Numerical Simulation of Physical Properties of Earth's Materials

Project Representative
Mitsuhiro Toriumi Institute for Frontier on Earth Evolution/Graduate School of Frontier Sciences, University of Tokyo

Authors
Mitsuhiro Toriumi Institute for Frontier on Earth Evolution/Graduate School of Frontier Sciences, University of Tokyo
Yosuke Ito Department of Earth and Planetary Sciences, University of Tokyo

MD simulations using direct deformation method to apply to diffusion type plasticity have been carried out by means of parallel computing with earth simulator. The direct deformation simulation of MgO can be conducted by anisotropic stress conditions on single crystal induced Shottkey vacancies. The deformation can be measured by anisotropic mean migration distances of vacancies.

The results can be obtained as follows: the anisotropic diffusion was possibly simulated by this method by applying the differential stress, and secondly the negative activation volume and negative activation enthalpy for anisotropic diffusion were obtained, and thirdly the diffusion creep resulted from anisotropic diffusion is proportional to the differential stress. These results are consistent with those obtained previously by indirect method.

Keywords: flow law, viscosity, simulation rheology, vacancy, direct deformation

1. Introduction

The target of the numerical study of rheology of earth materials is to obtain the flowage characterization both in the mantle and the crust. The rheology must be the controlling parameter of dynamics of the earth's processes, and the solid earth simulation program requires strongly flow law and frictional law of the mantle and crust materials in the wide range of pressure, temperature and water pressure. However, the experimental study is limited below 5 GPa and theoretical understanding of rheology is very limited, because of no realistic model on plastic deformation of polycrystalline materials (Karato et al., 1995).

The project of simulation rheology group also involves dislocation and vacancy dynamics in simple compounds not only of MgO, MgSiO3, and Mg2SiO4 but also of clay and zeolite minerals. Further, water structure and its effect on rheology, and shear zone and plate boundary dynamics having solid reaction of hydrous minerals and deformation are also investigated by using ES.

2. Results

The direct MD rheology of MgO has been performed as following;

1. Introduction of neutral vacancy in periclase,
2. anisotropic stresses are applied instead of confining pressure condition,
3. migration of vacancy can be measured from mean square distance of vacancy,
4. anisotropy of vacancy diffusion under stressed periclase can be obtained as a function of pressure, temperature and differential stress.
5. and the diffusion controlled solid state flow rate can be determined from the anisotropy and diffusivity of vacancy.

The MD simulation experiments have been carried out in conditions from 5 to 100 Gpa and from 1000 to 5000 K in the differential stress ranging from –10 to 10 Gpa. The diffusion constant was calculated from the mean square distance of vacancy migration divided by duration time followed by Einstein' relation. The basic cell size was in this case 3000, because the step size was need over nanoseconds. This is why the anisotropic diffusion experiments of vacancy require the enough precision in the determination of diffusivity even by full ES system (512nodes). Here simulation experiments were based on the Ito's tabling MD method which reaches 1.5 power calculations on square n for n-body problem of MD.

In Fig. 1 the calculation scheme for anisotropic diffusion under anisotropic stress condition is presented and it is suggested the difference in space scale between natural and MD system studied here. Even in this nanoscale rheology the long time experiments must be needed for precise determination of diffusion anisotropy. The simulation experimental results are shown in Figs 2 and 3. The figure 2 indicates the

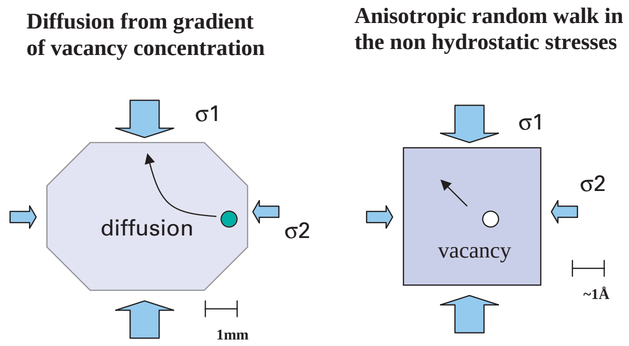


Fig. 1 Comparison of the grain scale deformation with nanoscale rheology controlled by vacancy diffusion. Left; grain scale diffusion creep (NH creep), and right; nanoscale deformation of crystal due to vacancy migration under non hydrostatic stresses.

anisotropy defined by D1/D2 vs temperature and pressure. It shows that the anisotropy ratio increases to unity with increasing temperature and pressure, indicating that the anisotropy decreases with these parameters. Considering the strain rate proportional to D1–D2 = D1(1–D2/D1), the strain rate should be largely controlled by temperature and pressure dependences of diffusion constant. On the other hand, the anisotropy ratio depends linearly on differential stress as shown in Fig. 3, suggesting that the strain rate is proportional to differential stress. Therefore, it is concluded directly that then diffusion controlled plasticity is just Newtonian as predicted by simple model on NH and Coble type creeps. This is the first results by direct anisotropic diffusion experiments by MD rheology. The figure 3 also indicates the symmetric relations in the negative and positive differential stresses, indicating scarce crystallographic orientation effects on anisotropic diffusion of vacancy in this study.

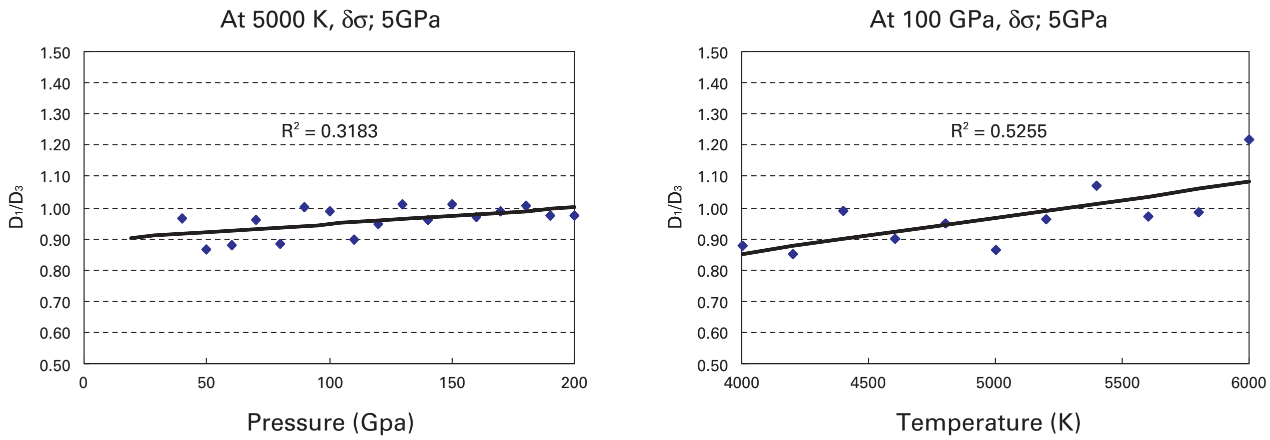
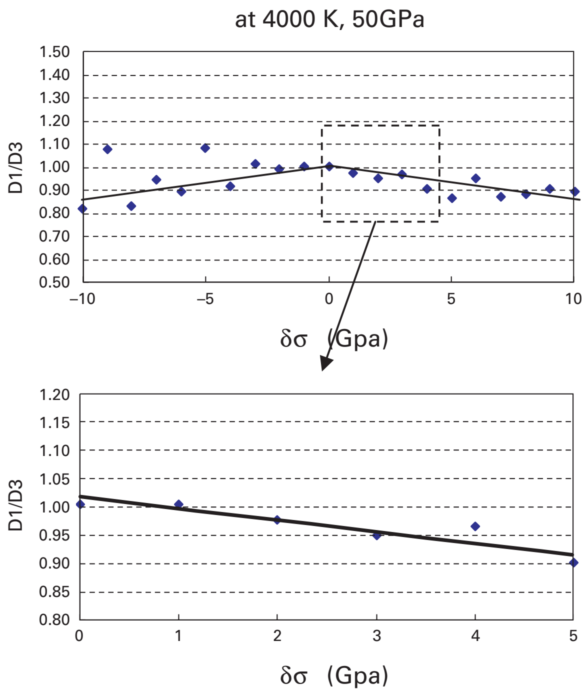


Fig. 2 Simulation results by MD method of anisotropic ratio of diffusion constant D1/D2 versus temperature (left) and pressure (right).



$$d\varepsilon/dt = D_1(1 - D_1/D_2)/G$$
$$= \text{const} \times \Delta\sigma/G$$

Fig. 3 Simulation results by MD method of anisotropic ratio of diffusion constant D1/D2 versus differential stress value, indicating the linear relation between them.

3. Discussion

The rheology of the Earth' mantle and crust has been studied by high temperature and high pressure creep experiments, but the ranges of these parameters were highly limited because of experimental difficulty (Yamazaki and Karato 2001). The upper bound of the experimental pressure is still 5Gpa in the normal case, but if the qualitative studies are involved, the upper limits extend to 20–30Gpa reaching the lower mantle conditions. The precise controls of differential stress strongly require the gas-medium experimental devices because of no friction between sample and device. This implies that the lower mantle rheology in experimental world is still beyond the science. The alternative approaches should be tired for investigation of the whole mantle dynamics together with earth evolution. Thus, the simulation rheology of earth materials is strongly needed.

Two schemes of simulation rheology are possible: one is the nanodynamics of dislocations and point defects (impurity ions and vacancies) using known models of creep, and the second is the direct simulation under the non hydrostatic stresses with MD simulation. The present study has been carried out to try the direct method of simulation rheology for mantle materials. The results indicate the diffusion controlled plastic flow depending linearly on the differential stress, indicating the Newtonian creep. This results show the available model of Nabarro - Herring creep having power exponent of unity (Ando 1989). That model is based on the thermodynamics of vacancy near the surfaces with neighboring grains, and thus it depends basically the grain shapes which changes with increasing plastic deformation. As a result, the strain rate by NH creep should be time-dependent but not steady state deformation.. However, the nanoscale deformation of crystal controlled by anisotropic diffusion of vacancies must be scale - invariant because vacancies should flow depending on stress configuration within a single crystal.

The temperature and pressure dependences of anisotropic diffusion do not mean the characteristics of the flow law, but the fast or slow diffusion coefficient must control the flow law in the temperature and pressure dependencies because of strain rate proportional to the difference between D1 and D2. The activation volume has been obtained as positive to negative value near the 70 Gpa and the activation enthalpy as 586 kJ/mol on MgO by means of MD method previously (Toriumi 2004).

References

Ando, K. (1989), Self-diffusion in oxides, Rheology of Solids and of the Earth, 57–82, Oxford University Press, Tokyo

Karato, S., S. Zhang, and H. Wenk (1995), Superplasticity in Earth's lower mantle: Evidence from seismic anisotropy and rock physics, Science, 270, 458–461

Toriumi, M., (2004), Numerical simulation of physical properties of earth materials. Annual report of the Earth Simulator Center, 2003–2004, 101–103.

Yamazaki, D., and S. Karato (2001), Some mineral physics constraints on the rheology and geothermal structure of Earth's lower mantle, Am. Mineral., 86(4), 385–391

計算地球物質科学による地球内部物質の物性評価計算

プロジェクト責任者
鳥海　光弘　　海洋科学研究開発機構／東京大学新領域創成科学研究科

著者
鳥海　光弘　　海洋科学研究開発機構／東京大学新領域創成科学研究科
伊藤　洋介　　東京大学地球惑星科学専攻

地球内部物質の計算科学的レオロジイの研究目的はマントルおよび地殻における流動則とその特徴量を決定することにある。地球物質のレオロジイは地球内部のダイナミックスを支配している基本的性質であり、このためレオロジイにより流動則や摩擦則を温度と圧力および水蒸気圧の関数として精度よく決定する必要がある。しかしながら、実験的研究の可能な範囲は高々50 kb以下であり、一方理論的な理解も多結晶体の結晶転位や点欠陥の集団的な運動のために、困難で未開拓な状態である。

分子動力学法による格子拡散型の変形に対する直接計算は多体問題と精度の問題で長時間ステップの計算を必要とするために現在のところ地球シミュレータでしか実行可能ではない。直接変形計算法は非静水圧下の条件で結晶内に閉じ込めた空孔を異方的に移動させることによって実現される。ここではMgOについて直接変形計算法によって流動則を決定しようと試みた。この計算には十分な精度の拡散係数を必要とするため、MD計算の時間をピコ秒まで行った。

計算結果は第一に、異方的拡散が非静水圧下で起こり、第2に異方的流動の活性化体積、活性化エンタルピーは負であり、第3には、異方的流動から得られる直接歪速度は加えられた差応力に1次で比例したことである。これらの結論は従来からの簡易モデルと調和的である。

キーワード：流動則，粘性率，計算レオロジイ，空孔，直接変形