Acceleration of molecular dynamics and its application to self-diffusion of lower mantle MgO

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1 introduction

Knowledge of rheological properties of materials of Earth's interior is required to reveal the whole dynamics of the Earth. The rheological properties are controlled by defects (vacancies, dislocations, or grain boundaries). By studying of properties of defects by MD (molecular dynamics), the rheological properties may be revealed. However, MD calculations of such the defects have been difficult for it required many atoms and costs too much calculation times. In this study, MD calculations are accelerated by technological developments at first. Next, self-diffusion of MgO of lower mantle is studied by developed program. This presentation will introduce the details of this study.

2 Technical developments

Technical developments are based on well-known MD program MXDTRICL (Kawamura 1996). At first, bookkeeping method with cell partitioning method is incorporated to reduce large size dependence (O(N2)) of judgments of cutoff. Next, program is parallelized (with processes and threads) and vectorized to optimize for Earth Simulator. The developed program is names as SUPER-MXDTRICL. Benchmarks show that each of these methods is effective when the number of atoms is large. SUPER-MXDTRICL achieved 3.7 sec/step (128nodes) and 1.8 sec/step (512nodes) for 10^6 atoms on Earth Simulator.

3 Self-diffusion of MgO

MD calculation is performed for the systems that contain a pair of vacancies. 10^7 steps of MD calculations show good (25%) precisions of self-diffusion. Activation enthalpies of migration and formation are in good agreements of experimental results at ordinary pressure. Decreases of self-diffusion coefficients are linear at low (-20GPa) pressure, decrease with increasing pressure, and turn to be slight increase at high (60-100GPa) pressure. This behavior may be related with self-diffusion of MgO of lower mantle.

4 Summary

Calculation times of 10^6 atoms are reasonable and it can be said that the MD calculations of defect contained systems are turned to be possible. MD now reveals pressure dependence of self-diffusion of MgO and this success shows the usefulness of MD to study the properties of defects. In the future, MD will study the properties of more complex defects (dislocations and grain boundaries) and will reveal the rhelogical properties of Earth's deep interior.