

Fast water diffusion in silica glass

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Water diffusion in silicate glass is a fundamental process controlling physical and chemical aspects of magmatism, but fundamental aspects of diffusion in silicate glass are not fully understood. In this study, we report one-order of magnitude faster water diffusion than that reported previously, discovered in diffusion experiments of deuterated water in silica glass, and discuss the water diffusion mechanism by considering diffusion pathways in silica glass.

A SiO₂ glass sample and deuterated water (²H₂O) were enclosed in a silica glass tube and heated in a furnace at 900-750 degree C for 1-20 hours with a water vapor pressure of 50 bar. Deuterated water was used to trace water diffusion at low water-concentration region (<10ppm), where background hydrogen signals obscure a diffusion profile of ¹H₂O. Diffusion profiles of ²H in samples were measured by secondary ion mass spectroscopy (SIMS: Cameca ims-6f) at Hokkaido University.

The ²H intensity rapidly decreases from rim to core of the sample as observed in the diffusion experiment with ¹H₂O (Kuroda et al., 2018). This profile shape can be explained by a concentration-dependent water diffusion model in silica glass (Kuroda et al., 2018), where water molecules diffuse through the diffusion pathways formed by breaking Si-O-Si bonds through a hydroxyl formation reaction (H₂O + Si-O-Si = 2Si-OH). In this study, we found that the tail of deuterium profile extends further into the deep region of the sample. This suggests that a small fraction of deuterium-bearing species migrates with a faster diffusion rate and that the diffusion has weak concentration-dependence.

It has been known that noble gas diffusion through “free volume sites” in the dry silica glass structure, and that the activation energy and diffusivity depend on the atomic radius. The fast diffusion coefficient of water in the present study can also be explained by the relation between diffusivity and the size of diffusion species observed for noble gases. Therefore, we conclude that water molecules can diffuse through free volume sites, which provide faster diffusion pathways than those formed through a hydroxyl formation reaction. The concentration of free volume sites, estimated from the solubility of noble gases, is much higher than that observed deuterium concentration in a fast diffusion path in this study. This implies that free volume sites are not fully occupied by water molecules at water vapor pressure of 50 bar. The contribution of fast water diffusion may become larger under higher water vapor pressures, where the concentration of water molecules dissolved into free volume sites may increase as noble gases.

Keywords: water diffusion, silica glass, SIMS, diffusion mechanism