha} = \{\ln(2), \ln(5), \ln(20)\}$.

the semi-infinite crack is assumed to kink into material 2 by a finite length a . The angle subtended by the extended crack of length a with respect to the x -axis, termed the *kink angle*, is denoted by ω . In the following discussion, the semi-infinite crack will be called the *interface crack* and the extended crack segment the *kinked crack*. The loading parameters for the problem are characterized by mode-I and mode-II stress intensity factors corresponding to that of the interface crack denoted by K_1 and K_2 , respectively. The loading is typically described using a non-dimensional parameter called the *phase angle* or the *mixed mode ratio* $\gamma = \arctan(K_2/K_1)$. The parameter γ is an indicator of whether the loading is mode-I or mode-II dominant. For example, $\gamma = 0$ is mode-I loading and $\gamma = \pi/2$ is mode-II loading. Expressions for the asymptotic mode-I and mode-II displacement fields for an interface crack in terms of K_1 and K_2 is given by Eq. 3.37. In the bi-material problem studied in [7], it had been shown that the kink angle depends on two non-dimensional material parameters called the Dundurs' parameters α and β [106]. The material parameters $\mu_1, \nu_1, \mu_2, \nu_2$ are expressed

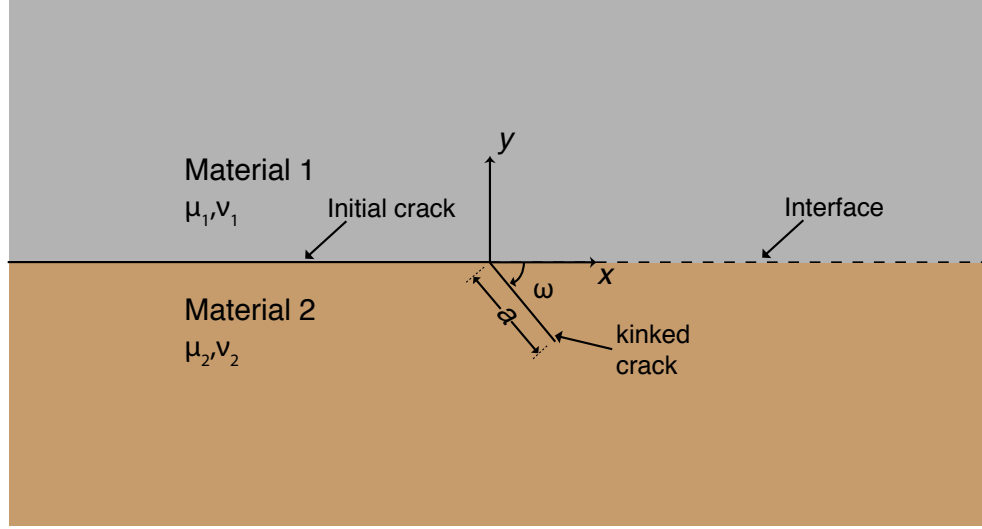


Figure 3.5: A schematic of a semi-infinite crack at the interface of material 1 (region shaded in grey) and material 2 (region shaded in brown), which kinks by an angle ω , on the application of far-field loading characterized by the mixed mode ratio γ . The symbol a is the kinked crack length.

in a non-dimensional form given by Dundurs [106] as follows:

$$\alpha := \frac{\mu_1(1 - \nu_2) - \mu_2(1 - \nu_1)}{\mu_1(1 - \nu_2) + \mu_2(1 - \nu_1)}, \quad (3.33a)$$

$$\beta := \frac{1}{2} \left(\frac{\mu_1(1 - 2\nu_2) - \mu_2(1 - 2\nu_1)}{\mu_1(1 - \nu_2) + \mu_2(1 - \nu_1)} \right). \quad (3.33b)$$

The material parameter α can be interpreted as a relative measure of stiffness, with $\alpha = 1$ indicating that material 1 is rigid and $\alpha = -1$ indicating that material 2 is rigid. A similar interpretation for the parameter β is unclear. In this work, $\beta = 0$ because when $\beta \neq 0$, the crack faces of the interface crack are in contact [34, 107, 108]. In other words, there is interpenetration of the crack faces, which is unphysical. Therefore, in this work, only the case of $\beta = 0$ is considered. The mode-I and mode-II stress intensity factors of the kinked crack are denoted by K_I and K_{II} , respectively. They are expressed in terms of stress intensity factors of the interface crack, K_1 and K_2 , for the case of $\beta = 0$, as given in [7]:

$$K_I + iK_{II} = (c(\omega, \alpha) + \bar{d}(\omega, \alpha)) K_1 + i(c(\omega, \alpha) - \bar{d}(\omega, \alpha)) K_2, \quad (3.34)$$

where $i = \sqrt{-1}$. The symbols c and d are complex valued functions of ω and α . The symbol $(\bar{})$ denotes the complex conjugate of a function.

Kinking of the interface crack

In this section, the procedure employed in [7] to predict the kink angle for a given loading γ and α is briefly reviewed. For a given loading γ , the interface crack is assumed to have kinked by an angle ω , forming an extended crack of length a . The kinked crack surfaces are free of traction. In [7], the kinked crack is considered to be a distribution of edge dislocations. To enforce traction-free conditions on the kinked crack segment, the stress fields from the interface crack and the distribution of edge dislocations are superimposed and set to zero. This leads to a singular integral equation which is solved numerically using Chebyshev polynomials. The complex valued functions c and d are tabulated for different values of ω . The energy release rate $\mathcal{G}$, given by

$$\mathcal{G} = q^{-2} \mathcal{G}_0 [|c|^2 + |d|^2 + 2\text{Re}(c \bar{d} e^{2i\gamma})], \quad (3.35)$$

is computed as a function of ω , where $|\cdot|$ denotes the magnitude of a complex number. In this equation, the symbols $q := \sqrt{1/(1+\alpha)}$ and $\mathcal{G}_0$ are the energy release rate of the interface crack and the symbol $\text{Re}(\cdot)$ is the real part of the complex number.

A crack growth criterion is necessary to compute the kink angle ω . Therefore, in [7], the crack is assumed to kink in the direction that maximizes $\mathcal{G}$ for a given α and γ . The kink angle is denoted by $\hat{\omega}$. For a given γ and α , the kink angle $\hat{\omega}$ can be computed by setting $d\mathcal{G}/d\omega|_{\omega=\hat{\omega}} = 0$ for $d^2\mathcal{G}/d\omega^2|_{\omega=\hat{\omega}} < 0$. This crack growth criterion is called the *maximum energy release rate criterion*. To compute $\hat{\omega}$ from Eq. 3.35, the functional form of the complex valued functions $c(\omega, \alpha)$ and $d(\omega, \alpha)$ are necessary. This would require solving the singular integral equation given in [7] and evaluating the coefficients for $c(\omega, \alpha)$ and $d(\omega, \alpha)$. To circumvent this issue, Veljkovic [8] proposed closed form approximations to the complex valued functions $c(\omega, \alpha)$, $d(\omega, \alpha)$, given as

$$c(\omega, \alpha) \approx \frac{1}{2} \sqrt{\frac{1}{1+\alpha}} \left(e^{\frac{-i\omega}{2}} + e^{\frac{-i3\omega}{2}} \right) \text{ and} \quad (3.36a)$$

$$d(\omega, \alpha) \approx \frac{1}{4} \sqrt{\frac{1}{1-\alpha}} \left(e^{\frac{-i\omega}{2}} - e^{\frac{i3\omega}{2}} \right). \quad (3.36b)$$

Note that the expressions for $\mathcal{G}$, $c(\omega, \alpha)$ and $d(\omega, \alpha)$ are specialized for the case of $\beta = 0$. I evaluated the accuracy of the approximate functions given in Eq. 3.36 by computing the kink angles using the approximate functions for the cases of $\alpha = \{0, 0.25, 0.5\}$ and comparing them to the data for the same provided in [7]. I first computed the energy release rate $\mathcal{G}$ (given in Eq. 3.35) by substituting the expressions for $c(\omega, \alpha)$ and $d(\omega, \alpha)$ from Eq. 3.36 for $0 \leq \gamma \leq \pi/4$. I then obtained $\hat{\omega}$ by maximizing the expression obtained for $\mathcal{G}$ with respect to ω for $0 \leq \gamma \leq \pi/4$. In Figure 3.6(a), the y-axis is the kink angle prediction corresponding to the maximum energy release rate criterion, which is denoted as $\hat{\omega}$. The x-axis is the mixed mode ratio γ for the case of $\alpha = 0$. The kink angle data obtained from [7] is shown using solid black circles and the kink angles computed using the approximate expressions for $c(\omega, \alpha)$ and $d(\omega, \alpha)$ from [8] are shown using thick solid red lines. It can be seen that $\hat{\omega}$ from [7] compares well with the $\hat{\omega}$ we have computed from [8]. Similar comparisons are made for $\alpha = 0.25, 0.5$ in Figure 3.6b and c, respectively. When comparing Figure 3.6a, b and c, it can be seen that the values of $\hat{\omega}$ computed using the work of [8] are less accurate for $\alpha = 0.5$ than for $\alpha = 0$ or $\alpha = 0.25$. Thus, it can be concluded that the approximate closed form solutions for $c(\omega, \alpha)$ and $d(\omega, \alpha)$ given in Eq. 3.36 should not be used for $\alpha > 0.5$.

To benchmark the modified RVFT model for interfaces, I propose to compute the kink angles for an interface crack for $\alpha = \{0, 0.25, 0.5\}$ and $0 \leq \gamma \leq \pi/4$. I considered a circular geometry as shown in Figure 3.7a, where an interface crack is modeled as a notch whose length is equal to that of the radius $R_0 = 1000$ mm. The region above the notch is material 1 and the region below the notch is material 2. An enlarged view of the notch root is shown in Figure 3.7b, where the coordinate axis is fixed at the notch tip and the vector subtending a polar angle θ with x-axis has a magnitude r . The kink angle $\hat{\omega}$ is measured clockwise with respect to the x-axis. The notch root radius is denoted by r_0 and $2r_0 = R_0/1000$. The finite width interface is shown using a dashed line segment and the width of the interface, i.e., $m\ell_0 = R_0/20000$. When the geometry is subjected to loading on the boundary (i.e., at $r = R_0$), the asymptotic displacement and stress fields pertaining to that of the interface crack hold at $r = R_0$. In other words, the process zone at the notch tip should be small enough such that stress fields and displacement fields obtained from linear elastic fracture mechanics for the interface crack should be valid far away from the notch tip. For example, if the asymptotic displacement fields corresponding to the interface crack are prescribed on the boundary of the circular geometry, then

the stress field obtained from FE computation should correspond to the asymptotic stress fields of the interface crack on the boundary. The non-dimensionalized asymptotic displacement field $\hat{u}_x$, $\hat{u}_y$ pertaining to that of an interface crack at $r = R_0$ is obtained from [91]. These fields, specialized for $\beta = 0$, are given for material 1 as

$$\hat{u}_x + i \hat{u}_y = \sqrt{\frac{1}{8\pi}} \left((3 - 4\nu_1) e^{i(\frac{\theta}{2} - \gamma)} - e^{-i(\frac{\theta}{2} + \gamma)} - i \sin \theta e^{i(\frac{\theta}{2} + \gamma)} \right), \quad (3.37a)$$

and for material 2 as

$$\hat{u}_x + i \hat{u}_y = \sqrt{\frac{1}{8\pi}} \left((3 - 4\nu_2) e^{i(\frac{\theta}{2} - \gamma)} - e^{-i(\frac{\theta}{2} + \gamma)} - i \sin \theta e^{i(\frac{\theta}{2} + \gamma)} \right). \quad (3.37b)$$

For material 1, the displacement field $u_x = \hat{u}_x |K| \sqrt{R_0} / \mu_1$ and $u_y = \hat{u}_y |K| \sqrt{R_0} / \mu_1$. Similarly, for material 2, $u_x = \hat{u}_x |K| \sqrt{R_0} / \mu_2$ and $u_y = \hat{u}_y |K| \sqrt{R_0} / \mu_2$. The symbol $|K| = (K_1^2 + K_2^2)^{1/2}$. In Eq. 3.37(a), the displacement component $\hat{u}_x$ for material 1 is evaluated to be the real part of the right side of the equation and the displacement component $\hat{u}_y$ is evaluated to be the imaginary part of the right side of the equation. Similarly, displacement fields $\hat{u}_x$ and $\hat{u}_y$ for material 2 are evaluated from Eq. 3.37(b). The non-dimensionalized stress components $\hat{\sigma}_{11}$, $\hat{\sigma}_{22}$ and $\hat{\sigma}_{12}$ of the asymptotic crack tip field of the interface crack at $r = R_0$, specialized for $\beta = 0$ are given as

$$\hat{\sigma}_{11} + \hat{\sigma}_{22} = \frac{1}{\sqrt{2\pi}} \left(e^{-i(\frac{\theta}{2} + \gamma)} + e^{i(\frac{\theta}{2} + \gamma)} \right) \quad (3.38a)$$

$$\hat{\sigma}_{11} - \hat{\sigma}_{22} + 2i \hat{\sigma}_{12} = \frac{e^{i\theta}}{\sqrt{2\pi}} \left(e^{i(\frac{\theta}{2} + \gamma)} \cos \theta - e^{-i(\frac{\theta}{2} + \gamma)} \right). \quad (3.38b)$$

The stress fields $\sigma_{11} = \hat{\sigma}_{11} |K| / \sqrt{R_0}$, $\sigma_{22} = \hat{\sigma}_{22} |K| / \sqrt{R_0}$, and $\sigma_{12} = \hat{\sigma}_{12} |K| / \sqrt{R_0}$. Using algebraic manipulations, the above equations can be solved to evaluate $\hat{\sigma}_{11}$, $\hat{\sigma}_{22}$ and $\hat{\sigma}_{12}$, respectively. (The manipulation is left out for the sake of brevity.) The asymptotic displacement fields $\hat{u}_x$ and $\hat{u}_y$ given in Eq. 3.37 are imposed on the boundary of the geometry for $K_1 = 91.6 \text{ MPa}\sqrt{m}$, $K_2 = 24.5 \text{ MPa}\sqrt{m}$, $\gamma = \pi/12$ and $\alpha = 0$. The stress components $\hat{\sigma}_{11}$, $\hat{\sigma}_{22}$ and $\hat{\sigma}_{12}$ from the FE solution at $r = R_0$ are shown using hollow red circles in Figure 3.8. The asymptotic stress fields given in Eq. 3.38 are plotted using a black solid line. It can be seen that they closely match the stress fields

from the FE solution. This verifies that the asymptotic conditions hold, and therefore the RVFT computations correspond to the case of semi-infinite crack at the bi-material interface. The fracture toughness of material 1 and 2 is denoted by g_b . The fracture toughness of the interface shown in the Figure 3.7(b) is denoted by g_{int} . The ratio g_b/g_{int} is chosen appropriately so that for the cases of $\alpha = \{0, 0.25, 0.5\}$, the crack will always kink into material 2 (see [7] for details). Computations based on RVFT are performed for a given α and γ , such that K_1 and K_2 are increased proportionally keeping γ fixed, until the crack initiates at the notch tip and kinks into material 2, forming a crack of finite length. Representative contour plots of the damage field d from the RVFT computations corresponding to kinking of crack at the bi-material interface is shown in Figure 3.9(a) and (b), for $\gamma = \pi/12$ and $\gamma = \pi/6$, respectively for the case of $\alpha = 0.25$. The kink angle $\hat{\omega}$ is calculated by measuring the angle between the x-axis and the kinked crack segment, as shown in the figure. A series of RVFT computations are performed for $\alpha = \{0, 0.25, 0.5\}$ and $0 \leq \gamma \leq \pi/4$ and the kink angles $\hat{\omega}$ are determined. The kink angles $\hat{\omega}$ from RVFT are represented using solid green circles in Figure 3.6a, b and c for $\alpha = 0, 0.25$ and 0.5 , respectively. It can be seen that the kink angles compare reasonably well to the data obtained from [7].

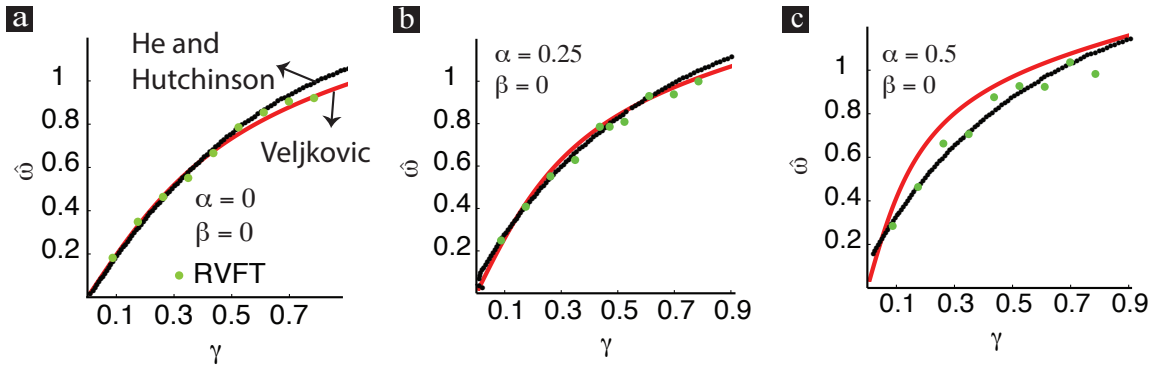


Figure 3.6: The subfigures (a-c) compare the kink angle ($\hat{\omega}$) solutions given in [7], denoted by hollow black circles, against the numerically obtained solutions from RVFT for $\alpha = 0, 0.25, 0.5$, respectively. The data obtained from RVFT computations are denoted by solid green circles. A comparison of the kink angles computed using the analytical approximations of $c(\omega, \alpha)$ and $d(\omega, \alpha)$, given in Eq. 3.36, from [8], is denoted by a solid red curve.

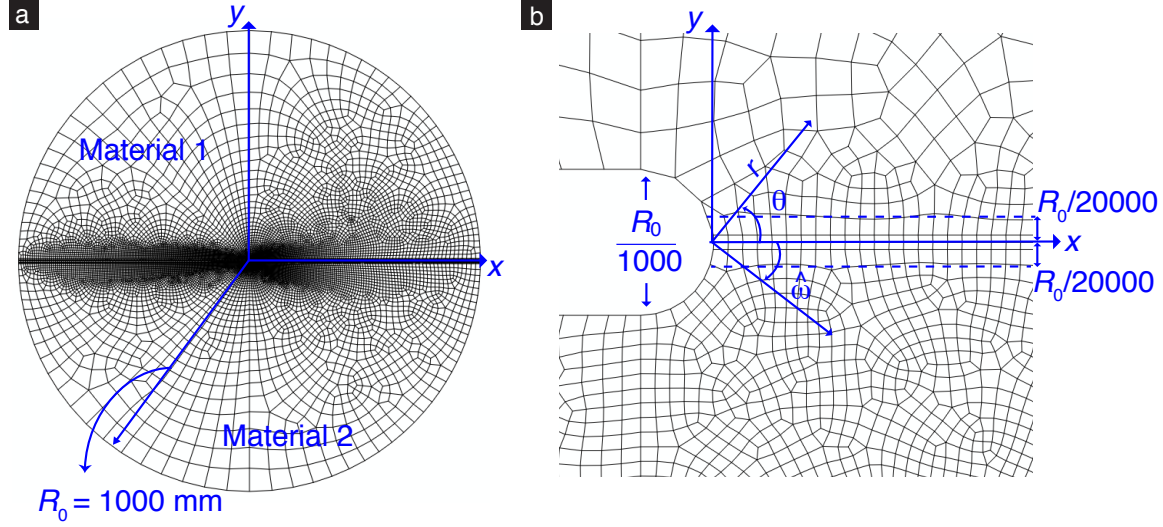


Figure 3.7: The finite element mesh of the notched circular geometry is shown in subfigure(a), where $R_0 = 1000$ mm is the radius and the notch length of the geometry. The geometry is subjected to asymptotic displacement fields $\hat{u}_x$ and $\hat{u}_y$ pertaining to that of an interface crack given in Eq. 3.37. The magnified region around the notch-tip is shown in subfigure(b), where the notch root diameter is $R_0/1000$. The x - y coordinate axis is located at the notch-tip. The polar angle θ and the kink angle $\hat{\omega}$ are measured counter-clockwise and clockwise with respect to x -axis at the notch-tip, respectively.

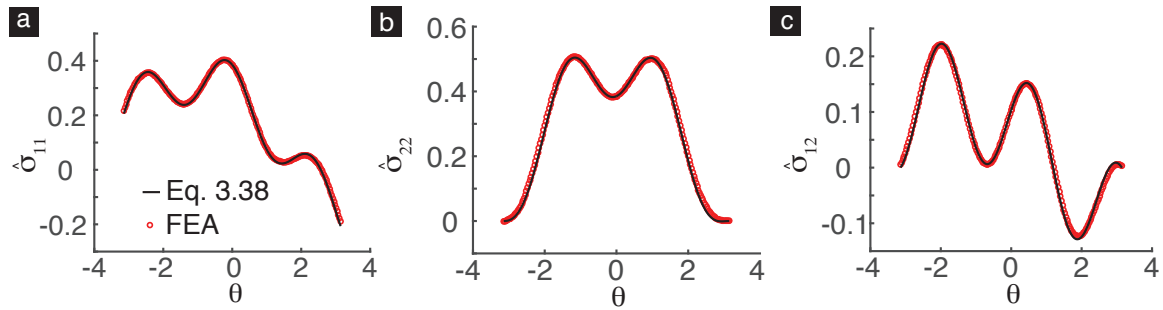


Figure 3.8: Subfigures a, b, and c show the variation of non-dimensionalized stress components $\hat{\sigma}_{11}$, $\hat{\sigma}_{22}$ and $\hat{\sigma}_{12}$ against angle θ (shown in Figure 3.7(b)) at $r = R_0$, respectively. The data obtained from FEA is denoted by hollow red circles and is compared to the asymptotic stress fields given in Eq. 3.38, denoted by a solid black line.

Crack trapping at the interface

In this section, we consider the identical semi-infinite crack at the bi-material interface and examine the condition under which the crack emanating from the tip of the interface crack remains trapped at the interface. The term crack trapping indicates that crack initiates at the tip of the interface crack and continues to grow along the interface. The occurrence of crack trapping is considered

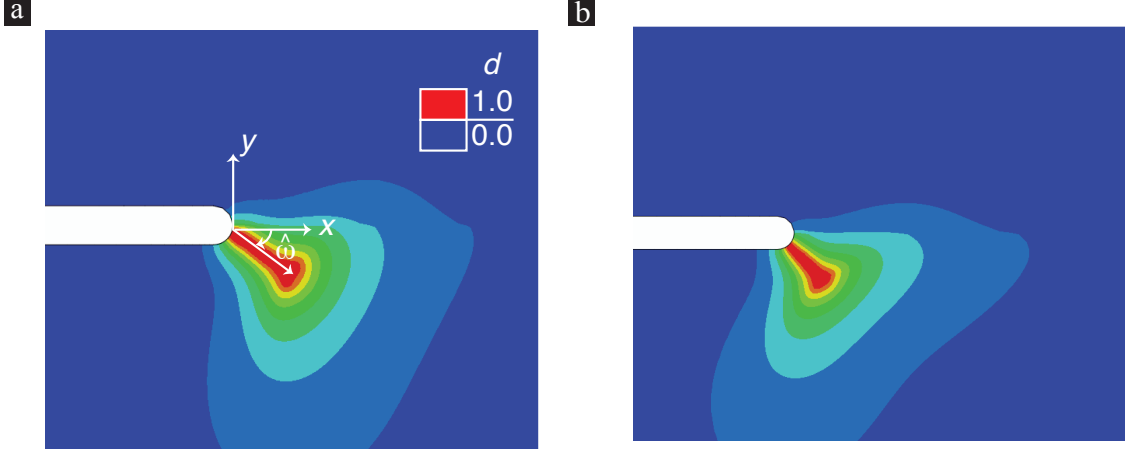


Figure 3.9: Subfigure (a) and (b) show the representative contour plots of the damage field d obtained from RVFT simulations for $\alpha = 0.25$, for the cases of $\gamma = \pi/12$ and $\gamma = \pi/6$, respectively. The crack is denoted by the field $d = 1$ and the kink angle $\hat{\omega}$ is measured clockwise from the x-axis.

in [7], where the authors state that as long as the material toughness (g_b) is sufficiently larger than the interface toughness (g_{int}), the crack will remain trapped at the interface. From Eq. 3.35, we can evaluate the ratio of the energy release rate of the kinked crack ($\mathcal{G}$) and the energy release rate of the interface crack ($\mathcal{G}_0$). Let $\mathcal{G}^*$ be the maximum of $\mathcal{G}$ with respect to ω for a given α and γ . Therefore, as long as $g_b/g_{int} > \mathcal{G}^*/\mathcal{G}_0$, the crack should remain trapped at the interface for a given loading γ and material property α . From the kink angle data (see the comparison of the solid red curve to the black circles in Figure 3.6), we can ascertain that the approximations for $c(\omega, \alpha)$ and $d(\omega, \alpha)$ are reasonable for $0 \leq \alpha \leq 0.5$. The quantity $\mathcal{G}^*/\mathcal{G}_0$ is computed using the approximations of $c(\omega, \alpha)$ and $d(\omega, \alpha)$, proposed in [8], from Eq. 3.35 for $\gamma = 3\pi/20$ and $\alpha = \{0, 0.5\}$. The variation of $\mathcal{G}^*/\mathcal{G}_0$ with α is denoted by a solid red curve in Figure 3.10. We carry out RVFT calculations by considering the same boundary value problem described in the previous section, by considering a circular geometry with interface crack of length R_0 , subjected to displacement boundary conditions $\hat{u}_x$ and $\hat{u}_y$ given in Eq. 3.37. The loading value $\gamma = 3\pi/20$ is an arbitrary choice; α varies between 0 and 0.5 and the values of g_b/g_{int} are chosen in the neighbourhood of $\mathcal{G}^*/\mathcal{G}_0$ as shown in Figure 3.10. For example, in the figure, when $\alpha = 0.1$ the quantity $\mathcal{G}^*/\mathcal{G}_0 \approx 1.4$, and therefore the ratio g_b/g_{int} is chosen in the neighbourhood of 1.4. Therefore, for $g_b/g_{int} = \{1.1, 1.3, 1.5, 1.7, 1.9\}$, RVFT computations are performed to verify whether the crack remains trapped or kinks into material 2. This is illustrated in Figure 3.10 by denoting the values of g_b/g_{int} for which the crack kinks into material

2 by green solid circles. The values of g_b/g_{int} for which the crack remains trapped at the interface is denoted by black solid circles. When the data in Figure 3.10 is compared to the crack trapping condition $g_b/g_{int} > \mathcal{G}^*/\mathcal{G}_0$, we can say that all the data points obtained from RVFT calculations below the red curve should represent when the crack is kinked, and above the red curve should represent when the crack is trapped. It can be seen that there are some data points above the red curve that indicate that crack kinking is observed, although crack trapping should have been observed. For example, let us again consider $\alpha = 0.1$, where $\mathcal{G}^*/\mathcal{G}_0 \approx 1.4$ and therefore for all $g_b/g_{int} < 1.4$, crack kinking should be observed. This is indeed true; when $g_b/g_{int} = \{1.1, 1.3\}$, crack kinking is observed. However, for $g_b/g_{int} = \{1.5, 1.7\}$ – which are values above the red curve – crack kinking occurs instead of crack trapping. Finally, for $g_b/g_{int} = 1.9$, crack trapping occurs. Therefore, we can conclude that RVFT computations qualitatively predict the phenomenon of crack trapping well, but the quantitative accuracy is low.

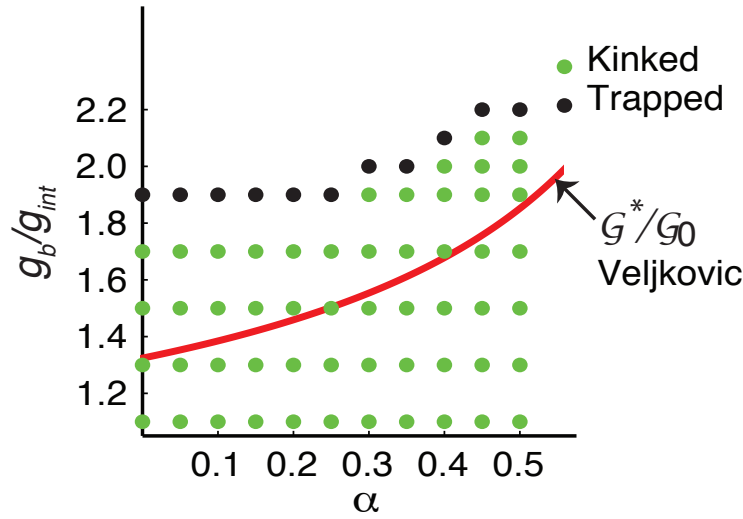


Figure 3.10: In this figure the phenomenon of crack trapping at the interface is studied where the crack grows along the interface for $g_b/g_{int} > \mathcal{G}^*/\mathcal{G}_0$. The quantity $\mathcal{G}^*/\mathcal{G}_0$ is obtained using approximations proposed in [8] and is denoted by a solid red curve. The solid circles are obtained from RVFT calculations. The green circle indicates the value of g_b/g_{int} at which a crack kinks into material 2. The black circle denotes the value of g_b/g_{int} for which the crack grows along the interface.

Chapter 4

Toughness enhancement in ceramic composites

Note: A version of certain sections of this chapter is under preparation for journal publication. Data and figures have been used with all co-authors' consent.

4.1 Introduction

In this chapter, I have applied the modified RVFT for interfaces to investigate toughness enhancement in the presence of weak interfaces. I find that crack deflection followed by crack arrest and crack re-nucleation is an important fracture mechanism that enhances toughness. Furthermore, the presence of weak interfaces is not always sufficient to enhance toughness, i.e., the geometry of the sample affects the fracture mechanism. In that respect, I have studied fracture mechanisms in rectangular and cylindrical geometries with weak interfaces. I find that toughness enhancement in cylindrical geometries is much lower than in rectangular geometries. This is because in cylindrical geometries, crack deflection occurs but crack arrest and crack re-nucleation does not. The different problems that I have studied are:

1. Two-dimensional (2D) analogs of micro-architectural designs in SBs and ceramic composites to gain insights into the operating toughness enhancement mechanisms;

2. Fracture mechanisms in three-dimensional (3D) geometries with lamellar architecture. I have specifically considered a 3D rectangular geometry with one interface and a 3D cylindrical geometry with one concentric interface.

4.2 2D analogs of structural biomaterials/ceramic composites

I have studied two 2D micro-architectures mimicking naturally occurring composites such as nacre. These are:

1. A multi-layered micro-architecture, where the bulk material has weak interfaces aligned parallel to the span of the geometry. The geometry has a v-notch oriented perpendicular to the interface and is subjected to three-point bending loading conditions.
2. A single edge notch geometry with a wavy interface aligned along the crack growth direction.

4.2.1 Multi-layered geometry

The motivation to study multi-layered geometries comes from the micro-architecture of nacre and spicules. As previously noted, spicules have a three dimensional micro-architecture where the bulk material (mineral phase) is arranged in concentric layers separated by the interface (organic phase). Multi-layered geometries, which can be considered two-dimensional analogs of spicules, have been studied extensively in the context of ceramics [9]. Clegg et al. [9] conducted experiments on Silicon Carbide (SiC), which is made into thin sheets and coated with graphite forming weak interfaces. The sheets are then pressed together to form a layered micro-architecture which can be seen in Figure 4.1 (a.ii). The work of fracture for the layered SiC-graphite material, which is notched and tested under three point bending, is 4625 Jm^{-2} , while that of monolithic SiC is 62 Jm^{-2} . The crack patterns in the layered material shown in Figure 4.1(a.ii) indicates crack deflection as a crack growth mechanism. Its load-displacement response (Figure 4.1a.i) indicates that the ceramic composite does not catastrophically fail once the peak load is reached, but instead shows step-like features beyond the peak load. This potentially enhances the toughness of the material. It is, however, unclear whether crack deflection is the only toughness-enhancing mechanism. Furthermore, any

correlation between the crack path and the observed step-like features in the load-displacement response is not well investigated. Therefore, I have studied crack growth in these multi-layered materials using the modified RVFT for interfaces.

I considered a two-dimensional geometry shown in Figure 4.1b, where the bulk material is separated by weak interfaces (represented by the region within the dashed grey line) that are aligned parallel to the span of the geometry. The interfaces are prescribed with a fracture toughness of g_I , while the bulk toughness is g_b such that $g_{int} \approx 0.1g_b$. The width of the interface is $m\ell = 0.05$ mm. The v-notch is oriented perpendicular to the interface and the geometry is subjected to three-point bending loading conditions. It is to be noted that the elastic properties are homogeneous throughout the material where the Young's modulus $E = 20.8$ GPa and the Poisson's ratio $\nu = 0.3$. Figure 4.1c shows the effect of the interfaces on the load-displacement response. From the figure, we can see that the geometry with 0 interfaces (monolithic or of homogeneous toughness g_b) reaches a peak load and fails in a brittle manner, as shown by an almost vertical drop in load after the peak load is reached. However, in the geometry with one interface, the load-displacement response shows a step-like feature after the peak load is reached similar to that seen in Clegg et al.'s work [9]. Let us examine the 3-interface case in detail and its crack path in Figure 4.1d. The peak load in the load-displacement response is denoted by the symbol A , and it drops almost vertically until B . The corresponding crack path can be tracked in Figure 4.1d using the same symbols. It can be seen that crack grows from the v-notch, i.e. point A up to the interface boundary at B , before it deflects at the first interface. When the crack deflects, the load gradually drops from B to C . Once the deflected crack penetrates into the bulk material, the load drops rapidly to point D , which corresponds to the boundary of the second interface. On keen observation, it can be noticed that the load-displacement curve from D to E is flatter than from B to C . This is because the second interface is closer to the region where the load-point displacement was applied, leading to compressive σ_{yy} that relaxes the stressed state. Therefore, the crack-driving force reduces, causing the crack to remain trapped at the second interface before it eventually penetrates into the bulk material. The trapping of the crack reflects as the almost horizontal step $C - D$ on the load-displacement curve, thus indicating an increased crack resistance. The same observation can be made in the case of the 4-interface simulation, where the load-displacement response shows the increased length of step size as the

crack impinges at the second, third, and fourth interfaces. The same feature can be observed in the load-displacement curve of the multi-layered SiC-graphite material, where the step size increases as the applied displacement increases.

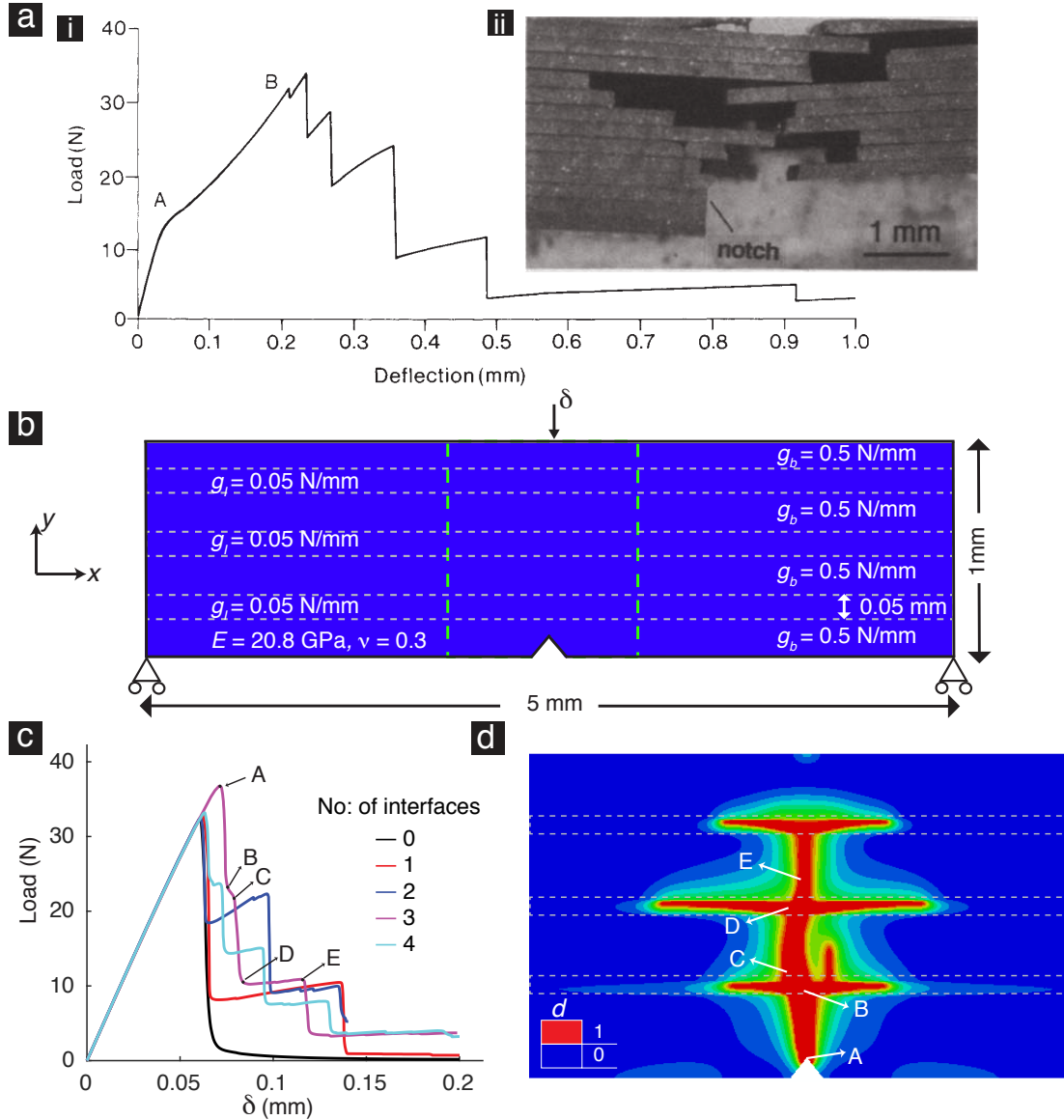


Figure 4.1: The subfigure (a.i) corresponds to the load-deflection response of a SiC-graphite composite. Its fracture surface is shown in subfigure (a.ii). The data is adopted from [9]. In subfigure (b), a schematic of a layered micro-architecture is depicted with layers prescribed with a fracture toughness of g_l and the bulk with a fracture toughness of g_b . The geometry has a v-notch and is subjected to three point bending loading conditions. Subfigure (c) shows the load-displacement response for 0 to 4 layers and subfigure (d) shows the crack path for a 3-layer composite. In subfigures (c) and (d) the crack path and the corresponding load points are indicated by points A,B,C,D,E in order to correlate the load-displacement behavior with the crack path.

4.2.2 Wavy interface

We have discussed in detail how toughness is enhanced due to the presence of weak interfaces in SBs. Can the geometric features of the interface enhance fracture toughness? For example, rams have wavy interfaces in their skull called suture joints that enhance toughness [109]. Suture joints that enhance toughness are also found in the beaks of woodpeckers [110]. There have been experimental studies to determine the role of wavy, weak interfaces in enhancing toughness [111, 112], and several models have been used to understand how this may occur [46, 113, 114]. However, the role of other factors, such as the amplitude of waviness on toughness enhancement, is not well understood because the models do not predict the crack path. Tracking the crack path is necessary to design wavy interfaces that maximize toughness.

In this section, we review how the interface geometry affects the toughness of the material by computing the work of fracture for straight and wavy interfaces. The interfaces are prescribed with a fracture toughness of g_I , while the bulk toughness is g_b such that $g_{int} \approx 0.01g_b$. The geometries for straight and wavy interfaces are shown in Figure. 4.2a.i and a.ii, respectively. The geometries are subjected to far-field displacement in the y direction (Mode-I loading). The wavy interface from the notch-tip is initially horizontal up to a certain length so that peak load at crack initiation is identical to that of the straight interface case. The wavy shape of the interface has an amplitude/wavelength ratio equal to one. The load-displacement response for both the cases is shown in Figure 4.2b. The wavy interface geometry shows a higher work of fracture as compared to the straight interface case. When the interface is straight, the crack extends along the interface (Figure 4.2c). However, when the interface is wavy, the crack path is much more complicated (Figure 4.2d). In the wavy interface, the crack initially extends along the straight segment of the interface before it deflects along the interface. The deflected crack remains trapped at the interface before it renucleates and jumps into the bulk material. We can correlate this instability with that of the load-displacement behavior. Let us consider a region of the load-displacement curve shown in the inset of Figure 4.2b, where the segment $A - B$ has almost constant load and the segment BC indicates a sharp load drop. The crack path that traversed during the same region of load-displacement response is tracked in Figure 4.2(e). The crack path from A to B corresponds to the almost constant load scenario. The crack is trapped at the interface which enhances the toughness. Once the crack becomes unstable, it

leaves the interface and jumps into the bulk material (segment $B - C$), thus leading to a load drop. Therefore, crack growth in the case of a wavy interface is constituted by a series of crack-trapping events at the interfaces followed by crack jumps into the bulk material. These events appear as steps in the load-displacement response, and enhance the material's toughness.

There are several interesting observations that can be made during the crack growth process. The weak interface nucleates cracks even before the main crack intersects the interface (Figure 4.2e). We can identify the main crack which approaches the interface, and we can also see the formation of daughter cracks at the interface. Daughter cracks form because the effective interface toughness is weaker than the bulk material (almost $0.01 g_b$), so it fails due to the tensile stress field present ahead of the main crack. This phenomenon is similar to the Cook-Gordon mechanism [104], which postulates that the nucleation of daughter cracks at a weak interface is due the stress field of a crack approaching almost perpendicular to the interface.

4.3 Fracture mechanisms in 3D analogs of structural biomaterials

As previously mentioned, despite being primarily composed of brittle ceramics, some structural biomaterials (SBs), such as bones and shells, are remarkably tough [1, 3, 115, 116]. For example, nacre—the iridescent material found in mollusk shells—is composed of $>95\%$ aragonite by volume (a brittle, calcium carbonate mineral), yet it has a specific fracture initiation toughness on par with nylon and some iron alloys [116]. These tough SBs are often heterogeneous and are composed of alternating layers of ceramic and organic materials (see Figure 4.3). The arrangements of these layers, which we refer to as layered architectures, are thought to be responsible for the enhanced toughness observed in these SBs [117].

A number of SBs, including nacre and bone, have served as models for the seminal research on understanding these connections [21, 40]. Recently, the anchor spicules of the marine sponge *Euplectella aspergillum* (*E. aspergillum*) have been added this group of model SBs [117–120]. The anchor spicules are hair-like fibers that attach *E. aspergillum* to the soft sediment of the sea floor where it lives (see Figure 4.4 (A)–(B)) [121]. Each of the thousands of anchor spicules in an *E. aspergillum* sponge is approximately 10 cm long and $50\ \mu\text{m}$ in diameter. Viewed in cross-section,

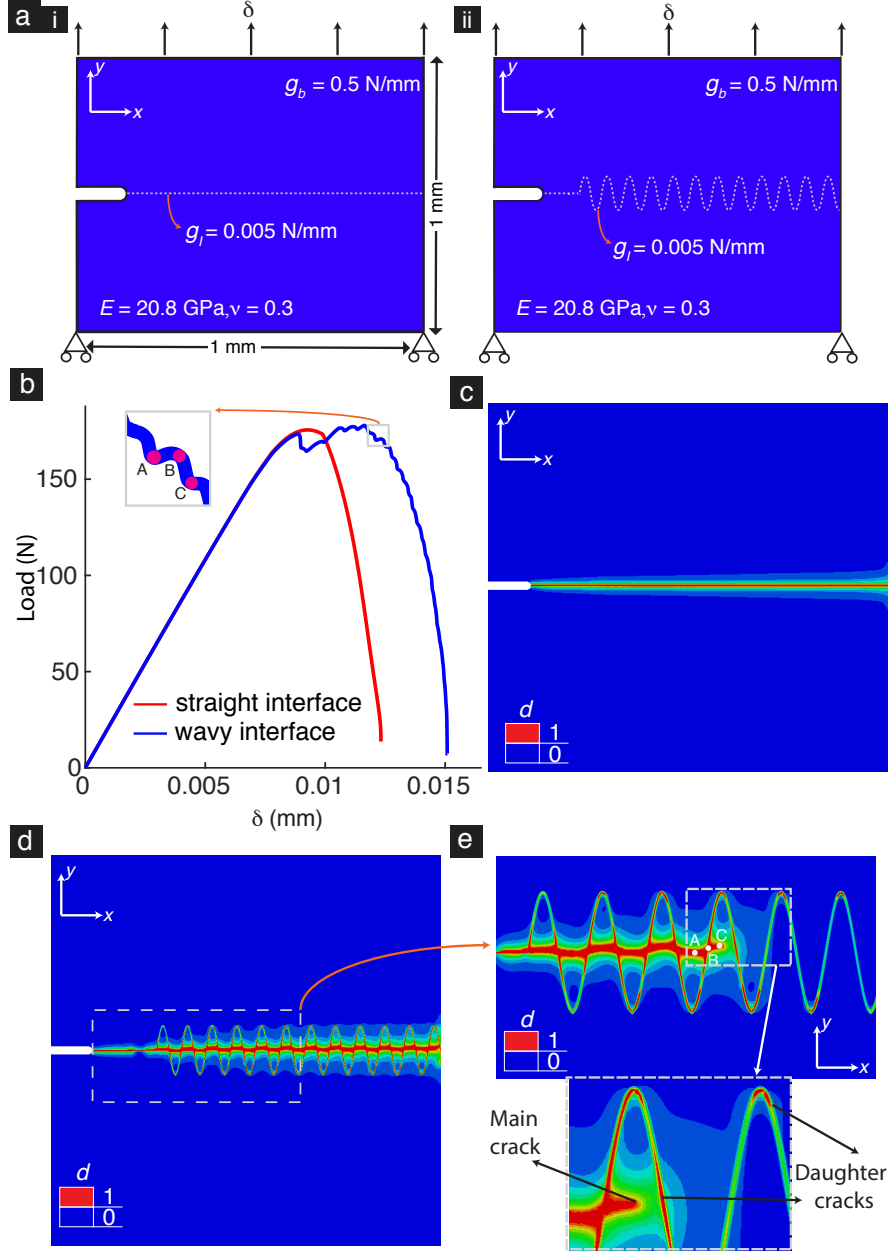


Figure 4.2: Subfigures (a.i) and (a.ii) describe the single-edge notch tension geometry with a straight interface and a wavy interface, respectively. In subfigure (b), the load-displacement response of the straight and wavy interface cases are shown. The load-displacement response for the wavy interface shows the occurrence of step-like features, as shown in the inset. Furthermore, the work of fracture for the wavy interface is higher than that of the straight interface. Subfigure (c) shows the crack path of a straight interface, while (d) shows the crack path of a wavy interface. In subfigure (e), a magnified view of a crack path shows crack trapping and crack jumping from the interface to the bulk material. Just ahead of the main crack, one can also observe the generation of daughter cracks at the interface.

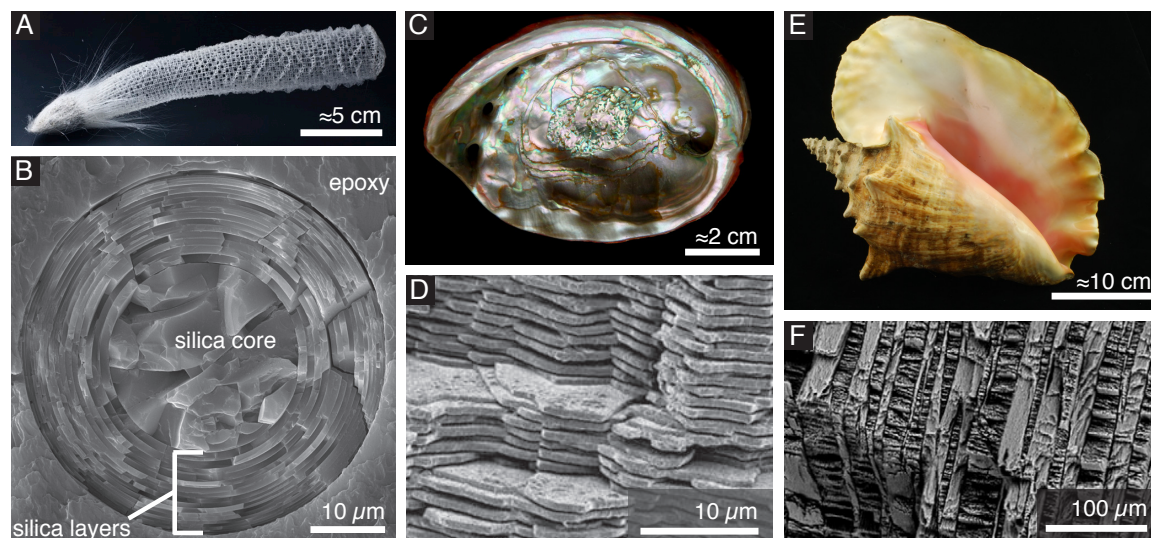


Figure 4.3: Examples of the layered architecture in SBs. (A) Skeleton of a *Euplectella aspergillum* sponge (modified from [10] copyright 2015, The National Academy of Sciences). (B) Concentric silica layers make up the cylindrical layered architecture of anchor spicules from *E. aspergillum* (modified from [10] copyright 2015, The National Academy of Sciences). (C) The iridescent shell of *Haliotis rufescens* (courtesy of John Varner). (D) The brick and mortar layered architecture of nacre consisting of staggered aragonite tablets (modified with permission from [11] copyright 2012, the Royal Society of Chemistry). (E) The shell of the queen conch (*Strombus gigas*) (courtesy of John Varner). (F) The crossed-layered architecture of the *S. gigas* shell, which consists of layers of aragonite (modified with permission from [12] copyright 2014, Elsevier).

an anchor spicule consists of a solid cylindrical core surrounded by ≈ 25 concentric, cylindrical layers (see Figure 4.3 B and 4.4 C) [10, 121, 122]. Both the core and the layers are composed of silica and adjacent silica layers are separated by a thin ($\approx 5\text{--}10\text{ nm}$ [121]) organic interlayer. Similar cylindrical layered architectures have also been found in spicules from a number of related sponge species [2, 123–125].

Many previous studies of *E. aspergillum* anchor spicules suggest that like the layered architectures of nacre and other tough SBs, the spicule's cylindrical layered architecture also enhances fracture toughness [117–120]. None of these studies, however, provide direct measurements of the *E. aspergillum* spicule's fracture toughness, nor by other means do they quantify how much the architecture enhances the spicule's toughness compared to that of its constituent silica. These measurements and comparisons are critical for determining whether the *E. aspergillum* spicules should be used as a template for bio-inspired materials with enhanced toughness.

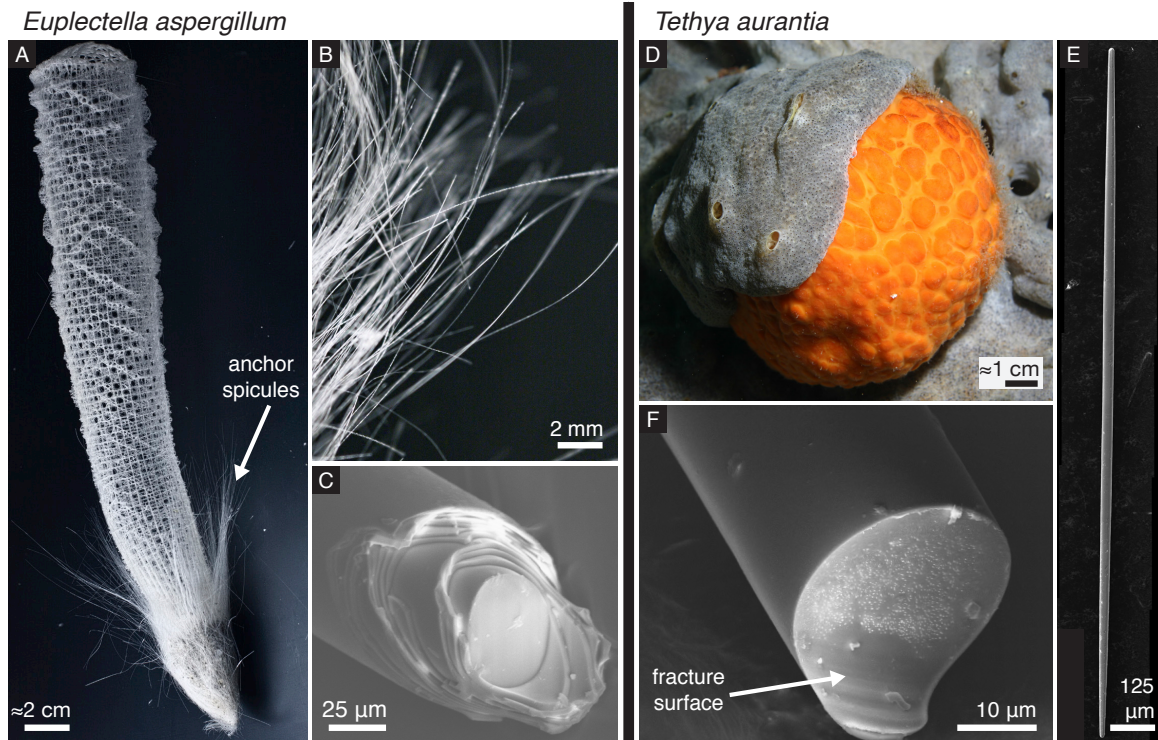


Figure 4.4: The skeletons and spicules of *E. aspergillum* and *T. aurantia* sponges. (A) The skeleton of the *E. aspergillum* sponge (modified from [10]). (B) The anchor spicules that fasten the sponge to the seafloor (modified from [10]). (C) The broken end of an *E. aspergillum* anchor spicule that was fractured in a three-point bending test showing its layered architecture (modified from [6]). (D) A *T. aurantia* sponge (image courtesy of Steve Lonhart/NOAA MBNMS). (E) A toothpick-like spicule found within the *T. aurantia* sponge (reproduced from [13] under the Creative Commons 4.0 BY license). (F) The exposed surface of a *T. aurantia* spicule that was fractured in a three-point bending test as the *E. aspergillum* spicule shown in (C) showing that it does not contain a layered architecture (modified from [6]).

4.3.1 Fracture toughness of spicules

In this section, I review a brief summary of the experimental work evaluating the fracture toughness of *E. aspergillum* spicules performed by Michael Monn. The fracture toughness of an *E. aspergillum* spicule is evaluated by conducting three-point bending fracture tests on *E. aspergillum* spicules. To quantify the toughness enhancement provided by the *E. aspergillum* spicule's architecture, its fracture toughness is compared to the fracture toughness of spicules from a related sponge, *Tethya aurantia* (*T. aurantia*) (see Figure 4.4D–F). The *T. aurantia* spicules have a similar chemical composition and bonding structure to the *E. aspergillum* spicules [2], but do not possess a layered

architecture (see Figure 4.4F) [13]. The *T. aurantia* spicules' fracture toughness using the same type of notched fracture test that is performed on the *E. aspergillum* spicules.

To compute the crack initiation toughness from the experiments on *E. aspergillum* and *T. aurantia* spicules, it is assumed that the crack front is straight and parallel to the notch root. The initial crack length is a and incremental crack length is denoted by Δa . The energy release rate G is given by

$$G(\Delta a; w_s) = -\frac{1}{2\sqrt{(a+\Delta a)(D-(a+\Delta a))}} \frac{d\Pi(\Delta a; w_s)}{d\Delta a}, \quad (4.1)$$

where $\Pi(\Delta a; w_s)$ is the system's potential energy when the crack is of length Δa , D is the diameter of the spicule, and the applied displacement is w_s . It follows from Irwin's analysis of Griffith's theory of fracture that the necessary condition for crack growth is $G(\Delta a, w_s) \geq R(\Delta a)$, where $R(\Delta a)$ is the material's crack growth resistance [126] and w_s is the applied displacement at pop-in. It is assumed that crack growth first occurs when $G(0, w_s) = R(0)$. Thus, the fracture initiation toughness $R(0)$ is given by

$$R(0) = -\frac{1}{2\sqrt{a(D-a)}} \left. \frac{d\Pi(\Delta a; w_s)}{d\Delta a} \right|_{\Delta a=0}, \quad (4.2)$$

where w_s is the applied displacement at pop-in. The overall toughness of the spicule is characterized by the average value of the crack growth resistance R denoted as $\langle R \rangle$. Furthermore, the $\langle R \rangle$ is shown to be equal to twice the work of fracture [22].

From the fracture tests, $\langle R \rangle$ of the *E. aspergillum* spicules is found to be higher than that of the *T. aurantia* spicules. Specifically, computing the ratio $\langle R \rangle^{(EA)} / \langle R \rangle^{(TA)}$ shows that the architecture increases $\langle R \rangle$ by a factor of 2.39. While this ratio is evidence that the *E. aspergillum* spicule's architecture does enhance toughness, we should put this enhancement in the context of enhancements observed in other SBs. The crack growth resistance of architected materials and their corresponding homogeneous ceramic constituents are denoted with the superscripts (arch) and (hom), respectively. By computing $\langle R \rangle^{(arch)} / \langle R \rangle^{(hom)}$ for nacre, bone, antler, and conch shell using work of fracture data available from literature (see Figure 4.5B and Table 4.1), it can be seen that the $\langle R \rangle$ enhancement in the *E. aspergillum* spicules is quite small. For example, $\langle R \rangle^{(arch)} / \langle R \rangle^{(hom)}$ for the conch shell exceeds 1000; several hundred times larger than the $\langle R \rangle$ enhancement in the *E. aspergillum* spicules.

It can be seen that $R(0)^{(\text{arch})}/R(0)^{(\text{hom})}$ can be as large as 250 in nacre, bone, antler and conch shell (see Figure 4.5A). In contrast, the measured $R(0)^{(\text{arch})}/R(0)^{(\text{hom})}$ is found to be only 1.07 for the *E. aspergillum* spicules. Thus, while the *E. aspergillum* spicules share a common architectural motif with many tough SBs, the measurements suggest that these seemingly similar architectures do not provide comparable enhancements to either the fracture initiation toughness or average crack growth resistance.

To investigate this difference in the toughness enhancements provided by the cylindrical and flat layered architectures, I have conducted 3D RVFT simulations comparing fracture mechanisms and the work of fracture in these structures.

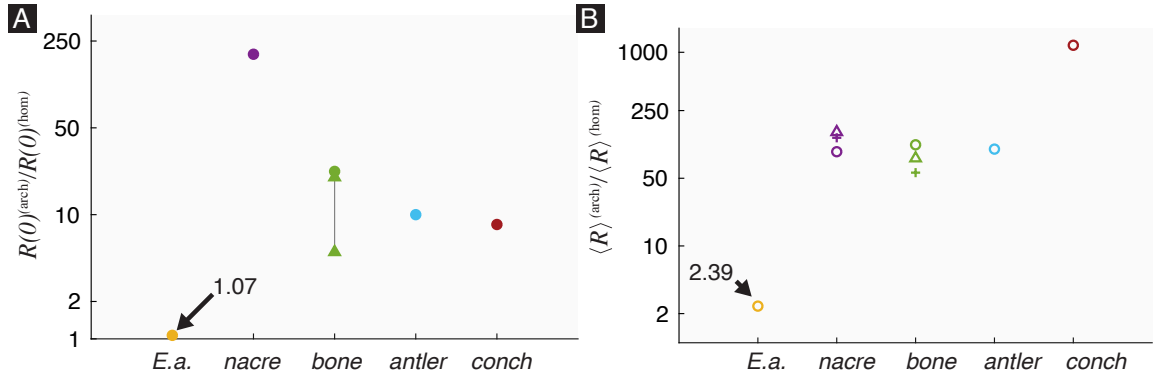


Figure 4.5: Comparison of the *E. aspergillum* spicule's toughness enhancement to the toughness enhancements of other SBs with layered architectures. (A) The initiation toughness enhancement metric $R(0)^{(\text{arch})}/R(0)^{(\text{hom})}$ of the *E. aspergillum* spicules and other SBs with layered architectures. We used the value $R(0)^{(\text{hom})} = 3 \text{ Jm}^{-2}$ of calcite as the control material for nacre and conch [14], and $R(0)^{(\text{hom})} = 10 \text{ Jm}^{-2}$ of hydroxyapatite [14] as the control material for bone and antler. (B) The average toughness enhancement metric $\langle R \rangle^{(\text{arch})}/\langle R \rangle^{(\text{hom})}$ of the *E. aspergillum* spicules and other SBs with layered architectures. We used the value $\langle R \rangle^{(\text{hom})} = 11 \text{ Jm}^{-2}$ of limestone as the control material for nacre and conch [15], and $\langle R \rangle^{(\text{hom})} = 70 \text{ Jm}^{-2}$ of hydroxyapatite [16] as the control material for bone and antler. In both (A) and (B), the values of $R(0)$ and $\langle R \rangle$ for nacre, bone, antler, and conch (*S. gigas*) were obtained from the literature (see Table 4.1). The multiple values for bone in (A) and for nacre and bone in (B) correspond to experiments performed by different research groups. The two green triangles connected by a line in (A) correspond to the range of values reported by [17]. Note that in both (A) and (B) the toughness enhancement metrics are plotted using a logarithmic scale.

Table 4.1: Summary of SB’s crack growth resistance data used to compute the toughness metrics in Figure 4.5. Statistical data, such as standard deviation (s.d.), standard error (s.e.), and sample number (N) are included when available.

Material	$R(0)$ [Jm^{-2}]	$\langle R \rangle$ [Jm^{-2}] ^{c)}	Ref.
nacre (<i>Pinctada margaritifera</i>)	587 ± 189 (mean $\pm$ s.d., $N=14$)	2068 ± 544 (mean $\pm$ s.d., $N=12$)	[40]
nacre (<i>Pinctada margaritifera</i>)	—	3300 ± 78 (mean $\pm$ s.e.) ^{d)}	[21]
nacre (<i>Pinctada margaritifera</i>)	—	2880 ± 260 (mean $\pm$ s.d.) ^{d)}	[127]
bone (<i>Homo sapiens</i>)	50–200	$11250^{\text{e)}$	[17]
bone (<i>Homo sapiens</i>)	224 ± 2 (mean $\pm$ s.d., $N=7$) ^{f)}	—	[44]
bone (<i>Papio anubis</i>)	—	15520 ± 2900 (mean $\pm$ s.d., $N=3$)	[128]
bone ^{a)}	—	8000 ± 524 (mean $\pm$ s.e.) ^{d)}	[21]
antler (<i>Cervus canadensis</i>)	$100^{\text{e)}$	$14000^{\text{e)}$	[129]
conch (<i>Strombus gigas</i>)	25 ± 7 (mean $\pm$ s.d., $N=4$)	26000 ± 14000 (mean $\pm$ s.d., $N=8$)	[130]
calcite ^{b)}	≈ 3	—	[14]
limestone	—	22	[15]
hydroxyapatite ^{b)}	≈ 10	—	[14]
hydroxyapatite	—	140	[16]

^{a)} The authors of this work did not specify the genus and species from which the bone specimens were obtained;

^{b)} Approximate values are given because the data was taken from a graph showing ranges of property values;

^{c)} Values were obtained for the work of fracture, γ_{WOF} , and were used to compute $\langle R \rangle = 2\gamma_{WOF}$;

^{d)} The number of specimens was not given in the referenced work;

^{e)} Values estimated from R -curve data;

^{f)} The reference provides the mode I stress intensity factor, K_I , at crack growth initiation. From this we estimated $R(0)$ to be K_I^2/E , where E is the Young’s modulus [17]. We take the value of E to be 18.6 GPa as per [131].

4.3.2 RVFT simulations of 3D analogs of nacre and spicules

The model material with a planar layered architecture consists of a notched beam with a rectangular cross-section whose width $W = 1$ mm, thickness $H = 1$ mm and length $L = 5$ mm. The beam is composed of two layers separated by a thin interface (see Figure 4.6 (A)). Similarly, our model material with a cylindrical layered architecture consists of a notched beam with a cylindrical cross-section composed of two layers separated by a cylindrical interlayer (see Figure 4.6 (B)). We constrained the cylindrical beam to have the same volume as the rectangular beam and therefore its diameter $D = 1.1228$ mm and length $L = 5$ mm. The notch length a in both beams is 0.2 mm.

In both beams, the interlayer has a thickness $t = 0.1$ mm and is located a distance $b = 0.2$ mm from the notch root. The Young's modulus $E = 20.8$ GPa and Poissons ratio $\nu = 0.3$ are the same in both the layers and the interlayer. However, the fracture toughness is $g_b = 500 \text{ Jm}^{-2}$ in the layers and $g_I = 0.5 \text{ Jm}^{-2}$ in the interlayer. The geometries are subjected to three-point bending loading conditions, by applying a displacement w_0 shown in Figure 4.6.

In Figure 4.6 (C) we show the load-displacement (F - w_0) response of the planar layered beam as well as that of a beam with the same geometry but without the interlayer. The monolithic beam exhibits typical brittle behavior with crack initiation occurring at $F \approx 25$ N leading to a large drop in F , which corresponds to abrupt crack growth, followed by a decrease in F until complete failure. The planar layered beam shows an almost identical response until the peak load is reached and first load drop occurs. After the first load drop, however, the load again increases before a second load drop occurs leading to complete failure. The crack path for the planar layered beam at $w_0 = 0.16$ mm is shown in Figure 4.6 (D). By examining the crack path at different values of w_0 , we observe three stages of crack growth:

1. A crack initiates at the peak load and grows until it reaches the interlayer. This corresponds to the first load drop from $F \approx 25$ N to $F \approx 9$ N. Once the crack reaches the interlayer, it is arrested.
2. The load then increases from $F \approx 9$ N to $F \approx 10$ N. During this increase, some amount of interfacial fracture occurs (see Figure 4.6 (D)) but the crack does not grow into the second layer. Thus, the increase in load corresponds to the crack being arrested by the weak interface.

3. Finally, the crack re-nucleates in the second layer, resulting in the second load drop from $F \approx 10$ N to $F \approx 5$ N. After the second load drop, the crack continues to grow through the second layer until complete failure occurs.

I computed $\langle R \rangle^{(\text{arch})} / \langle R \rangle^{(\text{hom})}$ from the force-displacement response of the planar layered beam to be 1.18. This toughness enhancement is caused by the combined effects of two toughening mechanisms: interfacial fracture, and crack arrest and re-nucleation.

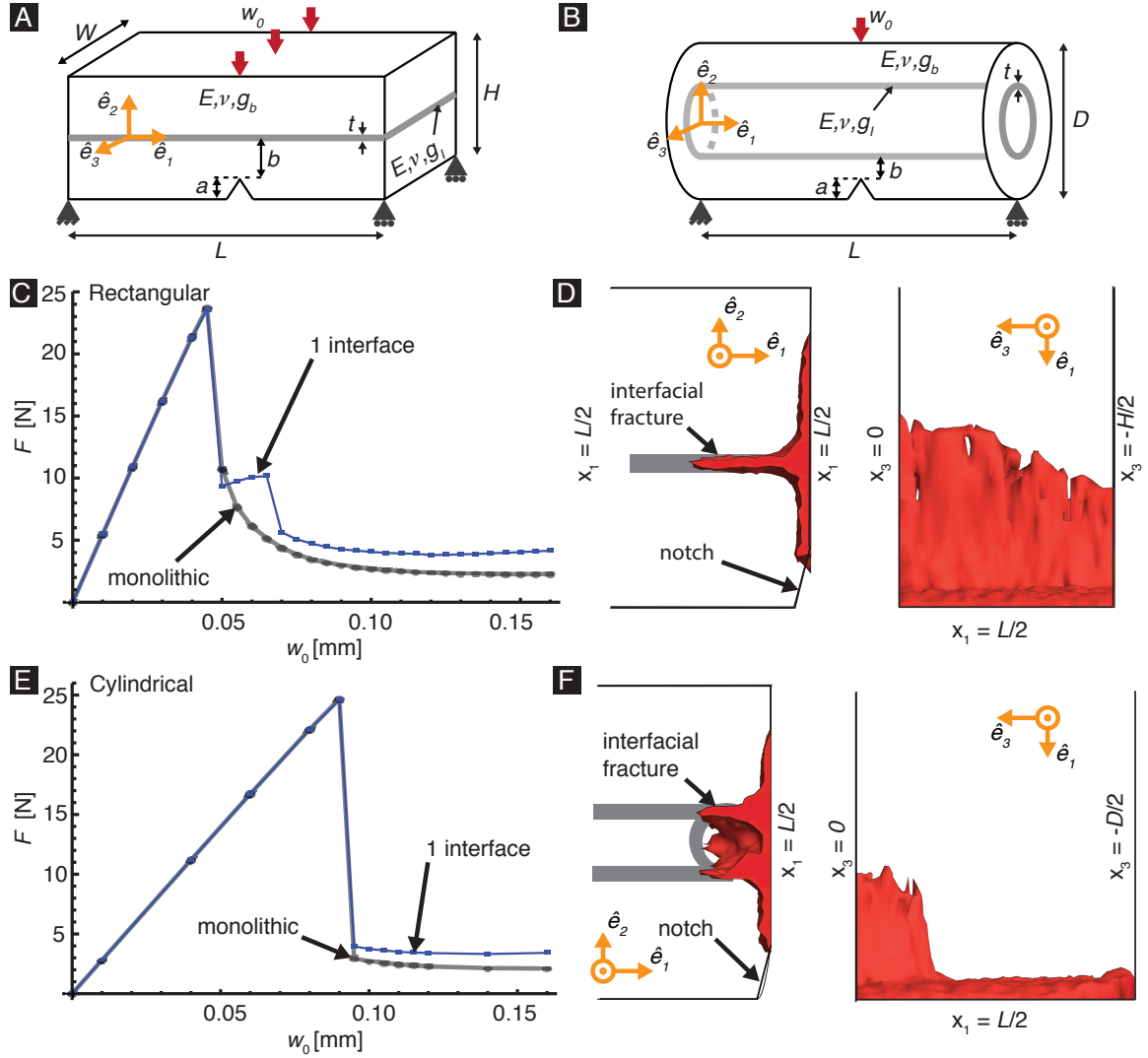


Figure 4.6: Regularized variational fracture model of beams with planar and cylindrical layered architectures. (A) Geometry of the notched layered beam with one planar interlayer shown in gray. (B) Geometry of the notched cylindrical layered beam with one cylindrical interlayer shown in gray. (C) Load displacement ($F-w_0$) response of the planar layered beam loaded in three-point bending. (D) Crack paths in the planar layered beam as seen from the planes whose normal vectors are $\hat{e}_3$ and $\hat{e}_2$. The red region corresponds to the crack path predicted by the RVF calculations at a displacement $w_0 = 0.16$ mm. (E) $F-w_0$ response of the cylindrical layered beam loaded in three-point bending. (F) Crack paths in the cylindrical layered beam as seen from the planes whose normal vectors are $\hat{e}_3$ and $\hat{e}_2$. The red region corresponds to the crack path predicted by the RVF calculations at a displacement $w_0 = 0.16$ mm. The gray curves in (C) and (E) correspond to monolithic beams with the same geometry and bulk properties.

Chapter 5

Design and testing of architected composites to show that weak interfaces enhance toughness

5.1 Introduction

From the literature survey in Chapter 1 and the fracture tests on spicules (courtesy of Michael Monn) in Chapter 4, characterizing the material properties of the constituents of SBs is not straightforward. The dimensions of the brittle and organic phase in SBs is in the order of micrometers and nanometers, respectively. Characterizing material properties at such small length scales is a complicated process. Therefore, I have pursued the design of composites that mimic the SBs using polymethyl methacrylate (PMMA) as the brittle phase and a network of interfaces composed of an adhesive. The advantage of designing these composites is that it helps us characterize the bulk material and the strength of the adhesive. Bio-inspired design and manufacturing of synthetic structures for enhanced toughness have been studied using manufacturing methods such as 3D printing, freeze casting, co-extrusion, sintering, fused deposition modeling, and laser engraving. Synthetic composites mimicking nacre-like architecture or conch-like architecture have been manufactured using fused deposition modeling (a form of 3D printing) and are found to show toughness properties

that are superior to their constituents [132, 133]. Freeze casting has been used to manufacture hybrid composites mimicking nacre that possess both superior strength and toughness as compared to nacre [134, 135]. Other methods such as SHELL (Sequential Hierarchical Engineered Layer Lamination) [136] have been used to study *Strombus Gigas*-like laminates and the role of hierarchy in their architecture, while methods such as sintering have been used to study nacre-like laminates [9]. However, these manufacturing techniques are not general purpose and versatile. For example, fused deposition modeling is confined to certain classes of materials like thermoplastics. SHELL has only been demonstrated in ceramics. Laser engraving creates small radial cracks which act as an array of defects forming weak interfaces [111]. Laser engraving is limited to materials with certain specific optical properties; and even then, it cannot be applied at regions that are deep within the bulk of the solid.

5.2 Conch shells as a model template for architecturing composites

As previously noted, the toughness of conch shells is several orders of magnitude higher than its constituent. The toughness enhancement in conch shells is almost an order of magnitude higher than nacre, although both nacre and conch are both composed of the same brittle phase aragonite. It is hypothesized that the complex architecture of conch shells is responsible for the toughness enhancement. A schematic of conch shells' architecture is shown in Figure 5.1, where the solid lines form the interfaces. These shells can be sectioned into outer, middle and inner layers. Each of these layers consists of first order lamella oriented 0° or 90° to each other. Within each of these first-order lamellae, there are second-order lamella oriented at an angle of $35^\circ - 45^\circ$ with respect to the first order lamella. Furthermore, within each of these second-order lamellae, there exist third-order lamella. Therefore, conch shells have multiple levels of hierarchy as compared to nacre or spicules. This hierarchy could potentially introduce more instances of crack deflection, crack arrest, and crack re-nucleation, thus contributing to the observed high toughness enhancement.

Using conch shell as a template to design architected composites, I have developed PMMA-based composites with three levels of hierarchy in a two-dimensional setting. PMMA is procured

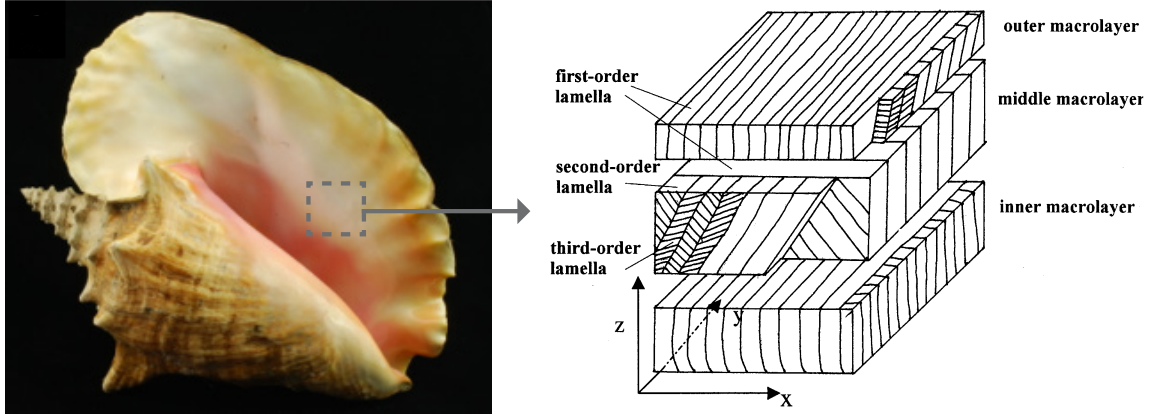


Figure 5.1: A schematic of the architecture of a conch shell, adapted from [18]. Conch shell is image courtesy of John Varner. Conch shells have a hierarchical architecture with shells sectioned into outer, middle and inner macrolayers. Within each of the macrolayers there exist first-order, second-order, and third-order lamella. The first-order lamella are oriented either at 0° or 90° , while the second-order lamella are oriented between $35^\circ - 45^\circ$ with respect to the first order lamella.

in the form of sheets and is laser cut and varied in the length and angle of the cuts in two dimensions ($x - y$ plane). The cut pieces of PMMA are assembled using a weak adhesive which forms the interface between the PMMA pieces. These composites can serve as a template to find out whether toughness enhancement occurs purely through interfacial fracture mechanisms. If so, is the enhancement significant?

5.3 Design of PMMA composites and the experimental procedure

Monolithic PMMA sheets are shown in Figure 5.2(A.i). The design to be architected is fed to the laser cutting machine. The PMMA sheets are adhered to a base layer of PMMA so that PMMA pieces remain intact after the laser cutting operation. The laser cut sample with various pieces is shown in Figure 5.2(A.ii). These PMMA pieces are detached from the base layer and the individual pieces are shown in Figure 5.2(A.iii). The PMMA pieces are then re-assembled with glue (Figure 5.2(A.iv)). The experimental setup is shown in Figure 5.2B, where the sample is mounted on a three-point bending fixture. The dimensions of the sample are shown in Figure 5.2B. The ratio $a/W = 0.25$ and $L/W = 2$, where a is the notch depth, L is the span and W is the width of the sample.

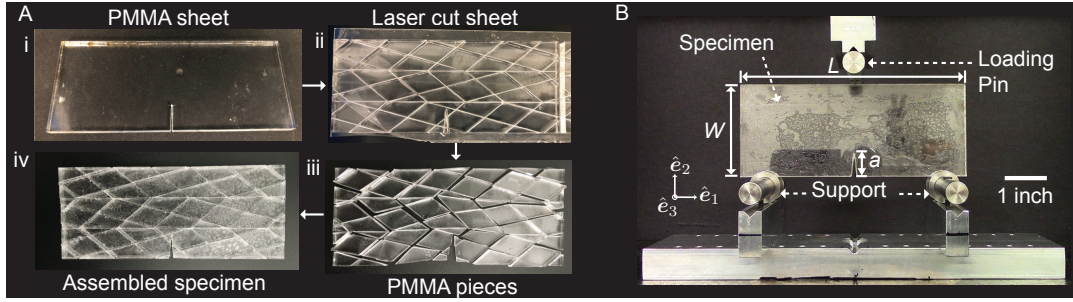


Figure 5.2: Subfigure A shows the specimen preparation process, where the PMMA sheet is laser cut on a base layer ((i) and (ii)) and the individual PMMA pieces are obtained (iii). Eventually these pieces are assembled back using a glue (iv). Subfigure B shows the three-point bending fixture, where L is the span of the specimen, W is the width, and a is the depth of the notch.

The Young's modulus for PMMA is characterized by using an un-notched sample with $L/W = 10$, so that Euler-Bernoulli (EB) beam theory results can be used to compute the Young's modulus [137]. A finite element (FE) model with linear elastic constitutive law is used to verify the prediction of Young's modulus from EB theory. The dimensions of the geometry in the FE model are chosen to be identical to those in the experiments. The Young's modulus from EB theory is given as the input to the FE model and the Poisson's ratio is chosen to be 0.35 [138]. The load-displacement response from the FE model subjected to three-point bending boundary conditions is compared against the experimental load-displacement response. The analysis ensures that PMMA shows linear elastic behavior and verifies the accuracy of EB theory.

Three-point bending notched fracture tests are conducted on three sample samples shown in Figure 5.3. The first sample is a monolithic sample with no interfaces (Figure 5.3(A)). The second sample is the architected composite with several crisscrossing interfaces (composed of a weak adhesive) shown in Figure 5.3B. The interfaces are organized as first-order lamella, second-order lamella, and third order lamella using blue dashed lines, red dashed lines and green dashed lines, respectively. Therefore, the architected composite mimics the conch shell architecture in a 2D sense. The third sample, shown in Figure 5.3C, has an interface aligned with the notch tip, denoted by a green dashed line. This sample is used to characterize the toughness of the interface, i.e. whether the adhesive is tough or weak.

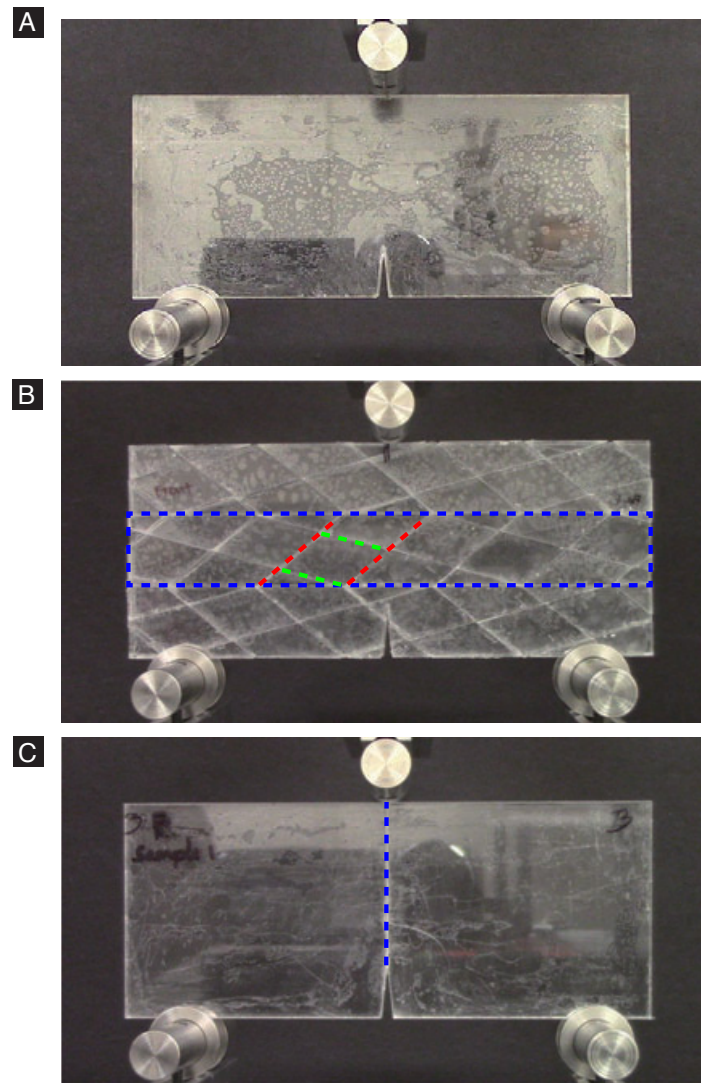


Figure 5.3: (A) The monolithic PMMA sample. (B) The architected PMMA composite where the first order, second order, and the third order of hierarchy is denoted using blue, red, and green dashed lines, respectively. (C) The sample with an interface (denoted using blue dashed lines) aligned parallel to the width of the sample from the notch tip.

5.4 Experimental results on un-notched and notched samples

5.4.1 Young's modulus measurements

To characterize Young's modulus of PMMA, un-notched specimens of aspect ratio $L/W = 10$ are tested under three-point bend loading conditions. A typical load-displacement response of one such specimen is shown in Figure 5.4A and the geometry of the specimen is shown as an inset. The stiffness k of the specimen is computed using a best-fit linear curve shown in Figure 5.4B. It can be seen that the best-fit linear curve compares well with the experimental data for $L/W = 10$. The stiffness k is computed to be 0.116 kN/mm. From EB theory, Young's modulus E is given as

$$E = \frac{L^3 k}{48I}, \quad (5.1)$$

where I is the moment of inertia and is equal to $BW^3/12$. The symbol B is the thickness of the specimen. For the specimen dimensions $L = 8.5$ inches, $W = 0.85$ inches and $B = 0.5$ inches, the Young's Modulus E is computed to be 2.28 GPa. The Young's modulus E from EB theory is given as an input to a three dimensional FE model with a linear elastic constitutive law. The geometry of the FE model is identical to the one shown in Figure 5.4A and the Poisson's ratio is taken to be 0.35 [138]. The comparison of the load-displacement response from the FE model against the experimental data in Figure 5.4C indicates that the E computed using EB theory is accurate. I also conducted an additional verification to ensure that prediction using EB theory is accurate. I compared the load-displacement response of FEA and the experimental data for an aspect ratio of $L/W = 2$ in Figure 5.4D, which shows close alignment. Therefore, from this analysis, it is concluded that PMMA shows linear elastic behavior and Young's modulus is about 2.28 GPa.

5.4.2 Fracture experiment results

Three point bend fracture experiments are conducted on the samples shown in Figure 5.3. The load-displacement response of the three samples is shown in Figure 5.5A. The corresponding crack paths are shown in Figure 5.5B. The crack path for the monolithic case (i.e. the sample with no interfaces) is shown in Figure 5.5B.i, and it can be seen that the crack initiates at the notch tip and

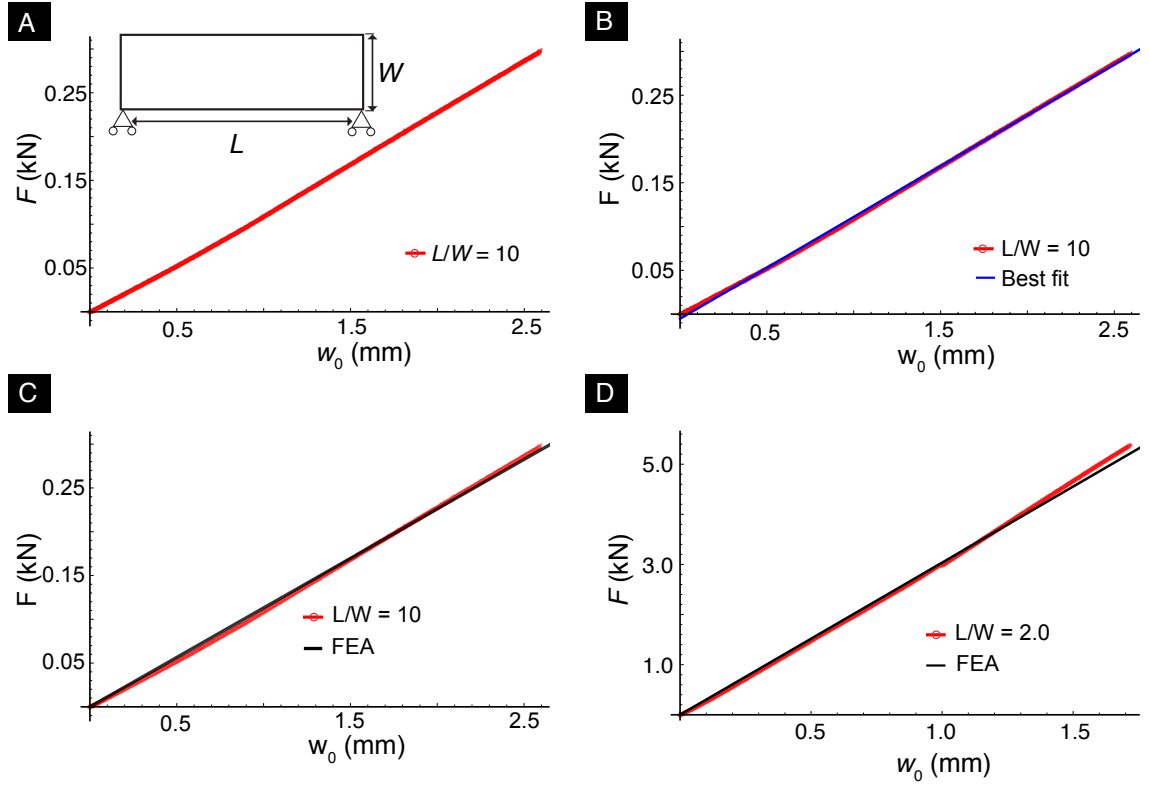


Figure 5.4: (A) In this figure the load-displacement ($F - w_0$) response for an un-notched sample with aspect ratio $L/W = 10$ is shown. (B) A linear best-fit curve is compared with the load-displacement response and the stiffness k is computed. (C) The load-displacement response from 3D finite element analysis (FEA), with a isotropic linear elastic constitutive law, is compared with the experimental data for $L/W = 10$. (D) The load-displacement response from the experiments and FEA is compared for $L/W = 2$.

extends in a direction parallel to the width of sample until failure. This crack path is typical of a brittle material subjected to mode-I loading conditions and this behavior is reflected in the load-displacement response. The sample reaches a peak load of 1.2 kN (which is approximately the crack initiation point) and then the load drops vertically to almost zero. This confirms that PMMA has a brittle behavior. In the architected sample (Figure 5.5B.ii), the crack initiates at the notch tip and deflects into the interface nearest to the notch tip. The crack is arrested at the interface before it re-initiates and grows into the next interface. Through a series of crack deflection, arrest, and re-initiation events, the crack eventually propagates in a zigzag manner until failure. The peak load for the architected sample is 0.45 kN. For the case of a solid with single straight interface (Figure 5.5B.iii), the crack grows along the interface parallel to the width of the sample reaching a peak load of 0.065 kN.

The overall fracture toughness is quantified using the work of fracture (WOF) defined in [22]. Work of fracture is defined as the area under the load vs. displacement response divided by two times the nominal crack area. The nominal crack area is determined by subtracting the notch length from the width of the sample and multiplying the result by the thickness of the sample. The WOF for the homogeneous solid, the architected composite, and the solid with a single straight interface is computed to be 262.6 J/m^2 , 2023.3 J/m^2 , and 170.2 J/m^2 , respectively. It can be seen that the architected composite is almost an order of magnitude tougher than the homogeneous solid. The solid with a single straight interface is the weakest among the three samples, indicating that the glue is indeed weak and does not contribute to the toughness. Therefore, from these systematic experiments, we can conclude that weak interfaces enhance WOF, i.e., overall toughness.

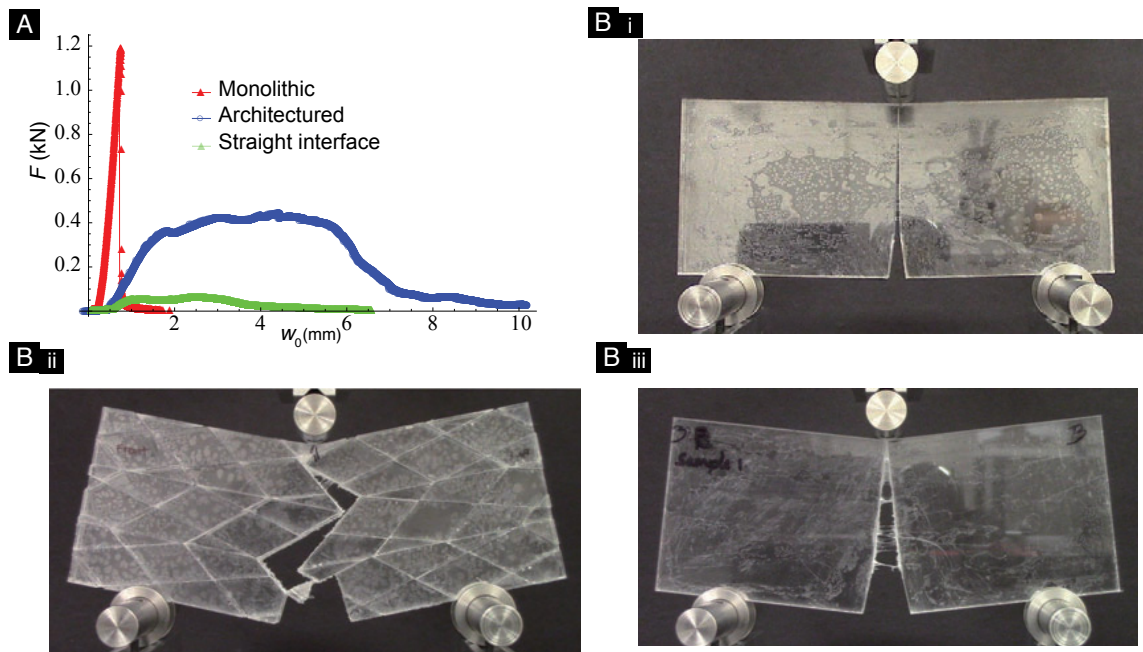


Figure 5.5: (A) In this figure, the load-displacement responses for monolithic, architected, and straight interface samples subjected to three-point bending are shown in red, blue, and green, respectively. The crack paths at the end of the test for monolithic, architected, and straight interfaces are shown in subfigures (B.i), (B.ii) and (B.iii).

Chapter 6

Conclusion

In this work, I have systematically investigated toughness enhancement mechanisms in ceramic composites through combined numerical and experimental. To this end, I developed a computational fracture mechanics tool based on RVFT to model composites composed of a brittle phase and a network of interfaces. I studied the toughness enhancement mechanisms in 2D and 3D architectures. Specifically, I predicted crack patterns and fracture mechanisms in planar lamellar architectures and concentric lamellar architectures. I have also explored the role of geometry on interfaces and developed composites composed of Polymethyl methacrylate (PMMA) with a network of interfaces. I have compared the toughness of the composites with that of monolithic PMMA samples. The notable contributions and conclusions from this work is summarized below:

1. I have developed a computational fracture model based on RVFT to model interfaces, by spatially varying the fracture toughness of the solid such that it is g_I in the interface region and g_b in the bulk solid.
2. The thickness of the interface is chosen to be $m\ell$, where ℓ is the regularization parameter ℓ . In the limit of ℓ going to 0, the interface thickness goes to 0, and the diffused crack region approaches a sharp crack region. I derived an analytical solution for the toughness of the interface, g_{int} in the limit of ℓ going to 0 and I found that the g_{int} depends on g_I , g_b and m .
3. I have verified the analytical solution for g_{int} numerically. For a single edge crack geometry under mode-I loading conditions, the critical energy release rate computed numerically for

crack initiation equals the analytical solution of the interface toughness, thus verifying the Griffith postulate of crack growth.

4. The modified RVFT model for interfaces connects very closely with studies in [7], where kink angles for a zero-thickness crack at the interface of a bi-material subjected to far-field loading conditions are predicted. I have shown that the kink angle predictions from RVFT agree well with those from [7] for different values of the Dundur's parameter α .
5. The load-displacement response predicted by the modified RVFT model for interfaces in 2D lamellar composites (SiC/graphite) compares qualitatively well with the experimental answer given in [9]. From the simulations, I discovered that the dominant fracture mechanism that enhances toughness is crack deflection at the interface followed by crack arrest and crack re-initiation at the interface.
6. From three-point bending fracture experiments, it is observed that toughness enhancement in spicules, which have a 3D concentric lamellar architecture, is significantly lower than that found in other SBs such as nacre, antler, or conch. From 3D RVFTI calculations on spicule-like architectures, I discovered that crack deflection is the fracture mechanism. Furthermore, crack arrest and crack re-nucleation is absent in these geometries. Therefore, I concluded that crack deflection alone does not enhance fracture toughness significantly.
7. I also designed PMMA based composites using the architecture of conch as a template. I computed the work of fracture (WOF) by testing notched PMMA composites under three-point bending loading conditions. I found that the WOF of a PMMA composite is almost an order of magnitude higher than that of a monolithic PMMA (homogeneous solid) sample. Furthermore, the sample with the interface aligned parallel to the width of the sample from the notch tip showed a lower WOF than the monolithic sample, indicating that glue was indeed weaker than PMMA.

6.1 Future Work

In this work I have demonstrated that by using RVFT based models, toughness enhancement mechanisms in ceramic composites can be understood. Furthermore, I have also developed a systematic methodology of developing such composites. The future work would comprise of calibrating the model parameters such as g_b , g_{int} in order to predict the crack paths in PMMA composites. The calibrated RVFT-based model can be used to study the role of hierarchy in a more systematic manner.

For example, using RVFT and numerical optimization algorithms, the optimal architecture for the interfaces in the PMMA composites that maximizes the structure's WOF in three-point bending tests can be obtained. In this optimization problem there are 12 design parameters, which are marked as $\theta_1^{(i)}, \theta_2^{(i)}, d_1^{(i)}, d_2^{(i)}$, where $i = 1, 2, 3$ in Fig. 6.1. These 12 parameters will be the arguments of the objective function in our optimization problem. For a given set of values for the 12 parameters, RVFT computation can be performed and the work of fracture from the force-displacement curve can be calculated. The WOF will be the value of the objective function in the optimization problem. Thus, the objective function in this case is only numerically defined. To solve the optimization problem, derivative-free optimization algorithms can be employed.

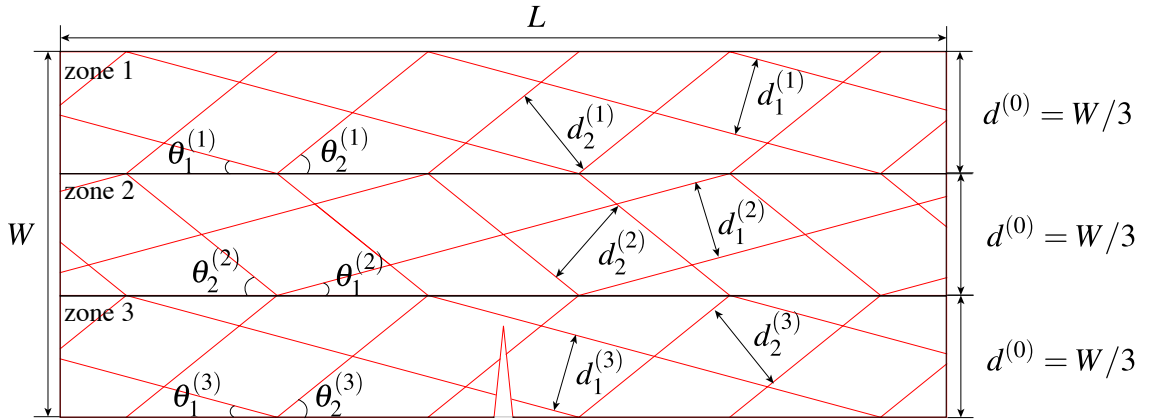


Figure 6.1: The design schematic for the 2D structure with criss-crossing interfaces.

I believe that this thesis work has laid a foundation for performing the numerical optimization of material architecture for maximizing toughness. I have demonstrated in this work that RVFT based models are robust and can predict toughness enhancement mechanisms with reasonable accuracy

in composites with weak interfaces. Extension of RVFT to non-linear material models, such as non-linear elastic solids, viscoelastic solids, and plastic solids, can lead to an exciting possibility of optimizing the architectures of composites such as metal-matrix composites and fiber-reinforced composites for maximum toughness.

Appendix A

Miehe's tension-compression split derivation of tangent stiffness matrix

Let us first evaluate the elastic strain energy $\psi(\lambda_1, \lambda_2, \lambda_3)$ in terms of the eigenvalues of ϵ :

$$\psi(\lambda_1, \lambda_2, \lambda_3) = \frac{\lambda}{2}(\lambda_1 + \lambda_2 + \lambda_3)^2 + \mu(\lambda_1^2 + \lambda_2^2 + \lambda_3^2) \quad (\text{A.1})$$

Now writing the operator split form of the $\psi(\epsilon)$:

$$\begin{aligned} \psi_0^+(\lambda_1, \lambda_2, \lambda_3) &= \frac{\lambda}{2} \langle \lambda_1 + \lambda_2 + \lambda_3 \rangle^2 + \mu(\langle \lambda_1 \rangle^2 + \langle \lambda_2 \rangle^2 + \langle \lambda_3 \rangle^2) \\ \psi_0^-(\lambda_1, \lambda_2, \lambda_3) &= \frac{\lambda}{2} [(\lambda_1 + \lambda_2 + \lambda_3) - \langle \lambda_1 + \lambda_2 + \lambda_3 \rangle]^2 + \mu((\lambda_1 - \langle \lambda_1 \rangle)^2 + (\lambda_2 - \langle \lambda_2 \rangle)^2 + (\lambda_3 - \langle \lambda_3 \rangle)^2) \\ \psi(\lambda_1, \lambda_2, \lambda_3) &= [(1-d)^2 + k] \psi_0^+(\lambda_1, \lambda_2, \lambda_3) + \psi_0^-(\lambda_1, \lambda_2, \lambda_3) \end{aligned} \quad (\text{A.2})$$

Hence, we can evaluate the σ as:

$$\begin{aligned} \sigma &= \sum_a^3 g_a \mathbf{n}_a \otimes \mathbf{n}_a \\ g_a &= \frac{\partial \psi(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_a} = [(1-d)^2 + k] \frac{\partial \psi_0^+(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_a} + \frac{\partial \psi_0^-(\lambda_1, \lambda_2, \lambda_3)}{\partial \lambda_a} \end{aligned} \quad (\text{A.3})$$

To evaluate the material elasticity tensor $\mathbb{C}$, (Bonet and Wood)

$$d_{ab} = \frac{\partial^2 \psi}{\partial \lambda_a \partial \lambda_b}$$

$$\mathbb{C} = \sum_a^3 \sum_b^3 d_{ab} \mathbf{n}_a \otimes \mathbf{n}_a \otimes \mathbf{n}_b \otimes \mathbf{n}_b + \sum_a^3 \sum_{b \neq a}^3 \frac{1}{2} \frac{g(a) - g(b)}{\lambda_a - \lambda_b} \mathbf{n}_a \otimes \mathbf{n}_b \otimes (\mathbf{n}_a \otimes \mathbf{n}_b + \mathbf{n}_b \otimes \mathbf{n}_a) \quad (\text{A.4})$$

Evaluating the above for the equations given in eq.A.2: Defining indicator functions:

$$\begin{aligned} H_1 &= 1 \quad (\lambda_1 + \lambda_2 + \lambda_3 > 0) \\ &= 0 \quad (\lambda_1 + \lambda_2 + \lambda_3 \leq 0) \\ H_a &= 1 \quad (\lambda_a > 0) \\ &= 0 \quad (\lambda_a \leq 0) \end{aligned} \quad (\text{A.5})$$

$$\begin{aligned} g_a &= [(1-d)^2 + k] (\lambda \langle \lambda_1 + \lambda_2 + \lambda_3 \rangle H_1 + 2\mu \lambda_a H_a \\ &\quad + \lambda [(\lambda_1 + \lambda_2 + \lambda_3) - \langle \lambda_1 + \lambda_2 + \lambda_3 \rangle] (1 - H_1) + 2\mu (\lambda_a - \langle \lambda_a \rangle) (1 - H_a) \end{aligned} \quad (\text{A.6})$$

where H_1 and H_a are defined in eq. A.5. Similarly, lets evaluate d_{ab} :

$$\begin{aligned} d_{ab} &= [(1-d)^2 + k] (\lambda H_1 + 2\mu \delta_{ab} H_a H_b \\ &\quad + \lambda (1 - H_1) + 2\mu \delta_{ab} (1 - H_a) (1 - H_b) \end{aligned} \quad (\text{A.7})$$

Appendix B

RVFT interface upper bound and lower bound

B.1 Distance function based on local coordinate system for the 2D problem

Let $\Omega \subset \mathbb{R}^2$ be a simply connected domain in $\mathbb{R}^2$ with C^2 boundary. Let $\alpha : [0, L] \mapsto \Gamma$ be an *arc-length* parametrization of Γ such that is $\|\alpha'(s)\| = 1$ and $\alpha''(s) = \kappa(s)N(s)$ where N is the unit normal to Γ and $\kappa(s)$ is the curvature of Γ . Details of the existence of a distance function and the tubular neighborhood $t(r)$ can be found in [139]. We can define a tubular neighborhood around the boundary with local coordinates (r, s) given by:

$$(x, y) = \alpha(s) + rN(s). \quad (\text{B.1})$$

r is simply the distance measured along the normal from the boundary and s just the parameterization coordinate. This coordinate system is orthogonal with Riemannian $\mathbf{g}$ metric with components:

$$g_{11} = 1 \text{ and } g_{22} = (1 - r\kappa(s))^2. \quad (\text{B.2})$$

Consequently, the area form on the tubular neighborhood is given by

$$dA = (1 - r\kappa(s)) dr ds, \quad (\text{B.3})$$

and for differentiable d it follows that

$$\|\nabla d\|^2 = \left(\frac{\partial d}{\partial r}\right)^2 + \frac{1}{(1 - r\kappa(s))^2} \left(\frac{\partial d}{\partial s}\right)^2. \quad (\text{B.4})$$

Note: The domain Ω is assumed to be convex, therefore, the curvature $\kappa(s) < 0$.

B.2 Upper bound

Let R be the largest value for which a tubular neighborhood coordinate system can be defined about Γ . We will assume $d \in \mathcal{V}$ (refer Eq. (3.14)) and that $d = 0$ for all $\mathbf{X} \in \mathcal{B}$ satisfying $\text{dist}(\mathbf{X}, \Gamma) > R$. Let us consider the energy functional given in Eq. (3.12) without the non-dimensionalization and denote it by I_ℓ . We can derive the non-dimensional form I_ε in the local coordinate system (r, s) by using the definition of gradient given in Eq. (B.4), the functional then becomes:

$$I_\ell[d] = \int_0^L \int_0^R \frac{g(r; m)}{2} \left(\ell \left[\left(\frac{\partial d}{\partial r}\right)^2 + \frac{1}{(1 - r\kappa(s))^2} \left(\frac{\partial d}{\partial s}\right)^2 \right] + \frac{d^2}{\ell} \right) (1 - r\kappa(s)) dr ds. \quad (\text{B.5})$$

As we did in the 1D problem, let us introduce non-dimensional variables $\varepsilon = \ell/R$ and $\hat{r} = r/R$ as follows: We can rewrite $I_\ell[d]$ as ,

$$I_\varepsilon[d] = \int_0^L \int_0^1 \frac{g(\hat{r}; m)}{2} \left(\varepsilon \left[\left(\frac{\partial d}{\partial \hat{r}}\right)^2 + \frac{1}{(1 - R\hat{r}\kappa(s))^2} \left(\frac{\partial d}{\partial s}\right)^2 \right] + \frac{d^2}{\varepsilon} \right) (1 - R\hat{r}\kappa(s)) d\hat{r} ds. \quad (\text{B.6})$$

As mentioned in section 3.3.2 that a trial function d^g defined in Eq. (3.17) would satisfy,

$$I_\varepsilon^* \leq I_\varepsilon[d^g]. \quad (\text{B.7})$$

Further, we also know that d^g depends only on $\hat{r}$. Therefore, we can drop the derivatives w.r.t the arc-length parameter s and obtain,

$$I_\varepsilon[d^g] = \int_0^L \int_0^1 \frac{g_\varepsilon(\hat{r}; m)}{2} \left[\varepsilon \left(\frac{\partial d^g}{\partial \hat{r}} \right)^2 + \frac{(d^g)^2}{\varepsilon} \right] (1 - R\hat{r}\kappa(s)) d\hat{r} ds. \quad (\text{B.8})$$

Therefore, the above functional can be re-written as

$$\begin{aligned} I_\varepsilon[d^g] &= \int_0^L \int_0^1 \frac{g_\varepsilon(\hat{r}; m)}{2} \left(\varepsilon \left(\frac{\partial d^g}{\partial \hat{r}} \right)^2 + \frac{(d^g)^2}{\varepsilon} \right) (1 - R\hat{r}\kappa(s)) d\hat{r} ds \\ &\leq \int_0^L \int_0^1 \frac{g_\varepsilon(\hat{r}; m)}{2} \left(\varepsilon \left(\frac{\partial d^g}{\partial \hat{r}} \right)^2 + \frac{(d^g)^2}{\varepsilon} \right) d\hat{r} ds \\ &= L \int_0^1 \frac{g_\varepsilon(\hat{r}; m)}{2} \left(\varepsilon \left(\frac{\partial d^g}{\partial \hat{r}} \right)^2 + \frac{(d^g)^2}{\varepsilon} \right) d\hat{r}. \end{aligned} \quad (\text{B.9})$$

Therefore, the above integral is a 1D integral in $\hat{r}$, which can be solved for the trial function d^g to obtain,

$$I_\varepsilon[d^g] \leq \frac{g_I}{2} \frac{\cosh\left(\frac{1}{\varepsilon}\right) + \cosh\left(\frac{2m\varepsilon-1}{\varepsilon}\right) \tanh\left(\frac{\alpha}{2}\right)}{\sinh\left(\frac{1}{\varepsilon}\right) + \sinh\left(\frac{2m\varepsilon-1}{\varepsilon}\right) \tanh\left(\frac{\alpha}{2}\right)} L \quad (\text{B.10})$$

which is the upper bound for the functional I_ε^* with L being the $Per(\Gamma)$.

B.2.1 Lower bound

As mentioned in section 3.3.2, we use the duality principles for convex functionals to obtain a lower bound for the variational problem I_ε^* in terms of the non-dimensional variables ε and $\hat{r}$ (refer B.2). Let the boundary at $\hat{r} = m\varepsilon$ be denoted by $\partial\mathcal{B}_{\hat{r}} \in C^2$ and by using the properties $\mathbf{P} \in \mathcal{A}$ (see Eq. (3.25)), the definition of g_ε (see Eq. (3.15))

$$\begin{aligned} I_\varepsilon^* &\geq \max_{\mathbf{P} \in \mathcal{A}} \min_{d \in \mathcal{V}} \int_\Gamma g_I \varepsilon d \mathbf{P} \cdot \mathbf{n} d\Gamma + \int_{\partial\mathcal{B}_{\hat{r}}} g_I \varepsilon d \mathbf{P} \cdot \mathbf{n} d\Gamma \\ &\quad - \int_{\partial\mathcal{B}_{\hat{r}}^+} g_b \varepsilon d \mathbf{P} \cdot \mathbf{n} d\Gamma - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon (\mathbf{P} \cdot \mathbf{P}) d\Omega - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon^3 (\nabla \cdot \mathbf{P})^2 d\Omega, \end{aligned}$$

Simplify the equation further using BCs of d given in Eq. (3.14), i.e., $d = 1$ is prescribed on Γ ,

$$I_\varepsilon^* \geq \max_{\mathbf{P} \in \mathcal{A}} \int_{\Gamma} g_I \varepsilon \mathbf{P} \cdot \mathbf{n} d\Gamma - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon (\mathbf{P} \cdot \mathbf{P}) d\Omega - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon^3 (\nabla \cdot \mathbf{P})^2 d\Omega. \quad (\text{B.11})$$

Thus, the above would give the optimal solution for $I_\varepsilon[d_\varepsilon^*]$ by maximizing over $\mathbf{P} \in \mathcal{A}$. Let us choose a trial function $\mathbf{P} = \mathbf{P}^g$ such that $\mathbf{P}^g = \nabla d^g$, where d^g is given in Eq. (3.17). On substituting for $\mathbf{P}^g$ in Eq. (B.11) we obtain,

$$I_\varepsilon^* \geq g_I \varepsilon \int_{\Gamma} \nabla d^g \cdot \mathbf{n} d\Gamma - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon \|\nabla d^g\|^2 d\Omega - \int_{\mathcal{B}} \frac{g_\varepsilon}{2} \varepsilon^3 (\Delta d^g)^2 d\Omega, \quad (\text{B.12})$$

which is the lower bound of the functional I_ε^* and where $\Delta(\cdot)$ is the Laplacian with respect to $\mathbf{X}$. To simplify this further we can transform the above functional to the local coordinate system $(\hat{r}, s)$ coordinates introduced in B.1 along with the non-dimensionalization. Let us also define Δd in $(\hat{r}, s)$ coordinate assuming the $d = d^g(\hat{r})$,

$$\nabla d = -\frac{1}{R} \frac{\partial d}{\partial \hat{r}} \mathbf{n}, \quad (\text{B.13a})$$

$$\Delta d = \frac{1}{R|1 - R\hat{r}\kappa(s)|} \frac{\partial}{\partial \hat{r}} \left(|1 - R\hat{r}\kappa(s)| \frac{1}{R} \frac{\partial d}{\partial \hat{r}} \right), \quad (\text{B.13b})$$

where $|\cdot|$ is the absolute value. On substituting Eq. (B.13) in to the lower bound inequality given in Eq. (B.12) and transforming the integral to $(\hat{r}, s)$ coordinate system we have,

$$\begin{aligned} I_\varepsilon^* \geq & -g_I \varepsilon \int_0^L \frac{\partial d^g}{\partial \hat{r}} (|1 - R\hat{r}\kappa(s)|) \Big|_{\hat{r}=0} ds - \int_0^L \int_0^1 \frac{g_\varepsilon}{2} \varepsilon \left(\frac{\partial d^g}{\partial \hat{r}} \right)^2 (|1 - R\hat{r}\kappa(s)|) d\hat{r} ds \\ & - \int_0^L \int_0^1 \frac{g_\varepsilon}{2} \varepsilon^3 \left(\frac{1}{|1 - R\hat{r}\kappa(s)|} \left[\frac{\partial}{\partial \hat{r}} \left(|1 - R\hat{r}\kappa(s)| \frac{\partial d^g}{\partial \hat{r}} \right) \right] \right)^2 (|1 - R\hat{r}\kappa(s)|) d\hat{r} ds. \end{aligned} \quad (\text{B.14})$$

Simplifying further, we have

$$\begin{aligned}
I_\varepsilon^* \geq & -g_I \varepsilon \left. \frac{\partial d^g}{\partial \hat{r}} \right|_{\hat{r}=0} L - \int_0^L \int_0^1 \frac{g_\varepsilon}{2} \left(\varepsilon \frac{\partial d^{g^2}}{\partial \hat{r}} + \varepsilon^3 \frac{\partial^2 d^{g^2}}{\partial \hat{r}^2} \right) (|1 - R\hat{r}\kappa(s)|) dr ds \\
& - \int_0^L \int_0^1 \frac{g_\varepsilon}{2} \varepsilon^3 \frac{1}{|1 - R\hat{r}\kappa(s)|} \\
& \left(\left[\kappa(s) \operatorname{sgn}(1 - R\hat{r}\kappa(s)) \frac{\partial d^g}{\partial \hat{r}} \right]^2 + 2 \left[\kappa(s) \operatorname{sgn}(1 - R\hat{r}\kappa(s)) \frac{\partial d^g}{\partial \hat{r}} \right] \frac{\partial^2 d^g}{\partial \hat{r}^2} \right) d\hat{r} ds.
\end{aligned} \tag{B.15}$$

The equation can be further simplified by introducing $\eta = \frac{\hat{r}}{\varepsilon}$ and $L = \operatorname{Per}(\Gamma)$ as follows,

$$\begin{aligned}
I_\varepsilon^* \geq & -g_I \left. \frac{\partial d^g}{\partial \eta} \right|_{\eta=0} \operatorname{Per}(\Gamma) - \int_0^L \int_0^{1/\varepsilon} \frac{g_\varepsilon}{2} \left(\frac{\varepsilon}{\varepsilon^2} \frac{\partial d^{g^2}}{\partial \eta} + \frac{\varepsilon^3}{\varepsilon^4} \frac{\partial^2 d^{g^2}}{\partial \eta^2} \right) \varepsilon d\eta (|1 - R\varepsilon\eta\kappa(s)|) ds \\
& - \int_0^L \int_0^{1/\varepsilon} \frac{g_\varepsilon}{2} \varepsilon^3 \frac{1}{|1 - R\varepsilon\eta\kappa(s)|} \\
& \left(\left[\kappa(s) \operatorname{sgn}(1 - R\varepsilon\eta\kappa(s)) \frac{\partial d^g}{\varepsilon \partial \eta} \right]^2 + 2 \left[\kappa(s) \operatorname{sgn}(1 - R\varepsilon\eta\kappa(s)) \frac{\partial d^g}{\varepsilon \partial \eta} \right] \frac{\partial^2 d^g}{\varepsilon^2 \partial \eta^2} \right) \varepsilon d\eta ds.
\end{aligned} \tag{B.16}$$

The last part of the integral corresponds to $o(\varepsilon)$ and higher order terms. Further, the trial function satisfies $\frac{\partial^2 d^g}{\partial \eta^2} = d^g$ and by using the Eqs. (3.15) and (3.17), we have

$$\begin{aligned}
I_\varepsilon[d_\varepsilon^*] \geq & -g_I \left. \frac{\partial d^g}{\partial \eta} \right|_{\eta=0} \operatorname{Per}(\Gamma_1) - \int_0^L \int_0^m \frac{g_I}{2} \left(\frac{\partial d^{g^2}}{\partial \eta} + \frac{\partial^2 d^g}{\partial \eta^2} d^g \right) d\eta (|1 - R\varepsilon\eta\kappa(s)|) ds \\
& - \int_0^L \int_m^{1/\varepsilon} \frac{g_b}{2} \left(\frac{\partial d^{g^2}}{\partial \eta} + \frac{\partial^2 d^g}{\partial \eta^2} d^g \right) d\eta (|1 - R\varepsilon\eta\kappa(s)|) ds + o(\varepsilon).
\end{aligned} \tag{B.17}$$

Taking $\lim_{\varepsilon \rightarrow 0} I_\varepsilon[d_\varepsilon^*]$ we have,

$$I_\varepsilon[d_\varepsilon^*] \geq -\frac{g_I}{2} \left. \frac{\partial d^g}{\partial \eta} \right|_{\eta=0} \operatorname{Per}(\Gamma). \tag{B.18}$$

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