Pressure effect of Self-diffusion in Periclase (MgO) by Molecular Dynamics

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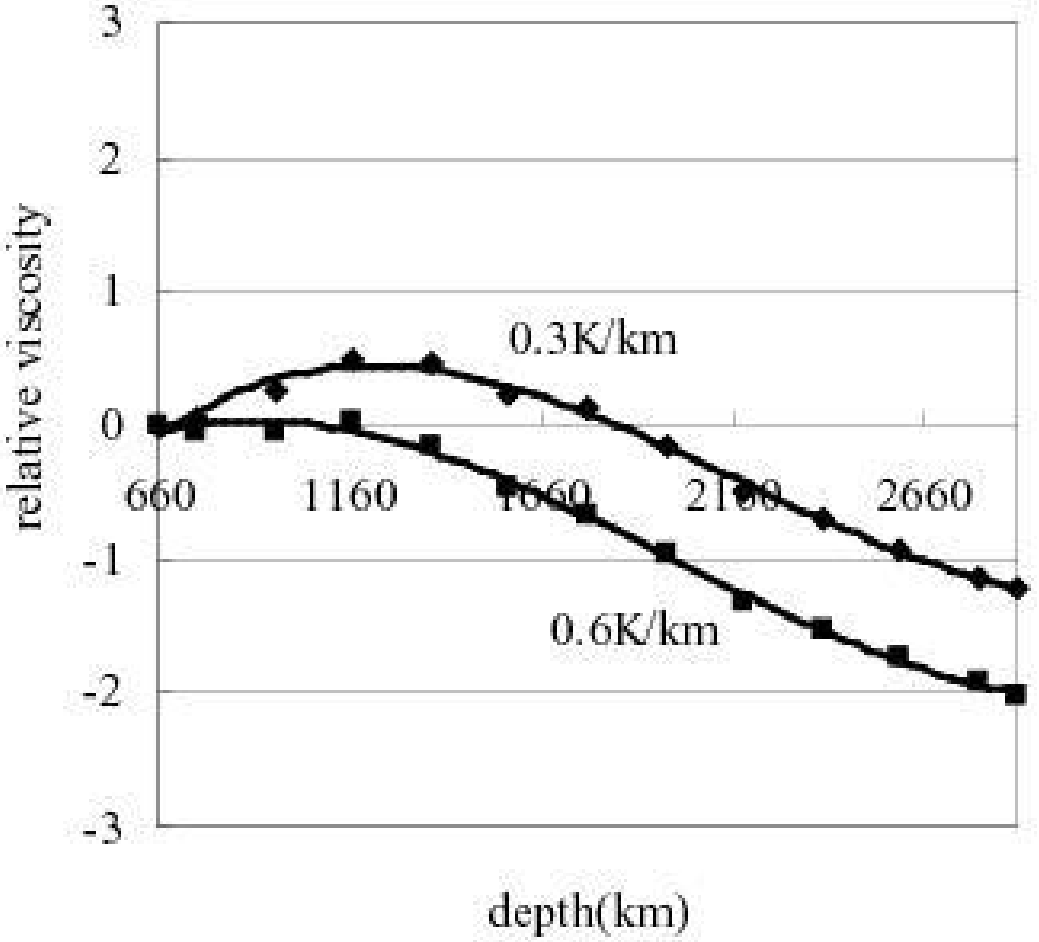
Pressure effect of self-diffusion in Periclase (MgO) was investigated by molecular dynamics (MD) and viscosity variation of lower mantle Periclase was predicted by employing the Nabarro-Herring model. Self-diffusion coefficients were derived directly from recorded trajectories of atoms. The MD calculations were performed at 2400-6000K and 0-140GPa.

Migration energy (Hm*) and formation energy (Hf*) of ordinary pressure (0GPa) are consistent with experimental data. Observed pressure dependence of self-diffusion coefficients were turned to be positive from negative with increasing pressure. The behavior of self-diffusion coefficients predicts softening of lower mantle periclase with increasing depth. We predict rate of reduction of the viscosity as 1.3 order (0.3K/km geothermal gradient) or 2.0 order (0.6K/km geothermal gradient).

Yamazaki et al., [2001] suggested that viscosity of the lower mantle is near that of weaker phase periclase in the place largely strained. The softening may be one of the causes of dynamic geological activities of the lower mantle, such as plume generation.


3
2
1
0
-1
-2
-3
relative viscosity
0.3K/km
0.6K/km
660
1160
2660
depth(km)