

# Viscosity and atomic-local-structures of basaltic melt under high pressure

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High pressure properties of basaltic melt are of importance in deep Earth science related to such as early magma ocean and subsequent differentiation processes (Agee 1998; Ohtani and Maeda 2001; Suzuki, *et al.* 2005)

Recently, experimental studies reported that the viscosity of basaltic melt decreases with increasing pressure (Allwardt, *et al.* 2007; Sakamaki, *et al.* 2013). They suggested based on the results of classical molecular dynamics simulation (Nevins and Spera 1998) and <sup>27</sup>Al magic-angle spinning nuclear magnetic resonance (Allwardt, *et al.* 2007) that this anomalous behavior is related to the coordination change of Al. However, other silicate melts which contain none of Al also show a common behavior of viscosity (McMillan *et al.*, 2009). It means that the microscopic origin of the anomalous pressure response of viscosity of the basaltic melt is still unclear. For this reason, in this study, we perform *ab initio* molecular dynamics simulations and analyze atomic-local-structures in basaltic aluminosilicate melt under pressure. At the last meeting, we reported the structural changes around Al atom. This time, we discuss relationship between the viscosity and structural changes not only around Al but other elements.

## Reference

- C. B. Agee, *Phys. Earth Planet. Inter.* **107**, 63 (1998)
- E Ohtani and M. Maeda, *Earth Planet. Sci. Lett.* **193**, 69 (2001)
- A. Suzuki, *et al. Phys. Chem. Miner.* **32**, 140 (2005)
- D. Nevins and F. Spera, *Am. Mineral.* **83** 1220 (1998)
- J. R. Allwardt, *et al. Am. Mineral.* **92**, 1093 (2007)
- P. E. McMillan and M. C. Wilding, *J. Non-Cryst. Solids.* **355** 722 (2009)
- T. Sakamaki, *et al. Nature Geoscience* **6**, 1041 (2013)

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