Molecular dynamics simulations of the hydration force and transport properties of a water film during 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 change in volume. For example, the serpentinization of peridotites or the hydration of periclase into brucite occurs with a molar volume increase of 40 % and 120 %, respectively. The thermodynamic 'force of crystallization' due to volume increase for the replacement of periclase by brucite is calculated to be about 1.9 GPa from thermodynamic considerations. However, recent experiments by Zheng et al. (2018) showed that the replacement reaction slows down significantly when the sample is subject to a confining pressure of only 30 MPa.

We hypothesize that for the brucite forming reaction to progress, the fluid film between the periclase-brucite grains needs to remain stable, and that under significant applied pressure, the fluid film may be squeezed out of the grain conctact. To quantify this effect, we have performed molecular dynamics simulations using LAMMPS together with CLAYFF force fields. The simulation cell consists of two periclase blocks with water in between. Several sets of simulations were perfomed by varying the crystallographic orientation of the blocks relative to each other and the pressure in the range 1 to 100 MPa.

Our results show that the pressure necessary to reduce the water film thickness sufficiently is on the order of 20-30 MPa. This pressure is much lower than the theoretical 'force of crystallization' and agrees with the pressure at which the periclase-brucite reaction slowed down in experiments, which substantiates the fluid-film hypothesis. These calculations are relevant to several geological systems where rock deformation is controlled by mineralogical transformations mediated by fluid-rock interactions at grain contacts, such as compaction in sedimentary basins, healing and sealing of fault zones, or serpentinization of the oceanic crust.