EGU24-11861, updated on 24 Jan 2025
https://doi.org/10.5194/egusphere-egu24-11861
EGU General Assembly 2024

Large scale molecular modelling of basalt surfaces and fracturing in basaltic glass

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How fracture initiate and propagate at the nanoscale controls the specific surface area available for fluid-rock interactions. Fracturing creates surface area and flow pathways, which control the flow mixing properties and reactivity. However, how fractures form at the nanoscale in basaltic glasses remains enigmatic. Here, we implement molecular dynamics simulations to reproduce fracture propagation in amorphous basalt. These simulations require large systems and long simulation times and are therefore currently depending on interatomic potentials rather than *ab initio* calculations. We have developed a machine-learned interatomic potential for basaltic glass that allow using molecular dynamics simulations to simulate fracture propagation at the nanoscale. This interatomic potential reproduces the mechanical properties of bulk solid and molten basalt over a wide range of temperatures and pressures. During a molecular dynamics simulation, bonds are formed and broken as the atoms and ions move. As a result, various species may form and migrate into the glass or towards the surface. In order to study how a basalt surface changes over time we looked at the cation-anion species on the surface and measured how long each species lived on the surface before the coordination changes. Our results show that the process zone around propagating cracks in basaltic glasses at the nanoscale is much larger than for instance when quartz breaks, and that cavities open ahead of the crack tip, and grow with time until they coalesce. A similar propagation process has been observed in fracture experiments on silica glasses at nanometer scale using atomic force microscopy and is reminiscent of the ductile fracturing process observed in metals. By training the interatomic potentials with water and carbon dioxide as fluids, we also aim to study how dynamic fractures may damage a basaltic glass and how the water and carbon dioxide enter these fractures in the wake of rupture. These simulations are relevant for carbon mineralization where a coupling between dissolution of the basalt and precipitation of carbonate minerals may lead to nanoscale fracturing of the rock.