

**Temperature and Pressure Effects on Diffusional Mg Isotopes in MgSiO<sub>3</sub> Liquid.** Haiyang Luo<sup>1</sup>, Bijaya B. Karki<sup>2</sup>, Dipta B. Ghosh<sup>2</sup>, Xiaobin Cao<sup>1</sup>, Huiming Bao<sup>1</sup>, <sup>1</sup>Department of Geology & Geophysics, Louisiana State University, Baton Rouge, LA 70803, USA, <sup>2</sup>Department of Computer Science, Department of Geology and Geophysics, Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803, USA

**Introduction:** Diffusional isotope fractionation (DIF) is an important parameter when disequilibrium systems are of interest, e. g. during crystal growth from a silicate melt. DIF was found to be large even at silicate melt temperatures [1,2,3,4]. Unlike simple diffusion of a molecular species in a dilute gas, it has been difficult to predict diffusional isotope fractionation factors for melt systems. Usually,  $\beta$  factor, a dimensionless empirical parameter, is used to describe the mass dependent diffusional isotope fractionation. The  $\beta$  factor is often assumed to be dependent on variables such as temperature, pressure, and chemical composition. However, the degrees of these variables' effect on the  $\beta$  factor are not explored. Here, we used first-principles molecular dynamic simulations to explore diffusional isotope effect of Mg in MgSiO<sub>3</sub> melt under a series of pressures (0 – 68 GPa) and temperatures (3000, 4000, 5000 K).

**Results and Discussion:** Our results show that, at a given temperature the  $\beta$  factor for diffusional Mg isotope effects decreases when pressure increases (Fig. 1). At 5000 K,  $\beta$  decreases from  $0.270 \pm 0.004$  to  $0.164 \pm 0.029$  with pressure increasing from 6 to 68 GPa (Fig. 2). At 4000 K,  $\beta$  decreases from  $0.255 \pm 0.007$  to  $0.182 \pm 0.040$  with pressure increasing from 1 to 60 GPa. At 3000 K,  $\beta$  decreases from  $0.288 \pm 0.014$  to  $0.239 \pm 0.024$  with pressure increasing from 0 to 10 GPa. We can attribute this decrease to the chemical environmental change of Mg in MgSiO<sub>3</sub> liquid at atomic level. At a constant volume, no clear trend is observed between the  $\beta$  factor and temperature, indicating that the temperature effect on the chemical environmental change of Mg is limited under the temperature range we explored.

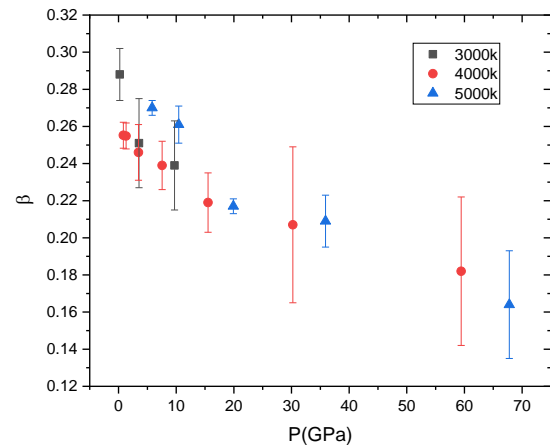


Fig. 1  $\beta$  versus pressure at 3000, 4000, 5000 K.

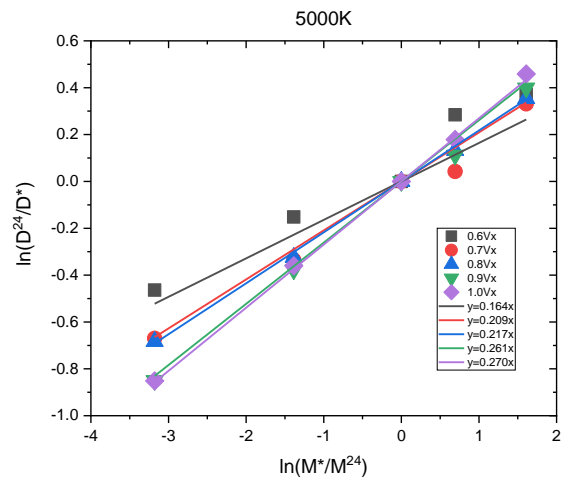


Fig. 2  $\ln(D^{24}/D^*)$  versus  $\ln(M^*/M^{24})$ .

**References:** [1] Richter FM et al. (1999) *GCA*, 63, 2853–2861. [2] Richter FM et al. (2003) *GCA*, 67, 3905–3923. [3] Richter FM et al. (2008) *GCA*, 72, 206–220. [4] Watkins JM et al. (2009) *GCA*, 73, 7341–7359.