Numerical Simulation of Physical Properties of Earth's Materials

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MD simulations with pairwise potential on MgO vacancies pair were conducted to obtain the Newtonian viscosity of lower mantle. The results are such that the viscosity of the upper half portion in the lower mantle shows uniform structure but in the lower half it rapidly decreases to the core mantle boundary by two orders of magnitude.

The ab initio MD calculation program designed by Tsuneyuki have installed on ES specially for magnesium aluminum garnet to apply to the vacancy, dislocation and hydrogen of MgO and $MgSiO_3$ and other silicates of deep mantle. The time consumed for this type of MD is available for actual simulation of earth' materials.

Keywords: vacancy diffusion, lower mantle, periclase, viscosity, molecular dynamics

1. Introduction

The aim of this research program is to obtain the constitutive law of earth's materials in the conditions ranging from shallow crust to deep mantle by means of the following simulations studies; (1) dislocation and vacancy structure and dynamics in MgO and $MgSiO_3$ in the lower mantle conditions using molecular dynamics method of pairwise potential and with ab initio calculation, (2) water structure and the physical properties in earth's materials using ab initio simulation, (3) shear zone structure and dynamics involving mineral reaction, water migration, localization, crack formation using granular system simulation. This year, we intend to perform the one million basic cell simulation studies of vacancy diffusion in MgO in very high pressure conditions for evaluation of the Newtonian viscosity of the lower mantle, and to conduct the installation study of the ab initio MD of garnet to tune up the parallel computing on ES.

2. Results

We investigated the molecular dynamic simulation of MgO to construct a neutral vacancies pair and to relax to the stable structure. Then it moves random walk from the initial position. The mean square distance of this random walk of the vacancies pair is temperature compensated diffusivity. The size of the basic cell reaches one million atoms. This type of simulation required in the estimation of the lower mantle rheology is to consider the density of vacancy pair and density of dislocation, because equilibrium densities of them depend on applied stress are very small in natural system. To conduct the simulation, the basic cell size is needed to be over one million atoms (Fig. 1).

Even using the ES, it is impossible to conduct the precise simulation of vacancy pair random walk for the relaxation process of vacancy migration need enough time.

Thus, the author (Ito) made a new algorithm utilizing table update method of near atomic position and velocities. As a result the n square calculation changes down to the n-1.5 power calculation, so that the times required for the 20 nanosecond relaxation experiments are possible in the evaluation of the Newtonian viscosity. In addition, the time studies for relaxation of vacancies pair are conducted and then it is concluded that the 20 ns experiments show enough narrow range of diffusivity compared with 4 ns experiments.

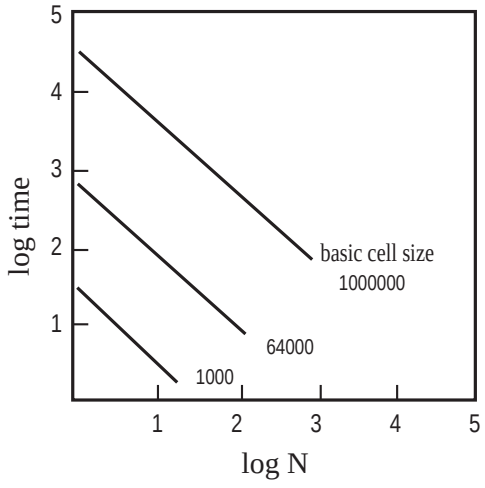

Fig. 1 Cpu time(second) vs size of parallel computing (number of nodes) for MD simulation of the 1000 to 1000000 atoms in the basic cell.

In the diagrams of the cpu time vs number of node of ES and the numbers of the basic cell atoms, we can immediately conclude that the n-1.5 power calculation is essential to realize the one million atoms molecular dynamic experiments in the available time scales.

The MD experiments were carried out in the range from 1900 to 6000 K and 20 to 150 Gpa. In the region below 4000 K the diffusivity of vacancies pair show a minimum near the 50 Gpa, and over 4000K it decreases monotonously. These results indicate that the activation volume of the vacancy diffusion decreases with increasing pressure from the positive value to the negative one through zero value at about 50 Gpa.

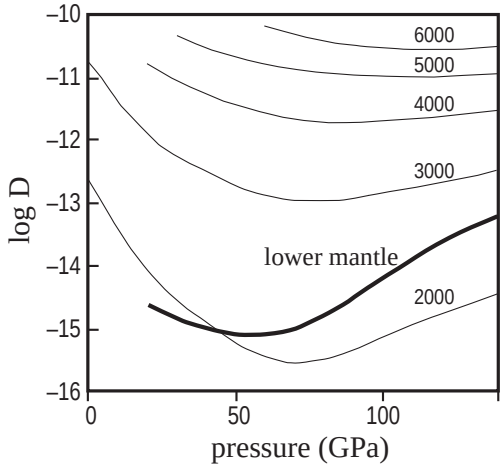

Fig. 2 Diffusion coefficient D (cm2/sec) as a function of pressure (Gpa) in the range from 1900 to 6000 K. The profile of the diffusion coefficient across the lower mantle is shown by broad line.

3. Application to the viscosity of the Earth's lower mantle

The viscosity of the solid materials can be defined as the derivatives of strain rate by stress. The strain rate and stress relation is commonly called as the constitutive law, and it should be classified into the linear law and non-linear law. The latter is the power law creep in general. The linear type is Newtonian creep (Wang et al., 1994) and representative model of the solid materials is the diffusion creep. This type of creep is governed by the lattice diffusion along the paths of grain boundary or of volume. In this case, the flow law of the Nabarro-Herring creep can be formulated as follows;

$$d\varepsilon/dt = AVD\sigma / RTd^2$$

where A = 13.3 and V = 2.44×10^{-5} m^3/mol, and D and d are diffusion coefficient and grain size, respectively.

Thus in the case of the lower mantle the diffusion creep is probably dominant because the stress condition in the lower mantle should be controlled by the convective flow, producing at most 10 MPa of differential stress, and because the lower mantle is seismically isotropic. Therefore, the dislocation creep type flow cannot be available in the lower mantle. Thus, we can think of the diffusion creep in the lower mantle rheology.

The pressure and temperature condition of the earth interior has been deduced from the seismic structure and the high pressure phase transition and phase reaction determined by the experimental investigations. The temperature reaches about 1500 K at 410 km and at 660 km it is about 1900 K because of olivine - m-spinel transition and post spinel transition, respectively (Ito and Katsura, 1989). The lower mantle geotherm may be considered to be nearly adiabatic because of its turbulent state.

Combining this geotherm with constitutive law obtained here, the entire viscosity profile of the lower mantle is deduced as shown in Fig. 2. It is concluded that the Newtonian viscosity in the region less than 70 Gpa keeps constant but it decrease rapidly to the core mantle boundary by the magnitude of two orders. The viscosity profile obtained here is important to the mantle convection pattern. The common assumption of the viscosity profile is such that the viscosity increases gradually to the core mantle boundary by two or three orders of magnitude, suppressing the strong turbulent convection.

4. Molecular dynamics with ab initio interaction calculation

In order to calculate the direct multibody potential in the earth's materials, we have to conduct the ab initio molecular dynamics simulation (Tsuneyuki 2002). Thus, Yoshiyuki and Tsuneyuki of our group have conducted the installation of ab initio MD on earth simulator using 1 to 10 nodes. The partition of the calculation flows of ab initio MD is such that the band indexing of electrons is shared to each node and calculation of basic planar wave function of electrons is by 10 nodes. A test simulation has been carried out on pyrope $Mg_3Al_2Si_3O_{12}$. It takes for 0.9 picoseconds about 33 hours (259.96 seconds), but the case of 1 node system needs 1552.21 seconds, compared with the time for SR8000 about 10948.63 seconds by 1 node.

5. Conclusions

We conducted the MD simulations with pairwise potential on MgO vacancies pair to obtain the Newtonian viscosity of lower mantle. The results are such that the viscosity of the upper half portion in the lower mantle shows uniform structure but in the lower half it rapidly decreases to the core mantle boundary by two order of magnitude.

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