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Dissolution and fracture properties of amorphous silica through classical molecular dynamics simulations

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Dr. Jessica Rimsza is from the Geochemistry Department of Sandia National Laboratories (Albuquerque, NM). She received her Ph.D. in Materials Science and Engineering from the University of North Texas (Denton, TX) in 2016 while working with Dr. Jincheng Du on atomistic simulations of oxide surfaces. She also served as a visiting scholar at Pierre and Marie Curie University (Paris, France) and the University of Electronic Science and Technology of China (Chengdu, Sichuan Provence, China) through the NSF Graduate Research Fellowship Program and the East Asia and Pacific Summer Institute respectively.

Dr. Rimsza's research focuses on the atomistic computer simulations of amorphous and crystalline oxide systems, including solid-liquid interfaces, brittle fracture of oxide structures, as well as defect formation and radiation effects. Her research has been funded by the Department of Energy (DOE), the National Science Foundation (NSF), and the Semiconductor Research Corporation (SRC).

Molecular modeling, including classical molecular dynamics simulation methods, have been widely applied to the understanding evolving surface structures and mechanical properties of oxides. Here, two different research questions will be presented, focusing on the dissolution and fracture properties of amorphous silica, and how modeling approaches have been applied to identify atomistic insight which could not be obtained from experimental analysis alone.

First, identification of the reactions and processes at water-silica interfaces are critical to predicting the chemical durability of silicate glasses, including nuclear waste glasses. Of interest is how intermediate phases, such as silica gel layers, affect the diffusion of water through the system and the dissolution rate. However, atomistic level information of the structure and dynamics at the glass-water interface is still missing, even for pure silica glasses. Simulations provide a unique opportunity to probe the processes which are responsible for the varying stability of interfaces which form during dissolution.

Second, crack propagation rates in amorphous silica increase in wet or humid environments changing the reliability of oxide systems. Increased reactions between water molecules and strained siloxane bonds located at the crack tip re suggested to cause early fracture of the system in subcritical conditions. Through molecular dynamics simulations of fracture in amorphous silica the fracture toughness and J-integral were calculated through upscaling of atomistic stress and displacement data. Analysis of the changing structural properties at the crack tip were used to investigate changes in the chemistry which control crack propagation in silicates in the presence of water.

These examples highlight the role of atomistic computational methods in investigating the variable structural and mechanical properties of complex amorphous oxides. 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.

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