
Contribution ID: **230** Type: **Oral 20 Minutes**

# Coupled chemo-mechanical fracture of silica in aqueous solutions

*Wednesday, 16 May 2018 10:08 (15 minutes)*

Crack propagation in silica may be enhanced in aqueous solution due to protonation of the silica surface and chemical reactions between the solution and strained siloxane bonds at the crack tip. To identify the coupled chemo-mechanical processes which govern silica fracture in the presence of pure and salt water, sub-critical fracture in amorphous silica has been investigated using molecular dynamics simulations and double-compression double-cleavage (DCDC) experiments. The molecular dynamics simulations have been performed with both a non-reactive and reactive force field. Using the reactive force field (REAXFF), slit cracks were introduced into models of amorphous silica and propagated as mode I fractures. The cracks were filled with reactive water molecules and different concentrations of NaCl. The simulation results confirm that the fracture toughness of silica in vacuum is greater than in aqueous solution. Using a reactive force field allows us to simulate water infiltration into the silica slit crack with reactivity: water dissociation allows for the hydroxylation of the silica surface, ion adsorption to the silica surface can affect the protonation of neighboring surface sites. The role of defect concentrations, crack tip radii, and solution composition on fracture toughness, surface structure, stress distributions, and crack depth will be discussed and qualitative comparisons between experimental and modeling results will be presented.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

## References

## Acceptance of Terms and Conditions

Click here to agree

**Primary authors:** CRISCENTI, Louise (Sandia National Laboratories); RIMSZA, Jessica (Sandia National Laboratories); JONES, Reese (Sandia National Laboratories); MATTEO, Edward (Sandia National Laboratories)

**Presenter:** CRISCENTI, Louise (Sandia National Laboratories)

**Session Classification:** Parallel 6-C

**Track Classification:** MS 4.23: Fluid flow-fracture phenomena in porous media