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Chemical-Mechanical Modeling of Subcritical-to-Critical Fracture in Geomaterials

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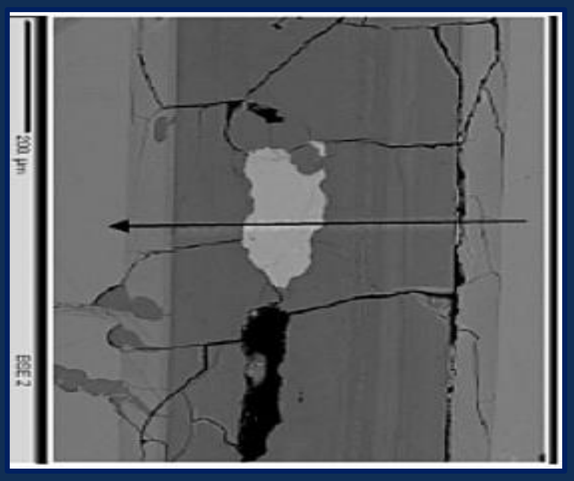
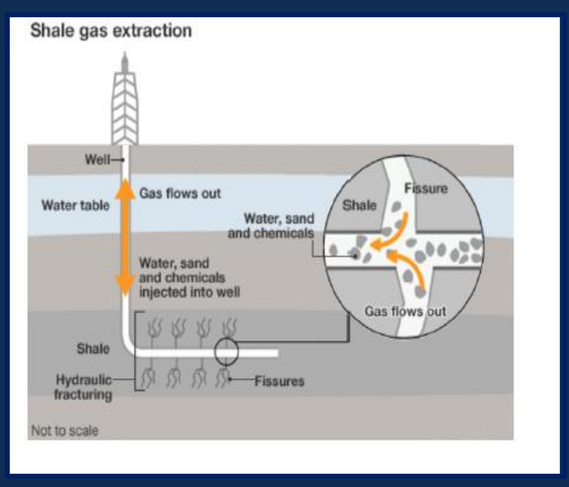




Exceptional service in the national interest

Objectives

- Develop a fundamental, atomistic-level understanding of the *chemical-mechanical* processes that **control subcritical cracks** in low-permeability geomaterials.
- Link atomic-scale insight to macroscale observables.
- Address how **chemical environment** affects **mechanical behavior**.

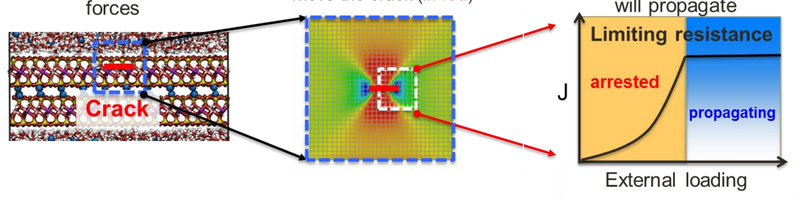
Atomistic to Continuum Scale Modeling

- A slit is inserted through bonds crossing a half plane
- A far-field continuum displacement boundary is applied on an annulus of atoms.
- Stress, displacement, and energy density fields are coarse-grained on a grid.
- Eshelby stress is formed and the J-integral is evaluated on the contour.

Molecular simulations sample atomic displacements, energies & forces

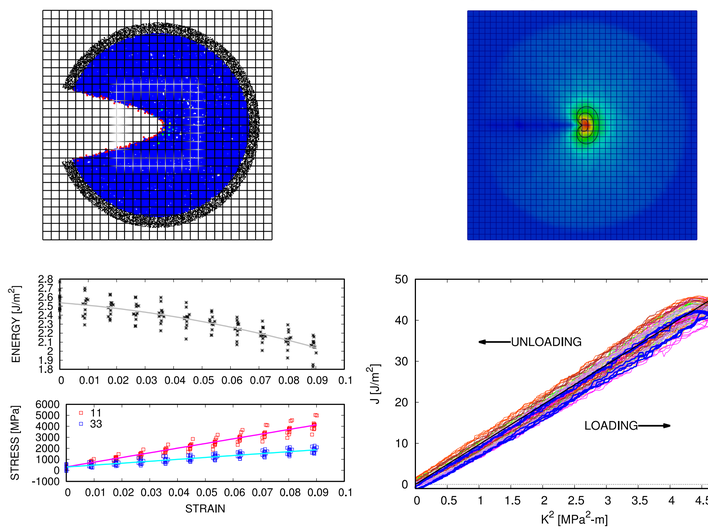
Eshelby stress fields use atomic data to characterize local energy available to move the crack (*in red*)

The J-integral is formed from the divergence of the Eshelby stress and determines if a crack will propagate



Modeling Dry Silica with a Non-Reactive Force Field

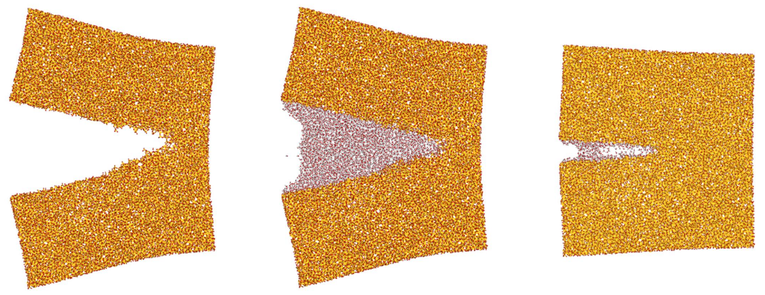
- Non-reactive force field (Tersoff) behaves more ideally or more according to linear elastic fracture theory than a reactive force field.
- Provides a good baseline of dry and non-reacting glass.



Fracture of Silica in Water

Investigate fracture in amorphous silica:

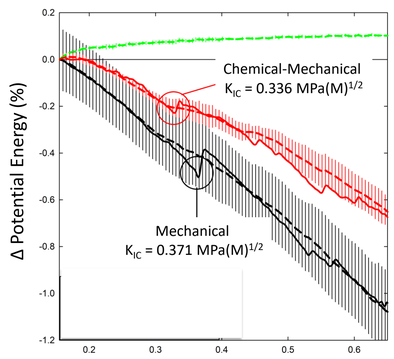
- SiO_2 is present in sandstone and shales
- ReaxFF potentials are well parameterized for Si/O/H systems
- Three different conditions were selected to isolate the impact of mechanical loading alone, water alone, and coupled chemical (water)-mechanical processes on crack tip propagation



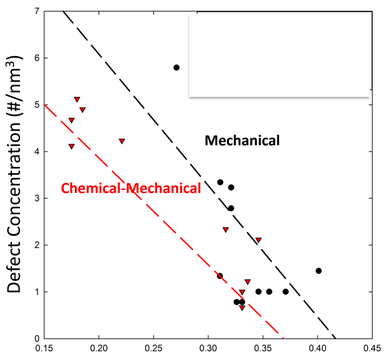
Mechanical (mechanical loading only)

Chemical-Mechanical (aqueous enviorment and mechanical loading)

Chemical (aqueous enviorment only)



Fracture toughness (K_{IC}) is defined by the first deviation of the potential energy from the expected trend. Fracture from chemical (H_2O)-mechanical effects occurred at 75% of the K_{IC} values from mechanical loading alone.

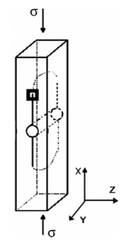


Immediately prior to crack propagation, the defect concentration is higher for systems that fracture at K_{IC} values of 0.25 MpaVm or less.

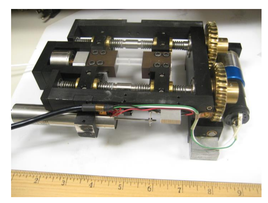
Experimental Setup

Objective: to obtain experimental data at the atom

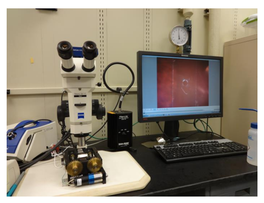
- Method: DCDC = Double Cleavage Drilled Compression
- Material: Silica parallelepipeds with holes
- Technique may be implemented with confocal microscope or AFM.



Schematic of glass rod and DCDC compression

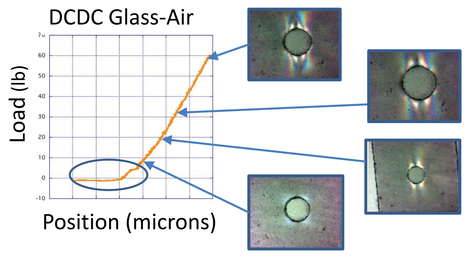


Glass rod in load frame



Confocal Microscope

Glass rod in environmental chamber



Stress fields observed in air

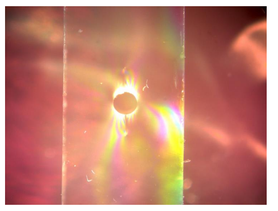
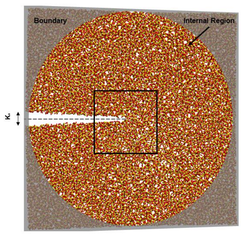
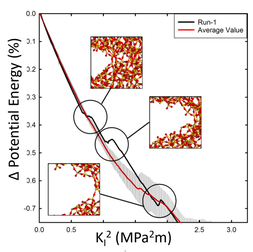


Image of stress field & first noticeable crack in DI water

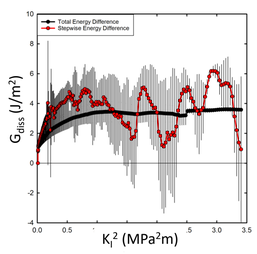
Fracture of Dry Silica using a Reactive Force Field



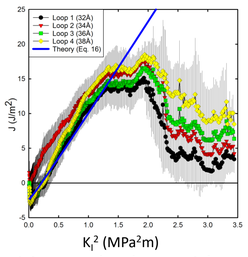
Schematic of silica system with slit crack. The J-integral is evaluated on contours (black).



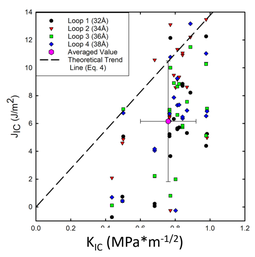
Discontinuities indicate fracture events. Crack tip morphology changes; bond breaking and rearranging occur.



Energy dissipation (Gdiss) highlights irreversible inelastic processes around crack tip.



J-integral values with increased loading & increasing loop sizes.



Fracture toughness (K_{IC}) and J-integral values for initial crack propagation.

Calculated
K_{IC}=0.76±0.16 MPaVm
J_{IC}=6.16±4.34 J/m²

Experimental
K_{IC}=0.78±0.04 MPaVm

Future Work

- Computationally add salts to water and investigate how salt changes crack surface structure and impacts fracture toughness
- Experimentally acquire results for loading in varying solution compositions
- Use developed techniques on other materials of geological significance.

Built on LDRD Laboratory Directed Research and Development

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