Investigation of hierarchical porous structures using phase-field fracture modeling informed by molecular dynamics simulation

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Abstract
The mechanical integrity of hierarchical porous structures depends on their pore morphology. To investigate the role of pore morphology on the mechanical and fracture behaviors of these complex systems, a multi-scale approach has been proposed. This paper shows how molecular dynamics simulations provide the means to extract material properties at the atomistic scale to further inform phase-field fracture technique at the continuum scale in an attempt to understand the mechanical response of these porous materials.

1. Introduction
Heiarchial porous structures offer superior properties and have been rapidly gaining interest from scientific and engineering communities for various applications such as energy and life sciences. Such porous strucutres are typically composed of pores from micro (<2 nm), meso (2–50 nm) to macro pores (450 nm). Moreover, the variation in pore shapes, sizes, and distribution in each scale substantially affect the mechanical properties including stiffness and strength of the porous materials leading to different macroscopic fracture responses. The wide variation of scales in pores demands a multi-scale evaluation of mechanical and fracture responses of the material under different loading conditions.

Although molecular dynamics (MD) simulations can provide detailed information about the material at the atomic scale, the limitation in domain size and simulation time associated with the scale makes it difficult to describe the material response under macroscopic loading conditions. On the other hand, continuum scale simulations are computationally efficient to predict the macroscopic response of the material but they lack the details of the underlying structures. MD-informed continuum simulation is one of the proposed approaches for overcoming the challenges associated with each scale while capturing the underlying physics of the system at a lower length scale. In this paper, we combine MD and phase-field (PF) fracture modeling approach to investigate the role of pore morophology at the atomic scale on macroscopic fracture behevior.

2. Results
In this study, LAMMPS, an open-source code along with a state-of-the-art reactive force field (ReaxFF) was used to conduct numerical analysis of various porous structures at the atomic scale. The hybrid formulation for the phase-field fracture technique was adopted in capturing the fracture behavior of porous silica. At the atomistic level, amorphous silica systems were subject to tensile loading with four distinct porous structures: (1) without a pore, (2) with a circular pore, (3) with a triangular pore, and (4) with a square pore. The simulation box is $29.41\times 29.41\times 1.51$ nm^3 in all cases. The porosity value of 2.27% remains the same for all cases. Tensile load is applied to all boxes while periodic boundary conditions are imposed. Material properties including Young's modulus, fracture energy release rate, critical tensile strength, and Poisson's ratio are obtained from MD simulations. These properties were then utilized in continuum-scale simulations of two benchmark problems: (i) single-edge notched shear and (ii) notched rectangular with three holes as shown in Fig.1. These two benchmark problems were selected to capture complex geometry as well as complex loading scenarios.

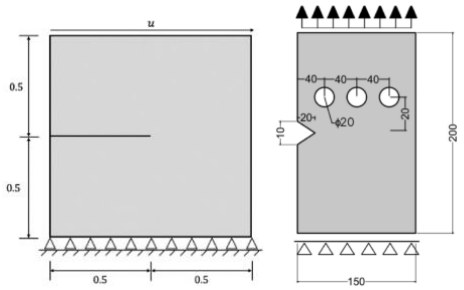

Fig.1 – Benchmark problems: single-edge notched shear and notched rectangular with three holes. All dimensions are in mm.

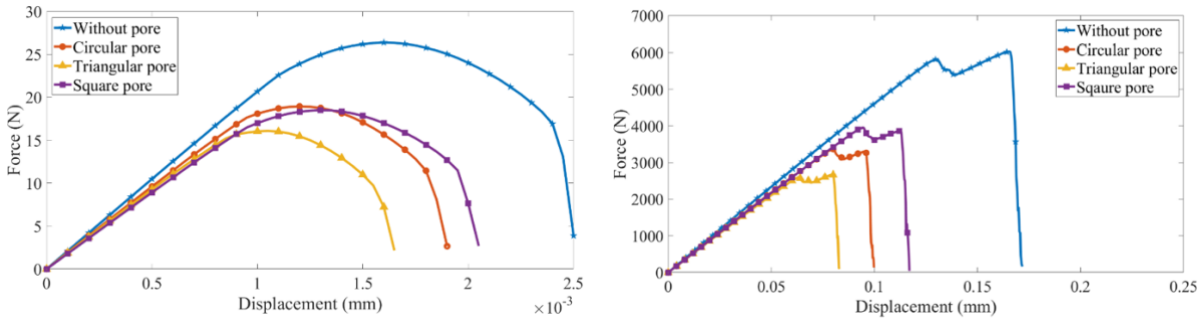

Fig.2 – Force-displacement curves for two single-edge notched shear (left) and notched rectangular with three holes (right).

The force-displacement curves shown in Fig. 2 clearly indicate the differences between all four cases for both benchmark problems. These plots highlight how the macroscopic response of porous silica is influenced by not only the porosity but also the pore shapes at the atomistic scale. Fig.3 shows different fracture patterns as a result of variations in the underlying atomistic model.

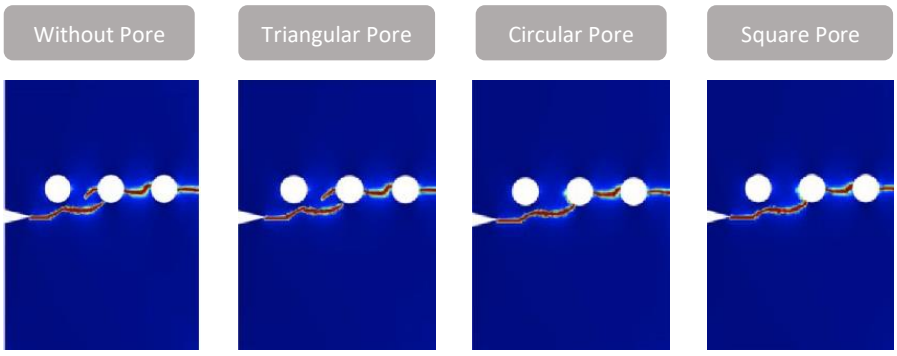

Fig.2 – Fracture response of notched rectanfular case with three holes for all four MD cases.

3. Conclusions

The MD-informed PF fracture approach illustrated the role of nano porosity as well as nano pore shapes on the macroscopic fracture response of amorphous silica under different loading scenarios.

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