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Molecular dynamics study of confined water in the periclase-brucite system under conditions of reaction-induced fracturing

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Reaction-induced fracturing may occur when dry rocks are exposed to water and undergo mineral transformations that involve a volume change. The volume increase associated with hydration reactions in rocks, like the hydration of periclase to brucite, requires a stable water film to be present at reactive grain boundaries. Recent experiments on the hydration of periclase observed that the replacement reaction slows down dramatically when the effective mean stress exceeds 30 MPa. We hypothesise that a stable fluid film is required for the brucite-forming reaction to progress, and when the applied pressure overcome the hydration force, the fluid film will collapse and be squeezed out of the grain contacts which will prevent formation of brucite. To quantify this effect, we run molecular dynamics simulations where our setup consists of two interfaces of either periclase or brucite surrounded by water, and we study the behaviour of the water film confined between two surfaces subject to compressive stress. The simulations are carried out using the ClayFF force field and the single point charge (SPC) water model in the molecular dynamics simulation program LAMMPS. Our simulations show that when the pressure reaches a few tens of MPa, the water film collapses. The process reduces the water film thickness to one or two water layers and reduces the self-diffusion coefficient of the water molecules by a factor of eight. When the water film thickness is less than two water layers, the water film thickness is smaller than the hydration shell around Mg^{2+} -ions, which will limit the ion-transportation. The observed collapse of the water film to a single layer at a normal pressure of 25-30 MPa might explain the observed slow-down of reaction-induced fracturing in the periclase-brucite system.