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Chemically Assisted Weakening of Calcium Oxide

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Chemically assisted fracturing can control permeability and deformation of rocks and manmade materials. Water weakening is an example of such chemically assisted process, where water molecules facilitate subcritical fracturing through hydrolysis reactions. The goal of our molecular modeling and experimental research is to identify molecular origins of water weakening in calcium oxide (CaO). To investigate this chemical-assisted fracture process, classical molecular dynamics simulations are used with the bond order-based reactive forcefield ReaxFF. Fracture was simulated via far field loading of a slit crack in tension under varying conditions, including vacuum and in an aqueous environment. The addition of water to the system resulted in CaO fracturing earlier and more often during dynamic loading, with a calculated reduction in fracture toughness of ~80%. Varying water concentration in the fracture was used to approximate humid v. bulk water conditions, and even lower humidity values significantly increased CaO fracture. In situ (in liquid) nanoindentation on dry CaO and CaO grains submerged in de-ionized water was also performed and dramatic water-weakening of CaO occurs. Nano-scale surface hardness and reduced modulus was quantified using nanoindentation, and upon exposure to de-ionized water at room temperature the CaO hardness decreased by 1-2 orders of magnitude, and reduced modulus decreased by 2-3 orders of magnitude. Overall, clear chemo-mechanical effects are identified in CaO, a common component of subsurface minerals that can be evaluated mechanistically through the use of reactive molecular dynamics simulations. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.