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Thermal conductivity of molten and glassy $NaAlSi_3O_8$, $CaMgSi_2O_6$, and Mg_2SiO_4 by non-equilibrium molecular dynamics at elevated temperature and pressure

Dane Tikunoff[1] and Frank J. Spera[1,*]

[1]Department of Earth Science, University of California, Santa Barbara, California 93106 , U.S.A.

Abstract

Non-equilibrium molecular dynamics (NEMD) simulations are used to compute the phonon thermal conductivity (k) for liquids and glasses of composition Mg_2SiO_4, $CaMgSi_2O_6$, and $NaAlSi_3O_8$ at 2000–4500 K and 0–30 GPa based on classical potentials. These compositions span the range of melt polymerization states in natural systems at ambient pressure. The NEMD results compare well with available laboratory measurements on molten $NaAlSi_3O_8$ and $CaMgSi_2O_6$ at 1 bar. Thermal conductivities decrease with increasing temperature (T), increase with increasing pressure (P), and at low pressure increase slightly as the mean coordination number of Si and Al around oxygen increases, in the sequence Mg_2SiO_4, $CaMgSi_2O_6$, and $NaAlSi_3O_8$. At 3500 K, the thermal conductivity of $CaMgSi_2O_6$ at 0, 10, 20, and 30 GPa is 1.1, 2.1, 2.5, and 3 W/mK, respectively. At ambient pressure (0.2 ± 0.15 GPa), k = 1.2 and 0.5 W/mK at 2500 and 4500 K, respectively, for $CaMgSi_2O_6$. For $NaAlSi_3O_8$ composition, k varies from 1.7 to 2.7 W/mK at 3050 K for pressures of 6 and 30 GPa, respectively. Mg_2SiO_4 liquid at ambient pressure (0.07 ± 0.16 GPa) is found to have thermal conductivities of 1.36 and 0.7 W/mK at 2500 and 4500 K, respectively. Tables giving computed k values for all compositions are included for state points studied. The trade-off between T and P implies that the phonon thermal conductivity of silicate liquids at mantle depths increases substantially (factor of 2–3) along isentropes.

Keywords: Thermal conductivity, molecular dynamics, silicate, mineral, amorphous, melt, temperature, pressure