The activation volumes of self-diffusions of MgO by Molecular Dynamics Simulations

Yosuke Ito[1], Mitsuhiro Toriumi[2]

[1] Earth and Planetary Sci, Univ of Tokyo, [2] Complexity S and E., Univ. Tokyo

The plastic deformation of rocks in earth's deep interior is controled by several microscopic mechanisms. Especially self-diffusion is one of the most important one of these mechanisms. The self-diffusion coefficients are strongly depended on temperature and pressure. The Temperature dependence is expressed by activation energy and the pressure dependence is expressed by activation volume. In this work the activation volume is given by Molecular Dynamics (MD) calculations. Interaction potentials are given by the empirical parameters which is based on Born-Mayer-Huggins model. The defects which cause the migration of atoms are assumed to be the pair vacancies of Mg sites and O sites. The formation and migration process are divided and the activation volumes are calculated for each other. The results of activation volumes are expressed by the following form

$V^*f(10^{-6}$ m^3/mol$) = -3.86*10^{-2}$ P (GPa) $+ 5.60$:(formation)
$V^*m(10^{-6}$ m^3/mol$) = -2.64*10^{-2}$ P (GPa) $+ 2.68$:(migration)
$V^* (10^{-6}$ m^3/mol$) = -6.50*10^{-2}$ P (GPa) $+ 8.28$:(sum).

The activation voulmes of formation has the large values at ordinary pressure and decreased with the increase of the pressure. The activation volume of self-diffusion is charactrized by this behavior of the activation volumes of formation. The activation volumes of migration becomes 0 at 100GPa and may become negative over 100GPa. In this work it is revealed that activation volume largely decreases with the increase of the pressure. Karato(1981) assumes that the pressure dependence of activation volume is equal to the compressivity V(P)/V(P=0). The compressivity of MgO is 0.75 at CMB (140GPa) (Mao and Bell, 1979). Our results give much more pressure dependence of activation volume and indicate that the possibility that the viscosity decreses with increase of pressure at deep part of lower mantle.