INTEGRATING SIMULATION, MACHINE LEARNING, AND EXPERIMENTAL APPROACHES FOR HIGH-THOUGHPUT SMALL-SCALE FRACTURE INVESTIGATIONS

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Abstract

The past decades have witnessed an increasing demand for characterizing fracture properties of materials at small scales due to the miniaturization of devices. While tremendous advances in experimental techniques have been achieved, researchers are still struggling with the knowledge gap between the experimental measurements and the fracture properties that need to be extracted. To bridge this gap, we propose a new paradigm for small-scale fracture investigations, in which delicate experiments, high-fidelity simulations, and advanced machine learning (ML) techniques are seamlessly integrated. Its feasibility and value are demonstrated in fracture toughness measurements: microcantilevers bending experiments and pillar indentation splitting experiments.

1. Introduction

Since the establishment of modern fracture mechanics, fracture toughness has been one of the fundamental properties that needs to be characterized in engineering design and manufacturing process. At macro-scales, there are many well-established methods that have been calibrated over decades and archived as standards such as ASTM Standards E1820 and C1421. However, there is an emerging demand for small-scale measurements due to the miniaturization of devices. In principle, most of the macro-scale testing methods can be downscaled using a geometrically similar specimen and identical loading conditions. However, for the most part, due to practical issues associated with microfabrication and loading machines, the small-scale testing configurations are substantially different from those for macro-scale tests, which inevitably involves complex geometries and boundary conditions. The resulting complexity of the deformation in the specimens makes it challenging to interpret the experimental results and extract the fracture toughness. To bridge this knowledge gap, there are several possible approaches including deriving analytical or semi-analytical solutions and performing simulations, but either their accessibility or accuracy has been largely questioned. Therefore, we propose a new class of solutions based on machine learning (ML) models, named "ML-based solutions", to overcome these limitations. ML provides a versatile platform to utilize all the information from experiments and simulations. Through delicate experiments, we can obtain all the necessary information for building high-fidelity computational models, allowing high-resolution simulations to calculate the target material property. By analyzing all the experimental and simulation data, ML models extract the knowledge of how to interpret experimental data accurately and rapidly. The establishment of ML-based solutions is essentially attributed to the state-of-the-art combination of experimental, simulation and ML approaches. The transformative impact of combining these approaches will be highlighted through the two example problems encountered in our micromechanical fracture testing of ceramic materials.

2. Results

First, we investigate a microfabricated cantilever-based fracture testing method and combine experimental data and simulations to evaluate the fracture toughness of brittle materials. To enable rapid and reliable interpretation of experiments in the absence of analytical solutions or computational resources, we develop a ML-based solution through careful analysis of simulation data. It is found that establishing an accurate ML-based solution is data-intensive. Advanced ML algorithms such as active learning and transfer learning can alleviate the need for a large amount of data and attain desired accuracy of a ML-based solution in a data-limited regime. Second, we investigate the fracture instability problem in the pillar indentation splitting experiment. A comprehensive understanding of the indentation fracture process is achieved by integrating the experimental observations and finite element simulations (including both cohesive zone modeling and *J*-integral). A simple scaling law is discovered and provides the backbone for extracting fracture toughness from experimental measurements. We also extend the concept of ML-based solutions to this problem and establish a predictive model for characterizing the indentation-induced instability and materials' fracture toughness.

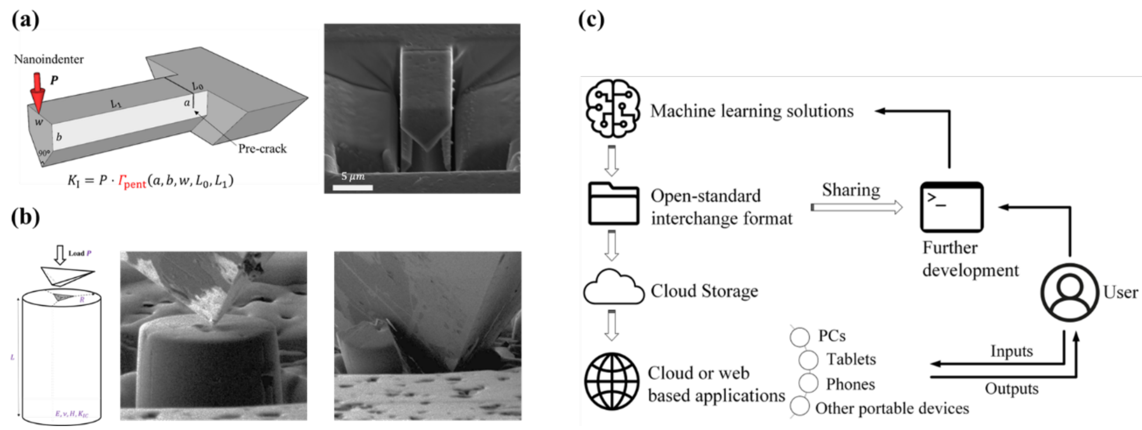

Figure 1: (a-b) Microcantilever bending and pillar splitting experiments for measuring fracture toughness. (c) Open-access ML-based solutions.

3. Conclusions

We have proposed a new paradigm for small-scale mechanical characterization of materials, in which delicate experiments, high-fidelity simulations, and advanced ML techniques are seamlessly integrated. Its feasibility has been explored in various scenarios: measuring fracture toughness through microcantilevers bending experiments and measuring fracture toughness through pillar indentation splitting experiments. The proposed paradigm has shown its promise in bridging the gap between experimental measurements and the extraction of target mechanical properties as well as enabling high-throughput small-scale fracture investigations.

References

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