Molecular Dynamics Study on Stress-Strain in Very Thin Film*

(Size and Location of Region for Defining Stress and Strain)

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The stress and strain in a very thin film under uniaxial tension are analyzed based on the motion of particles in the film by means of two-dimensional molecular dynamics (MD) simulation. The Lennard-Jones (L-J) potential is assumed as a two-body potential. The tensile load is applied by elongating the fundamental cell longitudinally. The numerical results show that the stress decreases considerably as the size of the region for defining the stress decreases. It is found that more than 130 particles are necessary in the region for the stress concept to be applicable in continuum mechanics.

Key Words: Computational Mechanics, Molecular Dynamics, Stress, Strain, Thin Film

1. Introduction

The manufacturing, processing and application techniques of thin films are being rapidly developed since the thin film is an essential basic element for advanced functional materials and devices. However, the mechanical and thermal properties of thin films are not fully understood because of experimental difficulties, i.e., knowledge concerning the properties is still insufficient. Hence, the values of physical quantities such as the coefficient of elasticity and thermal expansion obtained from the bulk material are used for the thin film⁽¹⁾.

In addition to the physical properties of the bulk, it is very important to investigate whether the macroscopic concepts established for continuum mechanics can be applied to microscopic elements such as thin film. Computer physics is one of the most powerful approaches for investigating microscopic elements

and structure. As a study on the application of a macroscopic concept, Kotake and Wakuri first clarified the mechanism of heat conduction of the thin film by using the MD simulation⁽²⁾, which was one of the computer physics techniques which was used in studies on crack initiation and propagation⁽³⁾⁻⁽⁷⁾, as well as estimation of macroscopic physical properties⁽⁸⁾⁻⁽¹⁰⁾.

The objective of this study is to understand qualitatively the stress and strain induced in a very thin film under uniaxial tension by means of two dimensional MD simulation. The stress and strain can be defined as physical quantities of molecular agglomerates; hence they strongly depend on the behavior of the molecular agglomerate. In this study, the stress and strain are defined as the physical quantity developed from the virial theorem⁽¹¹⁾ and as the change of distance between the molecules constructing the agglomerate, respectively. We discuss how to obtain the microscopic stress and strain from the motion of the molecular agglomerate. Furthermore, the relationship between the stress and strain levels and the molecular behavior, and the differences between the present stress and strain and those established in

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continuum mechanics are also clarified.

2. Computer Experiment Method

2.1 Thin film model and calculation method

The thin film configuration consisting of particles of atoms or molecules⁽¹¹⁾ is shown in Fig. 1. The force $F^{a\beta}$ of particle β on particle α is expressed as

$$F^{a\beta} = -\nabla \phi^{a\beta}, \quad (1)$$

where $\phi^{a\beta}$ is a pairwise potential between particles α and β , which is assumed to be the L-J (12-6) potential

$$\phi^{a\beta} = 4\epsilon \left\{ \left(\frac{\sigma}{r^{a\beta}} \right)^{12} - \left(\frac{\sigma}{r^{a\beta}} \right)^6 \right\}. \quad (2)$$

Here, $r^{a\beta}$ is the distance between particles α and β , and ϵ and σ the well depth and the length parameter, respectively. The force acting on particle α is then given by

$$F^a = \sum_{\beta} F^{a\beta}. \quad (3)$$

Denoting the mass by m , we have the following dimensionless position, length, velocity, force, time, energy, temperature and stress.

$$\begin{aligned} x^* &= \frac{x}{\sigma}, \quad l^* = \frac{l}{\sigma}, \quad v^* = \sqrt{\frac{m}{24\epsilon}} v, \quad F^* = \frac{\sigma}{24\epsilon} F, \\ t^* &= \sqrt{\frac{24\epsilon}{m\sigma^2}} t, \quad E^* = \frac{1}{24\epsilon} E, \quad T^* = \frac{k_B}{12\epsilon} T, \\ \sigma_{ij}^* &= \frac{\gamma}{24\epsilon} \sigma_{ij}. \end{aligned} \quad (4)$$

Here k_B is Boltzmann's constant and γ the specific volume. Hereafter, the asterisks are omitted. The

Fig. 1 Configuration of thin film and region defining stress and strain

equations of motion are transformed into the following difference equations:

$$v^a \left(t + \frac{\Delta t}{2} \right) = v^a \left(t - \frac{\Delta t}{2} \right) + F^a(t) \Delta t, \quad (5)$$

$$x^a(t + \Delta t) = x^a(t) + v^a \left(t + \frac{\Delta t}{2} \right) \Delta t. \quad (6)$$

The x -axis is taken in the direction of the thickness and the periodic boundary conditions are employed in the y direction in order to consider a film of infinite length, as shown in Fig. 1. In the fundamental cell, the numbers of particles are 16 and 18 in the x and y directions, respectively, for a total of 288 (16 × 18). In Eqs. (5) and (6), the time step of $\Delta t = 0.01$ is used because the period of thermal vibration of a particle is about 1–2. Tensile load is applied by elongating the longitudinal length, l_{yc} , of the fundamental cell by 0.2 % every 10^4 time steps.

In order to obtain the state of thermal equilibrium before applying the tensile load, the particles are set in motion during 10^4 time steps with $\Delta t = 0.005$. The stress and strain are calculated by averaging over the last 2000 time steps every 10^4 time steps. The potential is truncated at $4\sigma^{(2)}$.

2.2 Stress⁽¹¹⁾

The region S is defined as having k and l particles in the x and y directions, respectively, for a total of n ($k \times l$) particles, as shown in Fig. 1 by bold straight lines. Multiplying the equation of i -directional motion of particle α in the region by x_j^a and averaging with respect to time, we have

$$-\frac{1}{2t} \left(v_i^a x_j^a \right) \Big|_{-t}^t + \overline{v_i^a v_j^a} + \overline{x_j^a F_{iV}^a} + \overline{x_j^a F_{i\wedge}^a} = 0. \quad (7)$$

The third and fourth terms in Eq. (7) show the forces acting between the particles on the inside and outside of the region, respectively. The bar means the time average

$$\bar{f} = \frac{1}{2t} \int_{-t}^t f(\tau) d\tau. \quad (8)$$

Setting $t \rightarrow \infty$ in Eq. (7) and summing with respect to all particles in the region, we get

$$\sum_{a \in S} \overline{v_i^a v_j^a} + \sum_{a \in S} \overline{x_j^a F_{iV}^a} = - \sum_{a \in S} \overline{x_j^a F_{i\wedge}^a}. \quad (9)$$

Assuming that the forces due to the particles on the outside of the region, the right side of Eq. (9), act equally on the inside particles, we can define the stress as

$$\sigma_{ij(k \times l)} = \frac{1}{n} \sum_{a \in S} \overline{x_j^a \sum_{\beta \in S} F_{i\wedge}^{a\beta}}, \quad (10)$$

where $n_{\wedge}$ shows the number of particles on the outside of the region. From Eq. (9), the stress can also be expressed by

$$\sigma_{ij(k \times l)} = - \frac{1}{n} \sum_{a \in S} \overline{\left(v_i^a v_j^a + x_j^a \sum_{\beta \in S} F_{i\wedge}^{a\beta} \right)}. \quad (11)$$

If the time average can be written as an arithmetic

mean

$$\bar{f} = \frac{1}{K \cdot \Delta t} \sum_{k=1}^K f(k \cdot \Delta t) \quad (12)$$

so as to satisfy the numerical accuracy, Eq.(11) can be expressed by the relative distance between particles α and β .

$$\sigma_{ij(k \times l)} = -\frac{1}{n} \sum_{\alpha \in S} \left(\overline{v_i^\alpha v_j^\alpha} + \frac{1}{2} \sum_{\beta \in S} (x_j^\alpha - x_j^\beta) F_i^{\alpha\beta} \right), \quad (13)$$

Equation(13) has been extensively used^{(8),(12),(13)}. The stress expression of Eq.(10) cannot be expressed as the relative distance.

2.3 Strain

The strain is defined geometrically by the positions of particles. Using the least-squares method, we get the line segments $\overline{AB}$ and $\overline{CD}$ from the position, x_{ij}^a , of the outside particles forming region S shown in Fig. 1. Denoting as $\overline{l_{y(k \times l)}}$ the difference between the ordinates of the middle points of the line segments, the strain is

$$\varepsilon_{yy(k \times l)} = \frac{\overline{l_{y(k \times l)}} - \overline{l_{y0}}}{\overline{l_{y0}}}, \quad (14)$$

where $\overline{l_{y0}}$ is the reference length. The strain $\varepsilon_{xx(k \times l)}$ is defined in the same manner as $\varepsilon_{yy(k \times l)}$.

2.4 Energy and temperature

The potential, kinetic and total energies and temperature of region S are calculated from

$$E_{p(k \times l)} = \frac{1}{2} \sum_{\alpha \in S} \sum_{\beta \in S} \phi^{\alpha\beta} + \frac{1}{2} \sum_{\alpha \in S} \sum_{\beta \notin S} \phi^{\alpha\beta}, \quad (15)$$

$$E_{k(k \times l)} = \frac{1}{2} \sum_{\alpha \in S} v^\alpha \cdot v^\alpha, \quad (16)$$

$$E_{t(k \times l)} = E_{p(k \times l)} + E_{k(k \times l)}, \quad (17)$$

$$T_{(k \times l)} = \frac{2}{n} E_{k(k \times l)}. \quad (18)$$

3. Computer Experiment Results and Discussion

3.1 Reproducibility

Five computations are performed with different initial positions and velocities of particles. Figure 2 shows the stress-strain curves with respect to the fundamental cell having 16×18 particles. The stress is calculated using Eq.(11) and the strain by substituting $\overline{l_{y0}}$ obtained when $\sigma_{yy(16 \times 18)} = 0$ into Eq.(14). The five curves each of σ_{xx} , σ_{xy} and σ_{yy} are almost the same until σ_{yy} becomes maximum (for example, point G). It can be concluded that these computer experiments have good reproducibility. It is found that σ_{yy} increases nonlinearly with the increase of ε_{yy} . Suga et al. explained that the nonlinearity depends on the particle potential⁽¹⁴⁾. The particles are arranged in a single crystal, as shown in Fig. 1, until σ_{yy} becomes maximum. After that, the arrangement of particles is disordered because a dislocation is induced, and finally a slip appears. Consequently, the distance between particles in the tensile direction is suddenly changed.

Consequently, the tensile stress decreases suddenly, as shown in Fig. 2. For the discussion hereafter, the typical strains of $\varepsilon_{yy} = 0, 3.2$ and 6.4% , shown by points E, F and G, respectively, are selected. The values of σ_{xx} and σ_{xy} are almost constant in spite of the increase of load and are less than 3% of σ_{yy} at point G. They can be considered to be almost zero. Figure 3 shows the potential, kinetic and total energies in the fundamental cell. The kinetic energy is almost constant until point G. Assuming that the particles are argon atoms, we determine the temperature of $5-7$ K from Eqs.(18) and (4). The potential energy increases with the increase of strain. This result shows that the work due to the tensile load is stored as internal potential energy. Similar results are obtained for the other four computations.

3.2 Average with respect to time

In section 3.1, we showed the results obtained for setting $\Delta t = 0.01$ in Eqs.(5) and (6) and $K = 2000$ in Eq.(12). Here, we discuss whether the arithmetic mean expressed by Eq.(12) is suitable for averaging with respect to time, by comparison with the trapezoidal rule. As an example, σ_{yy} is dealt with in the region having 16×18 particles for $\varepsilon_{yy} = 6.4\%$. Table 1 shows the value of each term of Eq.(7) for one

Fig. 2 Stress-strain curve of 16×18 fundamental cell

Fig. 3 Energies in 16×18 fundamental cell

Table 1 Example of values of each term in Eq. (7)

	$-\frac{1}{2t} \left(v_i^\alpha x_j^\alpha \right) \Big _{-t}^t$ (a)	$v_i^\alpha v_j^\alpha$ (b)	$\overline{x_j^\alpha F_{iA}^\alpha}$ (c)	$\overline{x_j^\alpha F_{iA}^\alpha}$ (d)	(b) + (c)	(a) + (b) + (c) + (d)
arithmetic mean (one particle)	0.11261	0.00186	-1.97135	1.85638	-1.96949	-0.00050
trapezoidal rule (one particle)	0.11317	0.00186	-1.97143	1.85641	-1.96958	0.2×10^{-6}
arithmetic mean (average of particles)	-0.00182	0.00222	-0.12658	0.12617	-0.12435	-0.1×10^{-5}
trapezoidal rule (average of particles)	-0.00182	0.00222	-0.12658	0.12617	-0.12436	-0.2×10^{-6}

particle and for the average of 16×18 particles for the case when $K=2000$ in Eq. (12). There are differences between the arithmetic mean and the value obtained using the trapezoidal rule in the third and fourth decimal places of the first term and the third and fourth terms, respectively, for the case of one particle. The relative errors of these differences are less than 5%. However, we have the same values down to the fifth decimal place for each term for the average value of 16×18 particles. The value of the left side of Eq. (7), which must be zero, is less than 0.03% of the third term being the greatest absolute value of four terms. Results similar to those for σ_{yy} are obtained for σ_{xx} and σ_{xy} . Based on these numerical results, it can be concluded that the arithmetic mean is suitable under the conditions in which $\Delta t=0.01$ and $K \geq 2000$. Only then can the stress also be expressed by Eq. (13).

Equation (11) is applicable if the first term of Eq. (7) can be ignored by averaging with respect to time. As shown in Table 1, for the case of one particle, the first term amounts to 5.7% of the sum of the second and third terms or of the fourth term. Therefore, we must discuss the number of time steps, K . As an example, Fig. 4 shows σ_{yy} for $K=2000$ to 2×10^5 when $\epsilon_{yy}=6.4\%$. The number of particles in the region for defining the stress is varied from 16×18 to 1×1 because the first term depends on the number of particles, as shown in Table 1. As the number of particles becomes greater than 8×8 , the errors of σ_{yy} obtained from Eqs. (11) and (13) (shown by solid lines) for $K=2000$ relative to σ_{yy} for $K=2 \times 10^5$ become less than 1.5%. If the number of particles is 1×1 , the relative error is 4%. These relative errors imply that there is little effect due to K on the stress. However, the stress obtained from Eq. (10) (shown by dotted lines) fluctuates with K when K is small. If K is large, the stress becomes constant and agrees with that obtained from Eq. (11) or Eq. (13). The same effects due to K on σ_{xx} and σ_{xy} as on σ_{yy} can be found. From these results, it can be concluded that $K=2000$ is adequate if Eq. (11) or Eq. (13) is used. The length $\bar{l}_{i(k \times l)}$ for the calculation of strain is discussed in a similar manner as for the stress. Because the error of the length for $K=2000$ relative to that for $K=2 \times 10^5$

Fig. 4 Dependence of stress on number of time steps

is less than 0.15%, the effect of K on the strain is very small. The significant stress and strain can be obtained when $\Delta t=0.01$ and $K \geq 2000$. In other words, it is necessary to average them with respect to time over more than 20 periods of thermal vibration.

3.3 Strain induced in thin film and behavior of particle

The trajectories of particles are shown in Fig. 5 at three strain levels marked by points E, F and G in Fig. 2. Particles 1 to 5 are shown by numerals 1 to 5 in Fig. 1. If the particle is near the surface or the tensile load is large, then the particle moves about over a wider region. There are 100 time steps between the symbols marked on the trajectories on the right side of Fig. 5. In this figure, the period of thermal vibration is about 1~5 and the period is long when the tensile load is large. In order to determine the motion of particles more precisely, the probability of the distance between the instantaneous and mean particle positions being certain values during 2000 time steps is shown in Fig. 6. Figures 7 and 8 show the probabilities of the distances being certain values in the x and y directions between the neighboring particles. When the strain increases, the deviation of the distance in the tensile direction between the instantaneous and mean particle positions increases [Fig. 6(b)], that is, the particle moves over a wide area in the y direction. Moreover, the average value and the deviation of the distance between the neighboring particles in the y direction also increase [Fig. 7(b)]. We can find no

Fig. 5 Trajectories of particles

Fig. 6 Probability of distance between instantaneous and mean particle positions being certain values

significant change of the distance between the instantaneous and mean particle positions in the x direction [Fig. 6(a)], but there is a decrease of the average distance between the neighboring particles [Fig. 7(a)]. Results similar to those for particle 1 are obtained for particles 3 and 5. Figure 8 shows that particle 1 moves over a wider area than particles 3 and 5. From these results, it can be concluded that the deformation can be calculated from the statistical average of the distance between the neighboring particles, and the field of motion of particles is extended in the direction in which the distance between the neighboring particles is large. The deviation of the distance between neighboring particles is larger at the surface

than inside the thin film. This implies that lattice defects occur easily at the surface as the load increases.

3.4 Difference compared to stress and strain in continuum mechanics

In continuum mechanics, if the thin film is under simple tension, the stress and strain are uniform and independent of the size and location of the region for defining them. We will discuss whether the stress and strain obtained from Eqs.(11) and (14), respectively, have the same features as the stress and strain defined in continuum mechanics. Figure 9 shows the effect of the size of the region for defining the stress and strain on the stress-strain curve. The size of the region,

Fig. 7 Probability of distance between neighboring particles being certain values

Fig. 8 Probability of distance between neighboring particles being certain values

namely, the number of particles, can be from 16×18 to 2×2 . Then, the strain is obtained by substituting $\bar{l}_{y(k \times l)}$ for the case when $\sigma_{yy(16 \times 18)} = 0$ into $\bar{l}_{y0}$. The symbols on the stress-strain curves at $\epsilon \div 0, 3.2$ and 6.4% mean that the thin film is under the same state and the distance between the neighboring particles is also the same. As the number of particles decreases, the stress-strain curve shifts downward and the compliance increases. It is significant that the stress strongly depends on the number of particles even though the tensile load is the same. This result differs substantially from the concept of stress defined in continuum mechanics. On the contrary, if the number of particles increases, the stress-strain curve approaches a specific position. It is noted that, according to the symbols mentioned above, the number of particles has no effect on the strain, as for the strain in continuum mechanics.

If the region for defining the strain is small, the inaccuracy of the numerator is increased because the

Fig. 9 Effect of number of particles on stress-strain curve

denominator of Eq.(14) is small. Consequently, the stress-strain curve loses smoothness when the number of particles is 2×2 . Here, by substituting $\bar{l}_{y(k \times l)}$ for the case when $\sigma_{yy(k \times l)} = 0$ into $\bar{l}_{y0}$, the stress-strain curves are redrawn as shown in Fig.10 so that

$\sigma_{yy(k \times l)} = 0$ when $\epsilon'_{yy(k \times l)} = 0\%$. The symbols on the stress-strain curves mean that the distances between the neighboring particles are the same as those in the case of Fig. 9. It is noted that the stress decreases and the distance between the neighboring particles increases with the decrease of the number of particles when the strain is fixed. From Fig. 10, we can determine the relationships between the stress and the number of particles at $\epsilon'_{yy(k \times l)} = 0, 3.2$ and 6.4% , as shown in Fig. 11. The stress approaches a constant value as the number of particles becomes large. The relationship can be expressed by

$$\sigma_{yy(k \times l)} = A \exp\left(-\frac{\sqrt{n}}{3}\right) + B, \quad (19)$$

where A and B are constants, and is shown by the solid lines in Fig. 11. Assuming that n in Eq. (19) tends to infinity, we need an agglomerate of more than 130 particles to obtain a stress which is independent of the number of particles, that is, error relative to the stress at $n \rightarrow \infty$ is less than 3%. In other words, it is compatible with the macroscopic concept in continuum mechanics. On the other hand, if the number of particles is less than 50, the stress markedly decreases. If $n=1$, the stress cannot be defined because the second term on the right side of Eq. (11)

vanishes. Because the force acting between the particles is very small when $r^{ab} \geq 2$, we note that the particles marked by a to d in Fig. 1 have almost the same contributions to Eq. (13), which are almost independent of the size of the region for defining the stress. The number of these particles increases proportionally to the size of the region. When the region is large, the particles, labeled e, f and so on, which have almost the same contribution as particle d, appear inside the group containing particle d. The larger the size of the region is, the more particles e, f and so on there are. Consequently, the stress approaches a constant value with the increase of the size of the region for defining the stress. On the other hand, the number of particles at the corners of the region is small. Therefore, the contributions of these particles to Eq. (13) manifest when the size of the region is small. Figure 11 shows that the contribution is small.

Poisson's ratio is shown in Fig. 12. The abscissa is selected in the same manner as for Fig. 9. It is found that Poisson's ratio does not change with the size of the region for defining the stress. In continuum mechanics also, it does not change with the size of the region.

Fig. 10 Effect of number of particles on stress strain curve

Fig. 12 Poisson's ratio

Fig. 11 Effect of number of particles on stress

Fig. 13 Effect of location of region for defining stress and strain on stress strain curve

Now, we discuss the location of the region for defining the stress. If the size of the region is 12×12 , five locations can be selected in the x direction. The stress-strain curves for these five locations are shown in Fig. 13. There is no difference in the stress-strain curves. We obtained similar results for the region of 8×8 . It is evident that the stress-strain curve is independent of the location of the region.

4. Conclusion

The main conclusions obtained are summarized as follows.

(1) To obtain meaningful stress and strain values from the MD simulation, it is necessary to set the time step at about 0.01 and to average the stress and strain with respect to time over more than 20 periods of thermal vibration. Then, the stress is calculated using the forces acting between the particles which are in the region for defining the stress.

(2) The stress-strain curves obtained from the MD simulation have good reproducibility.

(3) Deformation can be calculated from the statistical average of the distance between the neighboring particles, and the field of motion of particles is extended in the direction in which the distance between the neighboring particles is large. The deviation of the distance between neighboring particles is larger at the surface than inside the thin film.

(4) As the size of the region for defining the stress decreases, the stress decreases and the compliance increases. This differs from the concept of stress defined in continuum mechanics. The size of the region for defining the strain has no effect on the strain.

(5) An agglomerate of more than 130 particles is necessary to obtain stress which is compatible with the macroscopic concept in continuum mechanics.

(6) The stress and strain are independent of the location of the region for defining them.

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