A Century of Fracture Mechanics: from Griffith Theory to Machine Learning Based Modelling

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Introduction

Fracture mechanics is a subject focusing on understanding and predicting fracture process of materials and structures. The past century has witnessed the development of fracture mechanics as both a field of fundamental science and an active engineering discipline. Integrating mechanics, mathematics and material science, the scientific questions studied under fracture mechanics includes fracture criteria, universal crack tip fields as well as failure/damage mechanisms of different material systems in various length scales. Combined with experimental characterization and advanced fabrications, fracture mechanics have guided engineering practices in predicting fracture loads, critical crack length and the growth rate of cracks under corrosive environments, which is essential in guaranteeing and improving structural reliability.

At the 100-year anniversary of the publication of Griffith's fracture paper [1], the present lecture is aimed to review some of the landmark basic theories in fracture mechanics, including the Griffith theory of energy release rate [1], Irwin's universal K-field [2] and G-K relation [3] in linear elastic fracture mechanics (LEFM), Dugdale-Barenblatt's cohesive crack models [4,5], the J-integral [6] and HRR field [7,8] in elastic-plastic fracture mechanics (EPFM), the JKR [9] and MD [10] models in adhesive contact mechanics and Paris' law of fatigue crack growth [11,12]. There have been tremendous applications of these fracture mechanics concepts in studying failure and structural reliability of engineering components and structures. Especially, recently emerged new materials and rapidly developed computational tools have presented novel challenges and opportunities for further advance of fracture mechanics in the second century. The lecture will continue with discussions of some recent advances in machine learning based modelling in fracture mechanics, including machine learning approaches to obtaining stress intensity factor (SIF) solutions and toughening 2D materials via topological effects and lattice asymmetry. We will end with some perspectives on some of the remaining outstanding problems in the field.

Review of some basic theories

During the past century, fracture mechanics has contributed a series of novel concepts regarding the fracture process of materials and formed a systematic framework to quantitively predict fracture behavior in various engineering scenarios, distinguishing fracture mechanics from other branches of mechanics. In this section, we review some of the landmark basic theories in the historical development of fracture mechanics as a branch of solid mechanics and engineering science.

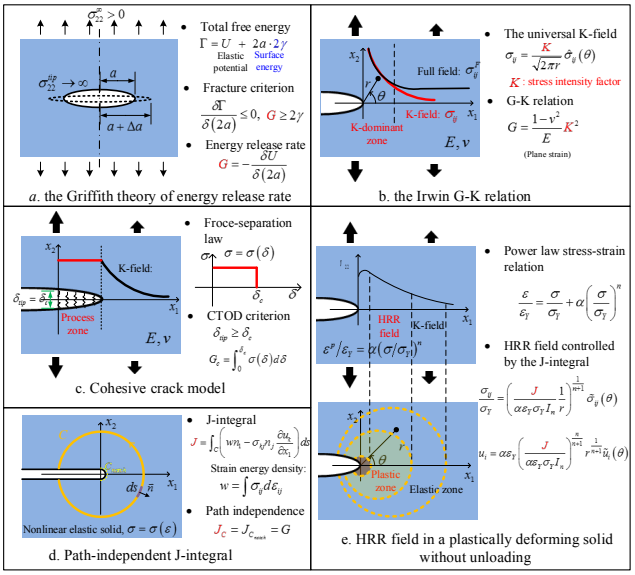

Figure 1. Basic theories and concepts developed in fracture mechanics.

Griffith's crucial development of a fracture criterion based on energetic arguments [1] marked the beginning of fracture mechanics. Before Griffith's theory, materials are thought to fail when the stress level reaches a critical valve. However, this stress-based criterion leads to a paradox when applied to the crack tip. Using linear elasticity, Inglis [13] found the stress at the tip of a *2a*-long crack in an infinite plate becomes singular as long as the remote load, σ_{22}^{∞}, is larger than zero (Fig. 1a). Under the stress-based criterion, this unbounded stress implies the crack will propagate at nearly zero load, which clearly violates experimental observations. To resolve this paradox, Griffith adopted an energy-based point of view and treated fracture as a process of releasing elastic energy and creating new surfaces. Correspondingly, Griffith pointed out the total free energy of the system, Γ, should include not only

the elastic potential energy, U, but also the surface energy, i.e.,

$$\Gamma = U + 2\gamma \cdot 2a\,, \tag{1}$$

where γ is the surface energy density. Based on laws of thermodynamics, Griffith proposed the total free energy should decrease during fracture and it is the balance between reduction in elastic energy and increase in surface energy as crack length extends that determines the critical condition for crack growth, i.e., the crack starts to propagate only if

$$\frac{\delta\Gamma}{\delta(2a)} \le 0 \;\; or \;\; G \ge G_c = 2\gamma\,, \tag{2}$$

where $G = -\partial U/\partial(2a)$ is the energy release rate with respect to the crack extension and G_c is the fracture energy of the material (Fig. 1a). Griffith further carried out experiments on glasses to measure the surface energy and validate the predictions of this energy release rate theory via fracture tests of glass tubes and spherical bulbs with cracks of various sizes. Different from the stress-based criterion, Griffith's theory of energy releases rate predicts the critical load of fracture depends on not only material properties but also geometry (length) of the pre-exiting crack.

While Griffith's theory addresses fracture from a global energy release rate point of view, George Irwin considered stress field near a crack tip and introduced the concept of stress intensity factor (SIF), *K*. Irwin [2,3] unveiled that there exists a universal K-field describing the asymptotic behavior of stress near the crack tip, which is independent of the global geometry and loading conditions,

$$\sigma_{ij}(r,\theta) = \frac{K}{\sqrt{2\pi r}}\hat{\sigma}_{ij}(\theta)\; as\; r \to 0\,, \tag{3}$$

where (r,θ) is the polar coordinate with origin at the crack tip and $\hat{\sigma}_{ij}(\theta)$ are universal angular functions (Fig. 1b). By calculating the work done to unzip the crack tip locally, Irwin showed that the universal crack tip field can be related to Griffith's global energy release rate via the following G-K relation,

$$G = \begin{cases} \dfrac{(1-\nu^2)}{E}K^2 & for\; plane\; strain \\ \dfrac{1}{E}K^2 & for\; plane\; stress \end{cases}. \tag{4}$$

where E is Young's modulus and ν is Poisson's ratio of the material. Correspondingly, the energy-based fracture criterion can also be written in terms of *K* as

$$K \ge K_c \tag{5}$$

where K_c is the toughness of the material. Irwin's G-K relation also provided a systematic way to calculate the energy release rate by solving boundary value problems in linear elasticity or, in some cases, to calculate the stress intensity factor from known energy release rate.

Because linear elastic constitutive relation is expected to fail eventually if stress keeps increasing in real materials, the stress singularity in K-field has raised some controversy. In reality, materials are expected to reach their strength within the so-called fracture process zone (PZ) near a crack tip (Fig. 1c). To account for the material behavior inside the PZ, the concept of cohesive crack models was introduced independently by Dugdale [4] and Barenblatt [5]. In such models, a force-separation law, $\sigma = \sigma(\delta)$, based on atomic interaction between upper and lower crack surfaces [11] or plastic yielding near a crack tip in a plane stress sheet [10] is imposed in a finite PZ at the crack tip and stress field does not go beyond a finite strength. Locally, crack is expected to propagate following the crack tip opening displacement (CTOD) criterion [14],

$$\delta_{tip} \ge \delta_c\,, \tag{6}$$

where δ_{tip} is the separation at the physical crack tip and δ_c correspond to the ending point of the force-separation law. It has been shown that the Griffith criterion in Eq. (2) is equivalent to the cohesive fracture criterion in Eq. (6) if 2γ is replaced with

$$G_c = \int_0^{\delta_c} \sigma(\delta)\, d\delta\,. \tag{7}$$

Another important landmark in fracture mechanics was the development of elastic-plastic fracture mechanics (EPFM) with key concepts including J-integral [6] and Hutchinson-Rice-Rosengren (HRR) field [7,8]. Rice [6] introduced the path independent J-integral,

$$J = \int_C \left(w n_1 - \sigma_{kj} n_j \frac{\partial u_k}{\partial x_1} \right) ds \tag{8}$$

where C is a contour enclosing the crack tip as shown in Fig. 1d, $w = \int_0^{\varepsilon_{ij}} \sigma_{ij}\, d\varepsilon_{ij}$ is the strain energy density of the nonlinear solid and $\vec{n}$ is the unit normal vector of the contour. Using its path independence property, it can be shown that J-integral corresponds to the energy release rate for a blunted notch in any non-linear elastic material or an elastic-plastic material without unloading,

$$J = J_{notch} = G\,. \tag{9}$$

Furthermore, the crack tip field in a power-law elastic-plastic material with stress-strain relation,

$$\frac{\varepsilon}{\varepsilon_Y} = \frac{\sigma}{\sigma_Y} + \alpha\left(\frac{\sigma}{\sigma_Y}\right)^n, \tag{10}$$

was solved by Hutchinson [7] and Rice and Rosengren [8], resulting in the so-called Hutchinson-Rice-Rosengren (HRR) field (Fig. 1e),

$$\frac{\sigma_{ij}}{\sigma_Y} = \left(\frac{J}{\alpha\varepsilon_Y \sigma_Y I_n} \frac{1}{r} \right)^{\frac{1}{n+1}} \tilde{\sigma}_{ij}(\theta) \tag{11}$$

$$u_i = \alpha\varepsilon_Y r \left(\frac{J}{\alpha\varepsilon_Y \sigma_Y I_n r} \right)^{\frac{n}{n+1}} \tilde{u}_i(\theta) \tag{12}$$

where I_n is a function of the power index n, $\tilde{\sigma}_{ij}(\theta)$ and $\tilde{u}_i(\theta)$ universal angular functions depending on plane

strain or plane stress condition. The HRR field then firmly established J-integral as the unique parameter that controls the crack tip field in a plastically deforming solid without unloading.

The development of fracture mechanics has also influenced the development of other related disciplines. For instance, for adhesion between deformable bodies, the boundary of adhesive contact area behaves similar to a crack front. This establishes an analogy between adhesive contact mechanics and fracture mechanics. In this sense, the Johnson-Kendall-Roberts (JKR) model [9] in adhesive contact mechanics can be thought of as Griffith's theory in a different context (adhesion), and Maugis's model [10] in adhesive contact mechanics are analogous to Dugdale-Barenblatt's cohesive crack models.

The concepts originated from fracture mechanics have been applied to address many engineering problems. For example, fatigue accounts for about 90% of failure in metals. Using the concept of SIF, the steady-state growth rate of a fatigue crack can be well described by the so-called Paris' law [11,12],

$$\frac{da}{dN} = C\left(\Delta K\right)^n \tag{13}$$

where a is the crack length, N is the loading cycle number, $\Delta K = K_{\max} - K_{\min}$ is the range of SIF and C and n are experimentally determined constants for any given materials.

Application of machine learning in fracture mechanics

Besides the celebrated achievements in producing fundamental knowledges and improving engineering performances during the past 100 years, fracture mechanics remains an exciting field for new discoveries and novel applications. With ever increasing rate of developments of new materials and novel computational tools, the study of fracture mechanics faces new opportunities and challenges. As some examples, we discuss below some recent advances in applications of machine learning in fracture mechanics. The intention here is to draw the attention of the research community to some of the open questions in this field.

1. A machine learning approach to LEFM

SIF is an important concept in LEFM and the experimental measurement of fracture toughness usually requires an accurate evaluation of SIF. Analytical and empirical solutions to SIF have been developed for specimens with relatively simple geometries. However, some recently developed advanced experimental methods, especially at small scales, involve complex specimen geometries. In such cases, neither analytical nor empirical solutions are feasible. Numerical simulations, such as finite element method (FEM), can provide a reliable solution. However, the construction and deployment of FEM simulations require time and expertise, which is impractical when dealing with large numbers of specimens with variations in dimensions. Therefore, the following question can be raised: is there any possible solution to SIF in complex fracture problems which can maintain accuracy and efficiency at the same time?

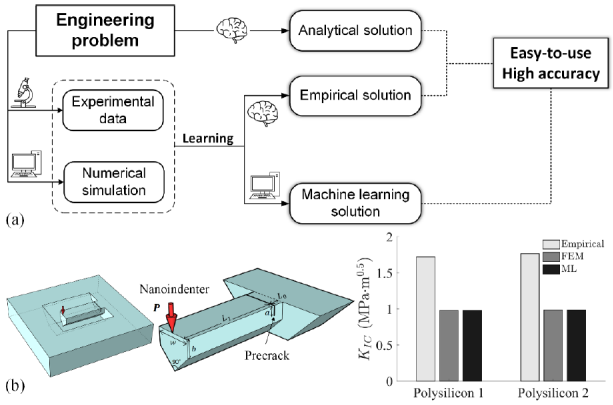

Figure 2. Machine learning solution to SIF for fracture samples with complex geometries.

Recently we have been exploring an innovative class of solutions based on machine learning, which can serve as a promising substitute when analytical and empirical solutions are not accessible (Fig. 2a). The feasibility and advantage of the machine learning solutions are demonstrated through the application in small-scale fracture toughness measurements of pre-notched pentagonal cross-section cantilevers (Fig. 2b). Specifically, regression tree-based and neural network-based solutions are obtained through training over a well-prepared data set. The obtained machine learning solutions can evaluate SIF accurately and rapidly (Fig. 2c), thus suggesting an approach to accelerate data interpretation in fracture toughness measurements on samples with more complex geometries.

2. A machine learning approach to topological toughening of graphene

For next example, let's discuss application of fracture mechanics to 2D materials, a relatively new class of materials that emerged over the last 15 years. As a most prominent example among hundreds of different 2D materials, graphene is the strongest material with a theoretical strength of 130 GPa. However, recent experimental measurements have demonstrated that graphene suffers a very low fracture toughness, close to that of ideally brittle solids [15]. Based on a fracture mechanics point of view, this low fracture resistance implies graphene is fragile under the presence of crack-like flaws. Therefore, how to toughen this atomically thin 2D graphene has become a key challenge for the study of fracture mechanics in 2D materials. As one attempt to resolve this problem, we have demonstrated the possibility of using the effect of topological defects, e.g., disclinations and dislocations, to enhance the fracture toughness of graphene [16]. By introducing the so-called topological toughening [17], we have generated tough graphene models, like rebar graphene [18], vein-patterned graphene and nacre-like graphene, with various toughening mechanisms, including crack tip blunting,

crack trapping, ligament bridging, crack deflection, daughter crack initiation and coalescence, pseudo-plastic deformation and snap-through among multi-stable states [19] (Fig. 3a).

Given the strong correlation between toughening mechanisms and topological effects, one interesting question can be raised: what is the optimal topological design for enhancing fracture toughness of graphene? This inverse design problem is challenging due to the strong nonlinear coupling between crack, topological defects and curvature in curved graphene samples. To address this challenge, we have been exploring the possibility of a machine learning based approach. By leveraging the strong learning ability of advanced machine learning algorithms, such as convolution neural networks (CNN) and conditional generative adversarial nets (cGAN), we have obtained machine learning models capable of classifying tough/brittle candidates (compared with the flat pristine graphene) given the out-of-plane geometry of the graphene samples within a finite design space. Further investigations showed machine learning models also can predict the important quantities regarding fracture/failure process, such as the distribution of maximal stress under the given load with high accuracy (Fig. 3c). Based on these preliminary results, we positively look forward to a machine learning based inverse design framework for topological toughening of graphene and other 2D materials.

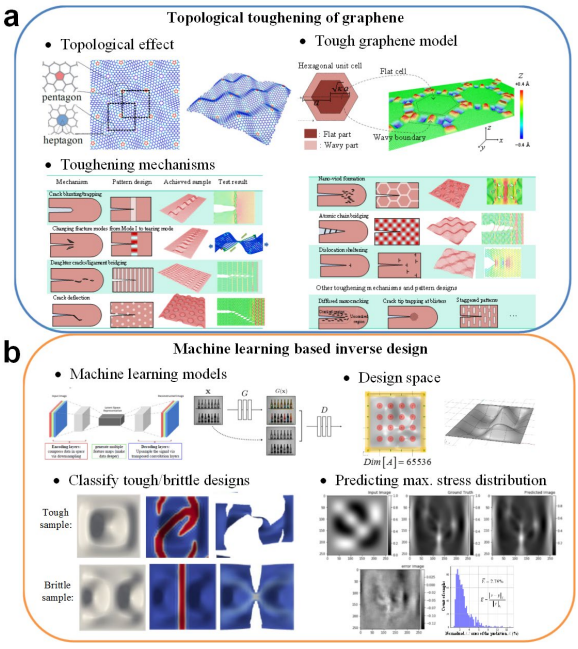

Figure 3. Topological toughening of graphene and machine learning based inverse design.

3. Machine learning based atomic simulations of fracture in heterogeneous 2D materials

In the third example, we present a machine learning based approach to conducting atomic simulations of fracture in 2D materials. For dealing with nanoscale materials, conventional fracture mechanics is not always sufficient. In particular, the fracture behavior of atomic heterostructures in some 2D materials can be highly influenced by the local atomic orders at the crack tip. While the detailed atomic structures are usually neglected in continuum models, current frameworks of atomistic simulations also have their shortcomings. For example, density functional theory (DFT) calculation are often prohibitively expensive for fracture simulations and classical molecular dynamic (MD) simulations often suffer from a lack of accurate interatomic potentials.

Recent advances in developing machine learning based interatomic potentials have provided a potentially viable way to bridge classical MD and DFT more effectively in simulating fracture with ab initio accuracy. Along this path, we showed some preliminary efforts to train an artificial neural network based on ab initio mechanical dataset to characterize the typical fracture behaviors of graphene and *h*-BN (Fig. 4a). These simulations captured repeated crack branching and deflection in *h*-BN and brittle fracture process in graphene. By comparing these two, we were able to identify a novel toughening mechanism induced by lattice asymmetry for *h*-BN (Fig. 4b). Careful analysis revealed that the crack branches and deflects due to the asymmetric edge elastic properties around the crack tip and crack edges swap their positions during propagation, which are only accessible in a asymmetric lattice like *h*-BN. Inspired by this example, simulations based on similar machine learning approaches are expected to be applicable to fracture study of other 2D materials.

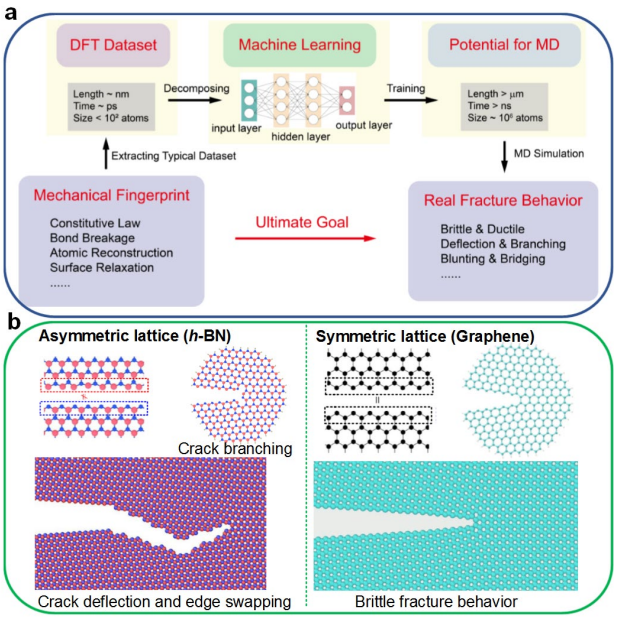

Figure 4. A machine learning based approach to atomic simulations of fracture in *h*-BN and graphene.

Outlook

This lecture is intended to review some of the landmark basic theories in fracture mechanics, beginning with the most celebrated paper of Griffith. Fundamental theo-

ries and concepts include Griffith's energy release rate of crack growth, Irwin's stress intensity factor and universal crack-tip field, Dugdale-Barenblatt's cohesive crack models, J-integral and HRR field in elastic-plastic fracture mechanics, JKR and Maugis' models in adhesive contact mechanics, as well as Paris' law of fatigue crack growth. These theories have fundamentally changed our view of fracture over the past century and will continue to play essential roles in interpreting and understanding material failure and design of next generations of advanced materials and structures.

With ever increasing pace of innovation in novel materials and powerful computational tools, new fracture problems and methodologies are also broadening the platform and opportunities for further development of fracture mechanics in this century. We have discussed some very preliminary examples of application of machine learning in fracture mechanics. To limit the scope of our discussion to problems closely related to the examples discussed here, a few open questions and potential research topics/directions are: 1) Can machine learning be used to predict the fracture toughness/crack growth rate/mechanism from observed complex fracture patterns under given load and sample geometry? 2) How can we optimize the training process of machine learning solutions in fracture mechanics? 3) As an inverse design problem, how can we systematically enhance the fracture toughness of graphene and other 2D materials through topological toughening and machine learning? 4) With the help of machine learning based modelling, can we build a theory to describe the interaction between crack, topological defects and curvature in 2D materials? 5) Can we use machine learning to identify the toughest 2D material? 6) What is the necessary and sufficient data set to train a machine learning based potential for reliable fracture simulations in 2D materials? 7) How can we balance the accuracy and efficiency in machine learning based modelling of fracture in 2D materials?

With endless developments of new materials and new experimental, analytical and computational tools, there will also be endless opportunities for fracture mechanics in the 21st century.

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