Evaluation of the diffusivity of dissolved ions through grain boundary of quartz and its application to the prediction of frictional healing

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Laboratory and field observations have shown that the frictional strength of a fault under stationary contact increases with time (frictional healing). The origin of frictional healing has been often interpreted as due to the increase in real contact area along fault surfaces. This interpretation was supported by the direct observation of increase of contact area of glass plates with time (Dietrich and Kilgore, 1994).
Slide-hold-slide (SHS) friction experiments (e.g., Frye and Marone, 2002; Katayama et al., 2015) have suggested that quartz shows relatively strong frictional healing compared to clay minerals and water plays a critical role for the frictional healing. In addition, temperature has a large effect on the frictional healing. The frictional healing is often characterized by the cutoff time (t_c) beyond which the frictional strength shows a linear recovery with the logarithm of time. SHS tests (Nakatani and Scholtz, 2004; Tenthorey and Cox, 2006) have suggested that t_c decreased from 1.2E+3 to 5.9E+1 sec as temperature increased from 200 to 927˚C. A plausible mechanism of rapid healing at high temperature is the enhanced contact area by the pressure solution under hydrothermal conditions (e.g., Tenthorey and Cox, 2006). To test whether the hypothesis can quantitatively explain such a healing behavior, the diffusivity of dissolved ions through intergranular water (intergranular diffusivity) is required for predicting the deformation rate by the pressure solution. The intergranular diffusivity of dissolved ions is, however, poorly constrained (He et al., 2013) because of the difficulty of experimental evaluation. In this study, we calculated the intergranular diffusivity of dissolved Si between quartz surfaces by molecular dynamics (MD) simulations.
In the MD simulations, water molecules and dissolved Si were sandwiched between quartz (1010) surfaces terminated with Si-OH groups. We calculated the diffusivity of dissolved Si in the direction parallel to the quartz surfaces. MD simulations were performed for the thickness of intergranular water from 0.5 nm to 2 nm and temperature from 150 to 350˚C.
As the thickness of intergranular water decreases from 2 to 0.5 nm, the diffusion coefficient of dissolved Si decreases by more than one order of magnitude. The activation energy of intergranular diffusivity ranges from 14 to 30 kJ/mol. Using the obtained intergranular diffusivity with the kinetic model of pressure solution, the increase in grain-to-grain contact area of quartz gauge (ΔA (m^2) were calculated as a function of time. Assuming that the strength recovery ΔT(MPa) is proportional to ΔA, we can calculate ΔT by the relationship of $\Delta T = (\Delta A_r / A_{r0}) C$ (A_{r0}: initial real contact area (m^2), C: cohesive strength (MPa)). Calculated t_c (9.4E+3 s at ˚C and 2.0E+2 s at 927˚C) by using the ΔT and time was roughly consistent with the experimental t_c in the SHS tests. The intergranular diffusivity obtained by this study is useful for extrapolating the relationship between time and strength recovery by SHS tests to natural systems and various time scales.

Keywords: Pressure solution, Frictional healing, Rate- and state-dependent friction law