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Transport properties and equation of state of 1-bar eutectic melt in the system $CaAl_2Si_2O_8$-$CaMgSi_2O_6$ by molecular dynamics simulation

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Abstract

Empirical potential molecular dynamics (EPMD) simulations of 1-bar eutectic composition liquid in the system $CaAl_2Si_2O_8$-$CaMgSi_2O_6$ have been conducted using the interatomic pair-potential of Matsui (1998). Simulations using ~10 000 atoms over a wide range of conditions (ρ: 2200–5000 kg/m^3; *T*: 1600–5500 K; *P*: 0–170 GPa) were used to derive an equation of state, determine self-diffusivities for all atoms, calculate melt viscosity, and investigate melt structures by coordination statistics. EOS results compare well to laboratory shock wave data up to ~25 GPa, diverging at higher pressure. Based on simulations of the end-member compositions of the join using the same potential, non-ideality in the volume of mixing at pressures below 10 GPa disappears at higher pressures. Ideal volume mixing at elevated pressure is consistent with inferences from laboratory shock wave studies of liquids in this system. The non-ideal volume of mixing at low pressure is directly correlated to structural differences between the end-member liquids and the mixing of cation-anion coordination polyhedra of differing volume. Self-diffusivities show reasonable agreement with laboratory values, with activation energies and activation volumes in the range 90–100 kJ/mol and 1–3 cm^3/mol, respectively. Shear viscosities at 3500 K span from 1.8×10^{-3} Pa·s at low *P* to ~4.4×10^{-3} Pa·s at ~14 GPa.

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