高圧下における玄武岩質メルトの粘性:第一原理分子動力学シミュレーション
Viscosity of Basaltic Melt under High Pressure: *ab initio* molecular dynamics simulations

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High-pressure behavior of basaltic aluminosilicate melt has been intensively studied due to its 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). 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 ^{27}Al magic-angle spinning nuclear magnetic resonance (Allwardt, *et al*. 2007) that this anomalous behavior is related to the coordination change of Al. However, so far there exist no ab initio simulations of basaltic melt in the pressure range, where the anomaly in viscosity is observed experimentally. In this study we therefore perform ab initio molecular dynamics simulations gradually changing volume and successfully reproduce a viscosity minimum in the pressure range corresponding to the experiments. We analyze relationships between the anomalous pressure response of viscosity and variations in the atomic-scale local structure.

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