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Diffusion in stishovite and $CaCl_2$-type silica from first-principles calculations: Implications for MORB viscosity in the lower mantle

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Both geophysical and geochemical observations document the widely distributed heterogeneities from small to large scales in the lower mantle. One of the primary interpretations for these compositional heterogeneities is the segregation of the subducted oceanic crust from subduction slabs. The rheological properties of the crustal components are essential for understanding the origin of this separation. Previous geodynamic simulations suggested that the segregation of the crustal components occurs near the core-mantle boundary. The viscosity applied in these models is usually only temperature- and depth-dependent, mainly because we still have very limited knowledge about the viscosity of individual minerals and the rheological behavior of the multi-phase system.

Since the lower mantle deforms as diffusion creep, ionic diffusion directly controls the mineral viscosity. Here, we reported first-principles results for Si and O diffusion of stishovite and $CaCl_2$-type silica and evaluated the relative viscosity of oceanic crust along different mantle geotherms. Our results show that the Si diffusion in $CaCl_2$-type silica has instinct negative activation volumes along <111> direction, leading to the Si diffusion enhancement with both pressure and temperature. We model the MORB composition as SiO_2 silica plus bridgmanite and consider the bulk viscosity as the weak phase forms an interconnected weak layer (IWL). Rheological weak CaCl2-type silica substantially reduces the crustal viscosity and could facilitate the segregation of subducted oceanic crust with increasing depths. The delaminated crustal fragments would be stirred and stretched sufficiently by the vigorous mantle convection and account for the ubiquitous heterogeneities in the lower mantle. Our results provide new constraints on the crustal rheology for the fine geodynamic simulations in the future to better understand the crustal recycling in the earth`s interior.

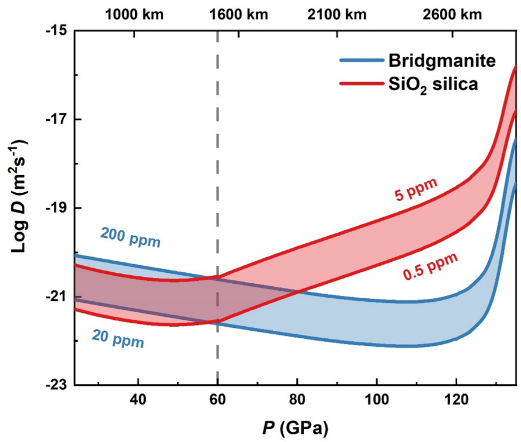

Fig. 1. Effective diffusion coefficient of stishovite and $CaCl_2$-type silica along geotherm compared bridgmanite

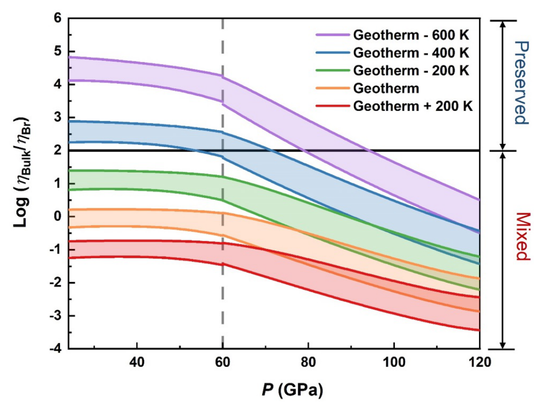

Fig. 2. Viscosity contrast between MORB (composed of 20 vol.% SiO_2 silica and 80 vol.% bridgmanite, η_{MORB}) and the bridgmanite dominant surrounding mantle (η_{Br}) with different crustal temperature.