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CALCULATION OF ELASTIC CONSTANTS OF QUARTZ IN MOLECULAR DYNAMICS SIMULATION

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1. Introduction

Molecular Dynamics (MD) simulation is a technique to compute the equilibrium and transport properties of a classical many-body system of which the nuclear motion of the constituent particles interacting via potential obeys the laws of classical mechanics. Recently, MD simulations are used in many respects instead of real experiments effectively for examining and modeling fundamental elastic behaviors of crystals[1),2)].

The simulations of NPT and NVT ensembles are carried out under uniaxial and tensile stress using 2-body interatomic potential for calculating elastic properties of quartz which is one of rock-forming minerals. We here report the results simulating the measurement of elastic compliance and stiffness which are calculated from stress-strain curves in single crystal.

2. Molecular Dynamics Simulation

For computing all forces between the particles, we treat the techniques used to solve the Newton's equations of motion for systems that we are aimed to simulate. The calculation of the force acting on every particle is the most time-consuming part of almost all MD simulations. A standard method for solving the ordinary differential equation is the finite difference method. One of the most widely used methods for integrating the equations of motion is the Verlet algorithm which is used in this study.

3. 2-body interatomic potential and ensembles

The 2-body interatomic potential function which we use is of the form:

$$U_{ij}(r_{ij}) = \frac{z_i\, z_j\, e^2}{r_{ij}} + f_0(b_i + b_j)\exp\left(\frac{a_i + a_j - r_{ij}}{b_i + b_j}\right) - \frac{c_i\, c_j}{r_{ij}^6} + D_{ij}[\exp\{-2\beta_{ij}(r_{ij} - r_{ij}^*)\} - 2\exp\{-\beta_{ij}(r_{ij} - r_{ij}^*)\}] \quad (1)$$

The function consists of the Coulomb term, the short range repulsion term, the Van der Waals term and the Morse term as a covalent force .

The MD simulations were carried out in NPT and NVT ensemble using the combination of the constant-temperature and the constant-pressure. For the constant-temperature MD simulation the velocities of atoms are rescaled at each time step. And the constant-pressure MD simulation was implemented by changing dimensions of axes and angles between these axes in the basic cell.

4. Calculation Models

Basic cells consist of 100 unit cells (5a×5b×4c, 900 atoms) and the unit cell had initial dimensions of a=4.912Å, b=4.912Å and c=5.390Å. The calculation was carried out to solve the equation of motion with a time increment of 2.0 fs. for quartz. Relaxation calculation keeping the temperature constant at 300K and the pressure constant at 0GPa is carried out for first 5000 time steps. And periodic boundary condition is adopted in three directions.

5. Evolutions of elastic compliance and stiffness for quartz

Key word : Molecular Dynamics Simulation, NPT and NVT ensemble, 2-body interatomic potential.

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Hookean elastic solids obey a linear Hooke's law, which states that the stress tensor is linearly proportional to the strain tensor:

$$\varepsilon_{ij} = S_{ijkl}\,\sigma_{kl} \qquad (2)$$

where ε_{ij} is the strain tensor, σ_{kl} the stress tensor and S_{ijkl} the elastic compliance, and the inverse of the elastic compliance is the elastic stiffness(C_{ijkl}). When a uniaxial compression is applied to a basic cell parallel to the principal axis, the principal strains are simply the unit relative displacements (normal strains) that occurs in the axis direction (Fig.1). And the shear strains are the half of the change of angles between principal axes (Fig.2).

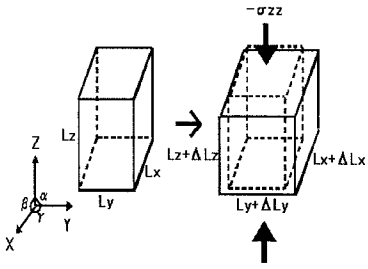

Fig.1 Model of simulation for normal strain

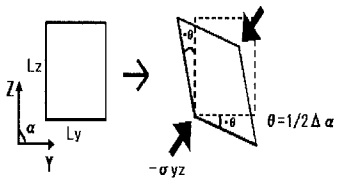

Fig.2 Model of calculation for shear strain

6. Results of calculation for elastic compliance and stiffness

As the results of MD calculations in NPT and NVT ensemble for quartz, elastic compliance and stiffness are determined by using the stress-strain curves. They are compared with experimental elastic constants in table 1. It shows that the elastic constants calculated by MD simulation agree well with the experimental data.

References

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2)N. Miyazaki and Y. Shiozaki, J. JSME, A-62, No.594, 1996.

Table 1 Elastic constants for quartz

Stiff-ness	Exp. (GPa)	MD (GPa)	Compli-ance	Exp. (1/GPa)	MD (1/GPa)
C_{11}	86.6	90.8	S_{11}	0.0128	0.0121
C_{12}	6.7	7.3	S_{12}	-0.0017	-0.0014
C_{13}	12.6	4.0	S_{13}	-0.0013	-0.0003
C_{14}	-17.8	16.3	S_{14}	0.0045	-0.0020
C_{33}	106.1	129.1	S_{33}	0.0097	0.0079
C_{44}	57.8	56.6	S_{44}	0.0201	0.0271

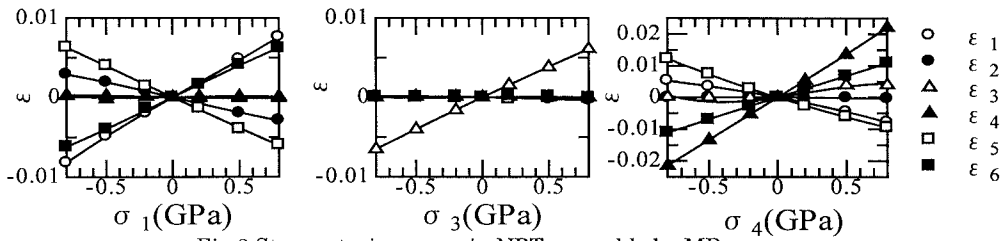

Fig.3 Stress-strain curves in NPT ensemble by MD

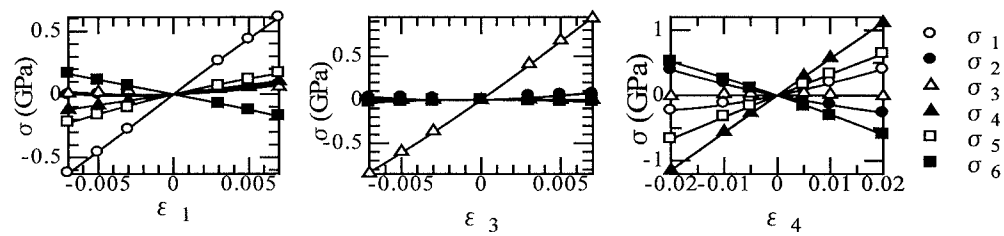

Fig.4 Stress-strain curves in NVT ensemble by MD