Calculation of Mechanical Properties of Solids Using Molecular Dynamics Method*

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We describe the calculation of mechanical properties of solids using the molecular dynamics method. The thermal expansion coefficient and elastic constants of α -Fe are calculated using an empirical potential, that is, the Johnson potential. The thermal expansion coefficient is calculated using a differential operation of the temperature dependence of the lattice constant obtained from the *NPT* ensemble molecular dynamics analysis. Reasonable agreement is found between the analytical results and measured data up to the phase transition temperature. The elastic constants are calculated from the stress-strain curves obtained from the *NVT* ensemble, the initial lattice constant of which is modified based on the result of the *NPT* ensemble. The analytical results agree reasonably well with the measured data up to 400 K.

Key Words: Computational Mechanics, Molecular Dynamics, Tensile Properties, Empirical Potential, Thermal Expansion Coefficient, Elastic Constants

1. Introduction

Material properties in extreme conditions such as extremely high or low temperature and extremely thin film hardly exist because their experimental measurements in such conditions are very difficult to obtain. When we calculate thermal stress during CZ (Czochralski) growth of a Si single crystal⁽¹⁾, we need the thermal expansion coefficient and elastic constants just below the melting temperature of the Si single crystal; however, no such data are available. Therefore, we can only rely on values extrapolated from the measured data obtained at temperatures far below the melting point and we cannot obtain reliable thermal stress of a Si single crystal during CZ growth.

The molecular dynamics (MD) method has been recently applied to various fields of science and engineering⁽²⁾ due to the recent development of high-performance supercomputers. In this method, the equations of motion for every molecule in a system are solved numerically to obtain its position and velocity, by which various material properties can be estimated using statistical mechanics⁽³⁾. The MD method provides a means of estimating material properties that have been difficult to measure. Although such applications of the MD method to practical materials have been made recently, there remain several problems. As regards the thermal expansion coefficient of a solid, it is easy to estimate using a lattice constant versus temperature curve obtained from MD calculations, and the thermal expansion coefficient of *c*-Si has already been calculated using the first-principle MD method⁽⁴⁾. The calculation based on the first-principle MD method is, however, hard to apply, considering that it requires a large amount of computer memory and computational time. Thus the use of empirical potentials which are compiled in handbooks⁽⁵⁾⁻⁽⁷⁾ is the most practical way of applying the MD method to the estimation of

* Received 29th May, 1996. Japanese Original: Trans. Jpn. Soc. Mech. Eng., Vol. 62, No. 594, A (1996) pp. 430-436 (Received 8th May, 1995)

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material properties. Either the fluctuation method^{(8),(9)} or the direct method^{(8),(10)}, in which elastic constants are defined as the initial tangent of a stress-strain curve obtained from the MD method, can be applied to the estimation of elastic constants of a solid. The former method is superior to the latter one in that it is capable of estimating the error of results⁽⁹⁾. On the other hand, the latter method provides additional information on material strength such as yielding due to dislocation generation⁽¹¹⁾. The direct method has been applied only to materials obeying the Lennard-Jones potential at very low temperature^{(8),(10)}, and has not been applied to the analysis of elastic constants of practical materials at high temperature. Establishment of a methodology for estimating elastic constants is of importance in obtaining not only elastic constants at extreme conditions but also accurate information on material strength in such conditions. In order to obtain reliable information on material strength, it is essential for the MD method to provide the accurate initial tangent of a stress-strain curve.

From the above background, we dealt with the calculation of mechanical properties of such a practical material as Fe using the MD method. The mechanical properties calculated were the thermal expansion coefficient and elastic constants, and they were calculated up to 400 K. The elastic constants were estimated by the direct method. The calculated values were compared with measured data.

2. Molecular Dynamics Method

2.1 General remarks

The MD method deals with Newton's equations of motion for N atoms or molecules which are subjected to forces from other atoms or molecules. Hereafter atoms or molecules are called particles. The equation of motion for a particle i is written as

$$m_i \frac{d^2 r_i}{dt^2} = F_i \left[-\frac{\partial \Phi}{\partial r_i} \right] \quad i=1, 2, \dots, N \quad (1)$$

where m_i , r_i and F_i denote mass, a position vector and a force vector of the particle i , respectively, and t and Φ denote time and total potential, respectively. These equations of motion are approximated by difference equations. Both initial conditions and boundary conditions are required for solving them. Both initial positions and velocities of particles are given as initial conditions. Initial velocities of particles are so determined that they are subjected to the Maxwell distribution; that is, a component of a velocity vector $\mathbf{v}$ at the temperature T is given by

$$\sqrt{\frac{m}{2\pi k_B T}} \exp \left\{ -\frac{mv^2}{2k_B T} \right\} \quad (2)$$

where v is one component of the velocity vector $\mathbf{v}$.

The equations of motion can be rewritten in a

nondimensional form using nondimensional positions x^* and r^* , velocity v^* , force F^* , time t^* , and temperature T^* which are defined as

$$x^* = \frac{x}{\sigma}, \quad r^* = \frac{r}{\sigma}, \quad v^* = \sqrt{\frac{m}{\epsilon}} v, \quad F^* = \frac{\sigma}{\epsilon} F, \quad (3)$$

$$t^* = \sqrt{\frac{\epsilon}{m\sigma^2}} t, \quad T^* = \frac{k_B}{\epsilon} T$$

where k_B , ϵ , σ and m denote the Boltzmann constant, interatomic potential depth, pseudo-diameter of a particle and particle mass, respectively.

2.2 NVT ensemble

The *NVT* ensemble MD method, in which the total number of particles N , system volume V and system temperature T are conserved, was used to calculate the elastic constants by the direct method. In this ensemble, the system temperature is kept constant by absorbing energy from a heat bath or discharging energy to it.

In the present analysis, we realized a constant system temperature by multiplying particle velocities by the following scale factor β at every certain time steps.

$$\beta = \left(\frac{T_{set}}{T} \right)^{\frac{1}{2}} = \left(T_{set} / \frac{2}{k_B N_{free}} \frac{1}{2} \sum_i^N m_i v_i^2 \right)^{\frac{1}{2}} \quad (4)$$

Here T_{set} and N_{free} denote a set temperature and the number of degrees of freedom of a particle, respectively. Equation (1) reduces to the following difference equations using the Verlet method⁽¹²⁾.

$$x_i(t + \Delta t) = x_i(t) + \Delta t v_i(t) + (\Delta t)^2 F_i(t) / 2m \quad (5)$$

$$v_i(t + \Delta t) = v_i(t) + \Delta t (F_i(t + \Delta t) + F_i(t)) / 2m \quad (6)$$

2.3 NPT ensemble

The *NPT* ensemble MD method, in which the total number of particles N , system pressure P and system temperature T are conserved, was used to calculate the thermal expansion coefficient. It is necessary to change system volume V to keep system pressure P constant. In this case, the conserved value is not internal energy E but enthalpy H defined by

$$H = E + P_E V \quad (7)$$

where P_E denotes external pressure, which is equal to system pressure in an equilibrium state.

In this ensemble, the position ρ_i and volume V of particle i are given as⁽¹²⁾

$$\rho_i^{n+1} = \rho_i^n + h \dot{\rho}_i^n + \frac{1}{2} \frac{h^2 F^n}{m L^n} - \frac{1}{3} h^2 \dot{\rho}_i^n \frac{\dot{V}^n}{V^n} \quad (8)$$

$$V^{n+1} = V^n + h \dot{V}^n + \frac{1}{2M} h^2 (P^n - P_E) \quad (9)$$

where $\rho_i = r_i / V^{1/3}$, and M and h denote the mass associated with the volume V and time interval, respectively. In Eqs. (8) and (9), the superscript n indicates a value at time step n , and $(\dot{})$ denotes differentiation with respect to time t . M is used as a parameter for suppressing the variation of P and V , hence a relatively large value is selected as its initial

Table 1 Crystal parameters of Fe

Temp[K]	Fe	Lattice constant[Å]	Crystal lattice
~1189	α -Fe	2.8665	b.c.c.
~1662	γ -Fe	3.6467	f.c.c.
~1808	δ -Fe	2.9315	b.c.c.

Table 2 Parameters of Johnson potential

Range(Å)	c_1	c_2	c_3	c_4
1.9 - 2.4	2.195976	3.097910	2.704060	7.436448
2.4 - 3.0	0.639230	3.115829	0.477871	1.581570
3.0 - 3.44	1.115035	3.066403	0.466892	1.547967

value and it is reduced to a small value when the system becomes stable. System temperature T is kept constant using the scaling method described in 2.3. Angle change between the axes of a unit cell is not permitted in the present NPT ensemble MD method.

System pressure can be calculated from the following equation using the virial equation⁽¹²⁾:

$$P = \frac{1}{3V} \left[\sum_i m v_i^2 + \sum_{i < j} r_{ij} F_{ij} \right] \quad (10)$$

where V and v_i denote system volume and the velocity of particle i , respectively. In order to keep system pressure P constant at P_E , V was increased, hence P was decreased, if $P > P_E$; conversely V was decreased, hence P was increased, if $P < P_E$.

2.4 Interatomic potential used in the analyses

The lattice structure of Fe changes as shown in Table 1 as the temperature increases. The interatomic potential used in the analyses was the Johnson potential⁽¹³⁾, from which the lattice constant and elastic constants of Fe at 0 K were reproduced; it is given by

$$\phi(r_{ij}) = -c_1(r_{ij} - c_2)^3 + c_3 r_{ij} - c_4 \quad (11)$$

$[\phi: \text{eV}, \quad r_{ij}: \text{\AA}]$

where c_1 through c_4 are parameters, the values of which are summarized in Table 2. According to a handbook on empirical interatomic potential⁽⁶⁾, the Johnson potential can be used not only for α -Fe but also for γ -Fe. The lattice structure of δ -Fe is the same as that of α -Fe, so that the Johnson potential was used for δ -Fe.

3. Calculation of Thermal Expansion Coefficient

3.1 Model for analysis and method of analysis

The model used in a thermal expansion coefficient analysis was a cubic unit cell composed of 64 unit lattices, in which four unit lattices are aligned along x , y and z ; hence the total number of atoms is 128 for α - and δ -Fe and 256 for γ -Fe. Cyclic boundary conditions were applied to all x -, y - and z - directions to calculate the thermal expansion coefficient of bulk Fe. The lattice constants shown in Table 1 were used as initial values for each crystal structure. In the present

Fig. 1 Lattice constant

Fig. 2 Thermal expansion coefficient

NPT ensemble MD method, no phase transition could be obtained at the temperatures shown in Table 1 probably because the angle change between the axes of a unit cell is not permitted. Thus atoms were rearranged at the phase transition temperature. A more flexible NPT ensemble is desired to simulate phase transition.

At a prescribed temperature, the lattice constant a was calculated from the volume V obtained from NPT ensemble MD method, and such a calculation was made at various temperatures to obtain temperature variation of the lattice constant. The thermal expansion coefficient α was calculated from the following equation:

$$\alpha = \frac{1}{a(273.15[\text{K}])} \left[\frac{da}{dT} \right]_{p=\text{const}} \quad (12)$$

A polynomial of a - T relation obtained from the MD method was used to calculate $(da/dT)_{p=\text{constant}}$.

$$a = \sum_{i=0}^n A_i T^i \quad A_i: \text{constant} \quad (13)$$

3.2 Results and discussion

Figure 1 shows the temperature variation of the

lattice constant of Fe obtained from the *NPT* ensemble MD method. This α - T curve was approximated by a 10th-order polynomial for α -Fe and a second-order polynomial for γ - and δ -Fe, and the thermal expansion coefficient α was calculated using Eq.(12). Figure 2 shows the analytical result compared with experimental data^{(14),(15)}. The present analytical result agrees relatively well with experimental data for α -Fe, but not for γ -Fe. Thus, application of the Johnson potential to the calculation of material properties of γ -Fe is questionable.

4. Calculation of Elastic Constants

4.1 Model for analysis and method of analysis

4.1.1 Method for calculating elastic constants

In a cubic crystal, the components of elastic constants matrix are given by the three independent elastic constants C_{11} , C_{12} and C_{44} as follows⁽¹⁶⁾:

$$\begin{Bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & & & \\ & C_{11} & C_{12} & & & \\ & & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{bmatrix} \begin{Bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{Bmatrix} \quad (14)$$

where stress σ_i and strain ε_i are defined as

$$\begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{zx} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix} \quad (15)$$

$$\begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{zx} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix} \rightarrow \begin{bmatrix} \varepsilon_1 & \varepsilon_6/2 & \varepsilon_5/2 \\ \varepsilon_6/2 & \varepsilon_2 & \varepsilon_4/2 \\ \varepsilon_5/2 & \varepsilon_4/2 & \varepsilon_3 \end{bmatrix} \quad (16)$$

The elastic constants can be calculated from σ_i - ε_i relations based on Eq.(14). In practice, by setting $\varepsilon_1 = \varepsilon_3 = \varepsilon_4 = \varepsilon_5 = 0$ in Eq.(16), we obtain the following relations for the calculation of the elastic constants:

$$C_{11} = \sigma_2 / \varepsilon_2 \quad (17)$$

$$C_{12} = \sigma_1 / \varepsilon_2 = \sigma_3 / \varepsilon_2 \quad (18)$$

$$C_{44} = \sigma_6 / \varepsilon_6 \quad (19)$$

4.1.2 Model for analysis

The model used in the elastic constants analysis was a cubic unit cell composed of 27 unit lattices, in which three unit lattices are aligned along x , y and z , hence the total number of particles is 54. An internal region S corresponding to one unit lattice was taken in a unit cell to calculate stresses that are defined by⁽¹⁷⁾

$$\sigma_{mn} = \frac{1}{N_s} \sum_i \left[\frac{mv_i^m v_i^n}{V_i} - \frac{1}{2V_i} \sum_j \frac{\partial \phi(r_{ij})}{\partial r_{ij}} \frac{x_{ij}^m x_{ij}^n}{r_{ij}} \right] \quad (20)$$

where N_s is the number of particles contained in the region S and V_i is the local volume of an atom and given by⁽¹⁸⁾

$$V_i = \frac{4\pi}{3} a_i, \quad a_i = \frac{\sum_j r_{ij}^{-1}}{2 \sum_j r_{ij}^{-2}} \quad (21)$$

4.1.3 Method for obtaining stress-strain relation

According to the method used by Iwaki⁽¹⁹⁾, tensile or shear loading was applied to a unit cell by varying its shape at every certain time steps, and after relaxation to thermal equilibrium, average stresses and strains were determined.

As shown in Eqs.(17) and (18), σ_1 , σ_2 (or σ_3), ε_1 and ε_2 are required for calculating C_{11} and C_{12} . The stresses σ_1 , σ_2 and σ_3 were obtained by increasing the unit cell length in the y -direction L by LC , as shown in Fig. 3. The normal strain in the y -direction ε_{yy} was calculated by

$$\varepsilon_{yy} = \frac{L_y - L_{y0}}{L_{y0}} = \frac{\Delta L_y}{L_{y0}} \quad (22)$$

where L_y is the length in the y -direction which was calculated from the average positions of particles located at the outer periphery of region S for stress calculations after a certain amount of deformation was applied to a unit cell, L_{y0} is its initial length, and $\Delta L_y = L_y - L_{y0}$. The symbols $\circ$, $\triangle$ and $\square$ in Fig. 4 show the calculated stress-strain relations at T of 5 K. The calculated stress-strain curves indicate good linearity in the lower strain region and nonlinearity and sharp drop of stress in the higher strain region.

Fig. 3 Model for calculating C_{11} and C_{12}

Fig. 4 Stress-strain curves for calculating C_{11} and C_{12} ($N=54$, $T=5$ K)

As shown in Eq. (19), σ_6 and ϵ_6 are required for calculating C_{44} . The stress σ_6 and strain ϵ_6 were obtained by deforming a unit cell by LC , as shown in Fig. 5. The shear strain ϵ_{xy} was calculated by

$$\epsilon_{xy} = \frac{1}{2} \left(\frac{\Delta L_y}{L_x} + \frac{\Delta L_x}{L_y} \right) \quad (23)$$

where ΔL_x and ΔL_y are, respectively, x - and y -displacements obtained from the average positions of the particles located at the outer periphery of region S for stress calculation. Figure 6 shows the calculated stress-strain relation. A linear relationship between stress and strain holds in the lower strain region.

4.1.4 A region for stress calculations Stresses can be estimated using Eq. (20). Iwaki⁽²⁰⁾ insists that both particles i and j in Eq. (20) should be taken so as to be included in the region S for stress calculations. In the present stress calculations, however, the particle i was taken in the region S , but all the particles within the range affected by the potential of the particle i were considered as the particle j which interacts with the particle i , so that some particles outside the region S were taken as the particle j . In Fig. 4, the stress-strain curve indicated by the symbol * is the result obtained using Iwaki's method. This

Fig. 5 Model for calculating C_{44}

Fig. 6 Stress-strain curve for calculating C_{44} ($N=54$, $T=5$ K)

result shows a higher stress at $\epsilon_2=0$ and a smaller slope, compared with the present method. As mentioned later, the slope of the stress-strain curve obtained from the present method provides reasonable elastic constants, so that Iwaki's method for stress calculations is doubtful.

4.1.5 Correction of initial stress A fixed value of lattice constant is used in the NVT ensemble MD calculation. Figure 7 shows the stress-strain curves of α -Fe obtained from the MD calculation using the lattice constant of $2.86 \text{ \AA}$ which is nearly equal to the lattice constant at T of 0 K. As shown in the figure, compressive stress increases at $\epsilon_2=0$ as the temperature T is increased. An initial compressive stress may be induced from constraining the thermal expansion of lattice by fixing the lattice constant of 0 K which is smaller than that of the corresponding temperature. In order to correct the initial compressive stress, we used the lattice constant obtained from the NPT ensemble MD method, the results of which are shown in Table 3, as a fixed value of the lattice constant corresponding to the temperature T . Figure 8 shows the stress-strain curves after correction of the initial compressive stress. Consequently all curves intersect at the origin.

4.2 Results and discussion

The calculated results of C_{11} , C_{12} and C_{44} are shown in Figs. 9 and 10, in comparison with experimental data⁽²¹⁾. C_{11} and C_{12} were respectively estimated by Eqs. (17) and (18), and C_{44} was estimated

Table 3 Lattice constants for correcting initial stress

Temp[K]	Lattice constant[Å]	Lattice constant[Å] (after correction)
100	2.86	2.86237
200	2.86	2.86643
300	2.86	2.87096
400	2.86	2.87553

Fig. 7 Effect of temperature on stress-strain curve

Fig. 8 Effect of temperature on stress-strain curve (after correcting initial stress)

Fig. 9 Elastic constants C_{11} and C_{12}

Fig. 10 Elastic constant C_{44}

using the following three equations.

$$C_{12} = \sigma_1 / \epsilon_2 \quad (24)$$

$$C_{12} = \sigma_3 / \epsilon_2 \quad (25)$$

$$C_{12} = (\sigma_1 + \sigma_3) / 2\epsilon_2 \quad (26)$$

Although there exist no experimental data in the lower temperature range, the MD results of C_{11} agree well with the experimental data⁽²¹⁾. As for C_{12} , when

the temperature is increased, the difference between the results of Eqs. (24) and (25) becomes large, and they deviate from the experimental data. However, the results of Eq. (26) which provide the average value of C_{12} calculated from Eqs. (24) and (25) agree reasonably well with the experimental data. On the other hand, the calculated results of C_{44} deviate from experimental data when the temperature is increased. At higher temperatures, a larger unit cell will be required for obtaining valid results because of large thermal fluctuation.

5. Conclusions

The thermal expansion coefficient and elastic constants of Fe are calculated using the *NVT* or *NPT* ensemble MD method. The following conclusions are derived from the present study.

(1) The Johnson potential, the parameters of which are determined so as to reproduce the lattice constant at 0 K, gives reasonable agreement with experimental data for α -Fe but not for γ -Fe. The applicability of the Johnson potential to γ -Fe is questionable.

(2) When stresses are calculated using the MD method, all particles not only within the region for stress calculations but also within the range affected by the potential should be considered as interacting particles.

(3) In the stress calculations using the *NVT* ensemble MD method, the lattice constant estimated from the *NPT* ensemble MD method should be used as a fixed value of the lattice constant corresponding to the temperature T to obtain a valid stress-strain curve.

(4) The elastic constants obtained from the MD method agree reasonably well with measured data up to 400 K. At higher temperatures, a larger unit cell will be required.

This study was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture.

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