

Structural and dynamical properties of Mg₂SiO₄ at high pressures

Tetsuya Morishita[1], Ritsuo Morishita[2], Toshikazu Ebisuzaki[2]

[1] Comp. Sci. Div., RIKEN, [2] Advanced Computing Center, RIKEN

<http://atlas.riken.go.jp/~tetsuya>

Molecular dynamics simulations were carried out to study structural and dynamical properties of Mg₂SiO₄ melts. Pair correlation functions $g(r)$, diffusion constants, and shear viscosity were obtained at several pressures (5GPa -- 29GPa). By compression, the coordination number of Si is gradually increased from 4 to 6, and SiO₄ tetrahedra are transformed to SiO₆ octahedra. Diffusion constants are not increased but decreased by compression, contrary to those of SiO₂ melts. We will also discuss the dependence of shear viscosity on pressure.