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# Shear viscosity and diffusion in liquid $MgSiO_3$: Transport properties and implications for terrestrial planet magma oceans

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## Abstract

Molecular dynamics simulations using a pair-wise additive potential are implemented to investigate self-diffusion (Mg, Si, and O) and shear viscosity of liquid $MgSiO_3$ in the density-temperature-pressure range 2350–5300 kg/m$^3$, 2500–5000 K, and 0–140 GPa, respectively. Self-diffusivity and shear viscosity are described by modified Arrhenian expressions, which feature a pressure-dependent activation volume. Activation energies for self-diffusion (Mg, Si, and O) and viscous flow are 99.6, 109.3, 97.4, and 95.3 kJ/mol, respectively; evidently oxygen mobility dominates liquid dynamics. Activation volumes for self-diffusion and shear viscosity at low (2–5 GPa) pressure are ~1 cm$^3$/mol with self-diffusion decreasing and shear viscosity increasing as pressure increases although there is a small interval near zero pressure within which diffusivity increases slightly with increasing pressure. Shear viscosity increases by a factor of 75 along the 3000 K isotherm from the top of the mantle to the core-mantle boundary. Along the 3000 K isentrope relevant to terrestrial magma ocean convection, shear viscosity increases by about a factor of three. The equivalence conditions between the Stokes-Einstein and Eyring transport models are derived. The Eyring model provides information on the size of the activated complex associated with viscous flow across the range in pressures relevant to the Earth's mantle and suggests that the number of atoms in the activated complex associated with shear flow decreases from ~8 atoms at low pressure to ~4 atoms at high pressure at 4500 K.

**Keywords:** Geochemical modeling, high-pressure behavior, mantle processes, composition of the mantle, transport properties, $MgSiO_3$