Molecular Dynamics Study of Stress Effects on Raman Frequencies of Crystalline Silicon*

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The effects of stress on the Raman frequencies of crystalline silicon are studied using molecular dynamics simulation both for uniaxial stress along the [100] direction and for biaxial stress which is isotropic in the (001) plane. The Tersoff potential is used to represent the interaction among the silicon atoms. Simulation results showed that the tensile stress causes the Raman frequencies to decrease. The conversion coefficients that are needed for converting the shifts of the Raman frequencies into the stress were obtained by comparing the simulation results with the dynamical equations for optical modes. The values obtained for the coefficients agreed well with the experimental values obtained by other works. The obtained relationship between the uniaxial stress and the Raman frequency for vibration in the [001] direction also agreed well with the experimental result we obtained using microscopic Raman spectroscopy.

Key Words: Molecular Dynamics, Computational Mechanics, Stress Analysis, Raman Spectrum, Raman Frequency, Optical Phonon

1. Introduction

As very-large-scale-integration (VLSI) devices have come to have fine and complicated structures with various thin films, high local stresses in these films have become a serious problem which leads to the deterioration in the reliability of the devices. Following this trend, it has become more important to measure and control these local stresses.

Micro-Raman spectroscopy has high spatial resolution with small penetration depth, so it is considered more powerful for measuring local stresses in VLSI devices^{(1),(2)} than other stress-measurement techniques such as X-ray diffraction and strain-gauge methods. Using micro-Raman spectroscopy, we can calculate stress in the following way. When stress is not present in a crystal, the crystal lattice vibrates with eigen frequencies corresponding to the spring constant. Eigen frequencies for the optical phonons with the

wave number of zero are called Raman frequencies. When stress is present, the Raman frequencies are shifted because the stress causes changes in the spring constant. Since these shifts of Raman frequencies have linear relationships with the stress, we can convert the shifts into the stress by using conversion coefficients that describe the changes in the spring constant. Therefore, precise values of the conversion coefficients are needed in order to calculate the stress precisely.

Although experimental values of the conversion coefficients for crystalline silicon have been published in a number of papers⁽³⁾⁻⁽⁵⁾, each paper uses its own different values, which lead to different values of stress. In this paper, by using molecular dynamics simulation, we study the effect of stress on the Raman frequencies of crystalline silicon, and we obtain the conversion coefficients both for uniaxial stress along the [100] direction and for biaxial stress which is isotropic in the (001) plane.

2. Analysis Method

2.1 Computation cell

The computation cell used is single crystalline silicon, which is a diamond-structure lattice as shown

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Fig. 1 Computational cell and coordinate system

in Fig. 1. This cell contains 216 atoms and the coordinate system is also shown in this figure, where the positive x , y , and z directions are in the $[100]$, $[010]$, and $[001]$ directions, respectively. Periodic boundary conditions are applied in all these directions.

2.2 Molecular dynamics simulation

We used the Tersoff potential to characterize interatomic interaction among silicon atoms because this potential accurately reproduces elastic properties of silicon⁽⁶⁾. Atom positions and velocities were calculated by numerically solving Newton's equations of motion using the Verlet algorithm⁽⁷⁾. The basic time step increment was set at $h=1 \times 10^{-15}$ s. And the temperature was set at 600K by using a velocity scaling method⁽⁸⁾. We investigated the effect of stress on the Raman frequencies, which are the peak frequencies of the Raman spectrum, in the following way. The stress was calculated by differentiating potential energy with respect to the strain⁽⁹⁾. Raman frequencies were then calculated from the phonon density of states. According to Wiener-Khintin's theorem⁽¹⁰⁾, the phonon density of states $Z_x(\omega)$ for the x direction is given by the following equation.

$$Z_x(\omega) = \left| \frac{1}{2\pi} \int f_x(t) \cos \omega t dt \right| \quad (1)$$

The same type of equation is given for the y and z directions. The summation for the integration in Eq. (1) runs over 6 000 time steps. The velocity autocorrelation function $f_x(t)$ in Eq. (1) is defined as

$$f_x(t) = \frac{2}{N} \sum_{i,j} [v_{xi}(t) - v_{xj}(t)][v_{xi}(0) - v_{xj}(0)] \quad (2)$$

Here, $v_{xi}(t)$ is the x component of the velocity of atom i at time t and N is the number of atoms. The summation in Eq. (2) runs over all the pairs of atoms i and j whose binding vectors are $(a/4, a/4, a/4)$, where a is the lattice constant.

Using the phonon density of states $Z_x(\omega)$ as the distribution function, Raman frequencies Ω_x for the x direction are given by

$$\Omega_x = \int \omega Z_x(\omega) d\omega / \int Z_x(\omega) d\omega \quad (3)$$

The same type of equation is given for the y and z directions. We applied the strain to the computation

cell and calculated the stress and the Raman frequencies in order to obtain the relationship between them. Using the obtained relationship, we can calculate the conversion coefficients which are needed for converting the shifts of Raman frequencies into stress. Details of the conversion coefficients are explained in the next section.

2.3 Conversion coefficients

Based on the lattice dynamical theory with the wave number of zero for silicon, the relationship between the stress and the Raman frequency for the x and z directions are given by Anastassakis et al.⁽³⁾ These relationships contain the definition of the conversion coefficients, which we want to calculate here. Because the derivation of the relationship is described in the original paper⁽³⁾, we show only the results here.

The relationship between the stress and the Raman frequencies for uniaxial stress along the $[100]$ direction is given by the following equations⁽³⁾.

$$\Omega_x - \omega_0 = \frac{1}{2\omega_0} (pS_{11} + 2qS_{12}) \sigma_x \quad (4)$$

and

$$\Omega_z - \omega_0 = \frac{1}{2\omega_0} [pS_{12} + q(S_{11} + S_{12})] \sigma_x \quad (5)$$

Here, ω_0 is the Raman frequency in the absence of stress, and Ω_x and Ω_z are the Raman frequencies in the presence of stress for the x and z directions, respectively. We can write $\Omega_y = \Omega_z$ because of the symmetry. Among publications, there is little discrepancy in values of ω_0 and the commonly used value is $\omega_0 = 520 \text{ cm}^{-1}$ ⁽³⁾⁻⁽⁵⁾. Here, cm^{-1} is usually used as the unit of frequency in the field of Raman spectroscopy. And S_{11} and S_{12} in Eqs. (4) and (5) are the 1,1 and 1,2 components of the elastic compliance constants, respectively. Using Young's modulus E and Poisson's ratio ν for uniaxial stress along the $[100]$ direction, we can write $S_{11} = 1/E$ and $S_{12} = -\nu/E$. Similarly, there is little discrepancy in the values of these elastic compliance constants used in publications, and the commonly used values are $S_{11} = 76.8 \times 10^{-13} \text{ m}^2/\text{N}$ and $S_{12} = -21.4 \times 10^{-13} \text{ m}^2/\text{N}$ ⁽³⁾⁻⁽⁵⁾. Coefficients p and q in Eqs. (4) and (5) represent the changes in the spring constant due to strain in the $[100]$ direction. Coefficient p describes the change for the $[100]$ direction, while q describes that for the $[001]$ direction. We call these coefficients the conversion coefficients because if we obtain the precise values of the coefficients, we can convert the Raman frequencies into the stress by using Eqs. (4) and (5). Although experimental values of the conversion coefficients for crystalline silicon have been published in a number of papers⁽³⁾⁻⁽⁵⁾, each paper uses its own different values, which lead to different values for the stress. In this paper we obtain the relationship between the stress

and the Raman frequencies by using the molecular dynamics method described in Section 2.2. And calculate the conversion coefficients p and q by comparing this relationship with Eqs. (4) and (5).

For the biaxial stress which is isotropic in the (001) plane, the relationship between the stress and the Raman frequencies is given by the following equations^{(3),(11)}.

$$\Omega_x - \omega_0 = \frac{1}{2\omega_0} [p(S_{11} + S_{12}) + q(S_{11} + 3S_{12})] \sigma_x \quad (6)$$

and

$$\Omega_z - \omega_0 = \frac{1}{\omega_0} [pS_{12} + q(S_{11} + S_{12})] \sigma_x \quad (7)$$

We can write $\Omega_y = \Omega_x$ because of the symmetry. The conversion coefficients p and q and the other coefficients ω_0 , S_{11} , and S_{12} are the same as those in Eqs. (4) and (5). Furthermore, equations that have the same coefficients are obtained for biaxial stress which is described by the principal axes in the [100] and [010] directions. We can thus use the same conversion coefficients in these cases. We here focus on uniaxial stress along the [100] direction and biaxial stress which is isotropic in the (001) plane.

3. Results and Discussions

3.1 Analysis results for uniaxial stress along the [100] direction

First, we calculate the elastic compliance constants S_{11} and S_{12} by using the simulation results for Young's modulus E and Poisson's ratio ν for uniaxial stress along the [100] direction; that is, the x direction. In our simulations, strain components ε_x , ε_y , and ε_z are input parameters, and stress components σ_x , σ_y , and σ_z are obtained as simulation results. Therefore, to apply uniaxial stress with the given value of ε_x , we need to obtain input values of ε_y and ε_z that make the stress components σ_y and σ_z zero. When the tensile strain $\varepsilon_x = 0.01$ is applied in the [100] direction, the values of the stress component $\sigma_z (= \sigma_y)$ for five input values (i.e., -0.0031 , 0.0030 , 0.0029 , 0.0028 , and 0.0027) of the strain component $\varepsilon_z (= \varepsilon_y)$ are obtained as shown in Fig. 2. Here, a negative value of the strain means compressive strain. The stress component was calculated by differentiating potential energy with respect to the strain⁽⁹⁾. Since Fig. 2 shows that $\sigma_z (= \sigma_y)$ vanishes when $\varepsilon_z = \varepsilon_y = -0.0029$, the obtained value of Poisson's ratio ν equals 0.29, which agrees well with the known value of 0.279⁽³⁾. When the tensile strain $\varepsilon_x = 0.01$ is applied, the values of the stress component σ_x for five input values of the strain component $\varepsilon_z (= \varepsilon_y)$ are obtained as shown in Fig. 3. As Fig. 3 shows that $\sigma_x = 1290$ MPa when $\varepsilon_z = \varepsilon_y = -0.0029$, the obtained value of Young's modulus equals 129 GPa, which agrees well with the known value 130

Fig. 2 Relationship between strain ε_z and stress σ_z for $\varepsilon_x = 0.01$

Fig. 3 Relationship between strain ε_z and stress σ_x for $\varepsilon_x = 0.01$

Fig. 4 Velocity correlation function $f_x(t)$ in the absence of stress and strain

GPa⁽³⁾. From these values obtained from molecular dynamics simulation, the components of the elastic compliance constants are obtained as $S_{11} = (1/129) \times 10^{-9} \text{ m}^2/\text{N} = 77.5 \times 10^{-13} \text{ m}^2/\text{N}$ and $S_{12} = (0.29/129) \times 10^{-9} \text{ m}^2/\text{N} = 22.5 \times 10^{-13} \text{ m}^2/\text{N}$.

Although the value of the strain, 0.01, is considered to be quite large, no dislocations were observed in our simulations because the computation cell was a perfect crystal containing no defects.

Next, we describe the stress effects on the Raman frequencies. These effects were investigated by using the method in Section 2.2. Figure 4 shows the calculated time evolution of the velocity autocorrelation function $f_x(t)$ defined in Eq. (2) in the absence of the stress, while Fig. 5 shows the result for the uniaxial stress with $\varepsilon_x = 0.01$ ($\sigma_x = 1290$ MPa). Both of these figures show that the frequency of $f_x(t)$ is about $15 \times$

Fig. 5 Velocity correlation function $f_x(t)$ for uniaxial stress with $\varepsilon_x=0.01$

Fig. 6 Phonon density of states $Z_x(\omega)$ in the absence of stress and strain

10^{12} Hz, which nearly equals 500 cm^{-1} . Therefore, the Raman frequencies are roughly estimated as 500 cm^{-1} . More precise values are calculated by using Eq. (3), which contains the phonon density of states defined in Eq. (1). From the results of $f_x(t)$ shown in Figs. 4 and 5, we calculated the density of states $Z_x(\omega)$, $Z_y(\omega)$, and $Z_z(\omega)$ by using Eq. (1). Figure 6 shows the obtained results for $Z_x(\omega)$ ($=Z_y(\omega)=Z_z(\omega)$) in the absence of stress. Figures 7 and 8 show the density of states $Z_x(\omega)$ and $Z_z(\omega)$ ($=Z_y(\omega)$), respectively, for the uniaxial tensile stress with $\varepsilon_x=0.01$ ($\sigma_x=1290 \text{ MPa}$). As shown in Figs. 6, 7, and 8, the peak frequency at which the density of states reaches the maximum value decreases due to the uniaxial tensile stress. By using Eq. (3) with the results for the density of states (Figs. 6–8), the Raman frequencies were obtained as $\omega_0=494.2 \text{ cm}^{-1}$, in the absence of the stress, and $\Omega_x=493.2 \text{ cm}^{-1}$ and $\Omega_z=491.7 \text{ cm}^{-1}$ for the uniaxial stress with $\varepsilon_x=0.01$ ($\sigma_x=1290 \text{ MPa}$). These values are shown in Figs. 6, 7, and 8 and show that the Raman frequencies also decrease due to the uniaxial tensile stress.

In addition to $\varepsilon_x=0.01$, we used the following three input values of strain ε_x : 0.005, 0.0025, and 0.0005. The obtained relationships between the stress σ_x and the Raman frequencies for Ω_x and Ω_z are shown in Fig. 9. These relationships are written as the following equations.

$$\Omega_x - \omega_0 = -7.75 \times 10^{-4} \sigma_x \quad (8)$$

Fig. 7 Phonon density of states $Z_x(\omega)$ for uniaxial stress with $\varepsilon_x=0.01$

Fig. 8 Phonon density of states $Z_z(\omega)$ for uniaxial stress with $\varepsilon_x=0.01$

Fig. 9 Relationships between stress and Raman frequencies for uniaxial stress along [100]

and

$$\Omega_z - \omega_0 = -19.4 \times 10^{-4} \sigma_x \quad (9)$$

Here, the unit of σ_x is MPa, while the unit of ω_0 , Ω_x , and Ω_z is cm^{-1} . Due to the symmetry, Ω_y equals Ω_z . Using microscopic Raman spectroscopy, we obtained the following experimental result for Ω_z .

$$\Omega_z - \omega_0 \approx -21 \times 10^{-4} \sigma_x \quad (10)$$

Equation (9) agrees well with Eq. (10). And by comparing Eqs. (8) and (9) with Eqs. (4) and (5), the conversion coefficients p and q are obtained as $p = -1.40 \times 10^{28} \text{ s}^{-2}$ and $q = -1.81 \times 10^{28} \text{ s}^{-2}$. These coefficients are obtained by the use of the following values already mentioned: $\omega_0=494.2 \text{ cm}^{-1}$, $S_{11}=77.5 \times 10^{-13} \text{ m}^2/\text{N}$, and $S_{12}=-22.5 \times 10^{-13} \text{ m}^2/\text{N}$. We will compare these results with published values at the end

of Section 3.3.

When the temperature is 150 K, the conversion coefficients were obtained as $p = -1.41 \times 10^{28} \text{ s}^{-2}$ and $q = -1.82 \times 10^{28} \text{ s}^{-2}$. Therefore, the coefficients are considered almost independent of the temperature.

3.2 Analysis results for biaxial stress isotropic in the (001) plane

By using the same kind of method as in section 3.1, to apply biaxial stress with the given values of ϵ_x and ϵ_y , we controlled the input value of ϵ_z so that the stress component σ_z is zero. Figures 10 and 11 shows the density of states $Z_x(\omega)$ ($=Z_y(\omega)$) and $Z_z(\omega)$ for the biaxial stress with $\epsilon_x = \epsilon_y = 0.01$ ($\sigma_x = \sigma_y = 1818 \text{ MPa}$). The values of the Raman frequencies $\Omega_x = 489.3 \text{ cm}^{-1}$ and $\Omega_z = 487.2 \text{ cm}^{-1}$, which are obtained from Eq. (3) by using the results for the density of states (Figs. 10 and 11), are shown in these figures. Comparing these figures with Fig. 6, we find that both the peak frequencies and the Raman frequencies decrease due to the biaxial tensile stress. In addition to $\epsilon_x = \epsilon_y = 0.01$ we used the following three input values: 0.005, 0.0025, and 0.0005. The obtained relationships between the stress σ_x and the Raman frequencies for the biaxial stress are shown in Fig. 12. These relationships are written as the following equations.

$$\Omega_x - \omega_0 = -27.0 \times 10^{-4} \sigma_x \quad (11)$$

and

$$\Omega_z - \omega_0 = -38.5 \times 10^{-4} \sigma_x \quad (12)$$

The coefficient -38.5×10^{-4} in Eq. (12) is about double

the coefficient -19.4×10^{-4} in Eq. (9). This result agrees well with the fact that the right side in Eq. (7) is exactly double the right side in Eq. (5). By comparing Eqs. (11) and (12) with Eqs. (6) and (7), the conversion coefficients p and q are obtained as $p = -1.40 \times 10^{28} \text{ s}^{-2}$ and $q = -1.80 \times 10^{28} \text{ s}^{-2}$. These coefficients are obtained by the use of the same values as before: $\omega_0 = 494.2 \text{ cm}^{-1}$, $S_{11} = 77.5 \times 10^{-13} \text{ m}^2/\text{N}$, and $S_{12} = -22.5 \times 10^{-13} \text{ m}^2/\text{N}$. These values of the conversion coefficients for the biaxial stress agree well with those for the uniaxial stress described in Section 3.1. Both these results for the uniaxial and biaxial stress are listed in Table 1 along with the values of p and q published in Refs. (3), (4), and (5). Table 1 shows that the results of this work agree well with the experimental values ($p = -1.43 \times 10^{28} \text{ s}^{-2}$ and $q = -1.89 \times 10^{28} \text{ s}^{-2}$) obtained by Chandrasekhar et al.⁽⁴⁾

3.3 Published experimental results

Here, we focus on the case for the uniaxial stress along the [100] direction. To investigate which published experimental result agrees best with the results of this paper, we compare Eqs. (8), (9), and (10) with Eqs. (4) and (5) in which published values of p and q are used. First, using the values in Ref. 4 (i.e. $p = -1.43 \times 10^{28} \text{ s}^{-2}$ and $q = -1.89 \times 10^{28} \text{ s}^{-2}$), Eqs. (4) and (5) are written as

$$\Omega_x - \omega_0 = -7.34 \times 10^{-4} \sigma_x \quad (13)$$

and

$$\Omega_z - \omega_0 = -20.4 \times 10^{-4} \sigma_x \quad (14)$$

Fig. 10 Phonon density of states $Z_x(\omega)$ for biaxial stress with $\epsilon_x = \epsilon_y = 0.01$

Fig. 11 Phonon density of states $Z_z(\omega)$ for biaxial stress with $\epsilon_x = \epsilon_y = 0.01$

Table 1 Values of coefficients p and q

	$p (10^{28} \text{ s}^{-2})$	$q (10^{28} \text{ s}^{-2})$
This work, uniaxial stress	-1.40	-1.81
This work, biaxial stress	-1.40	-1.80
Reference 3	-1.2	-1.8
Reference 4	-1.43	-1.89
Reference 5	-1.683	-2.630

Fig. 12 Relationships between stress and Raman frequencies for biaxial stress which is isotropic in the (001) plane

These equations agree well with Eqs.(8) and (9). Furthermore, Eq.(14) agrees well with Eq.(10), which was derived from our experimental results using microscopic Raman spectroscopy. On the other hand, by using the values in Ref. 3 (i.e. $p = -1.2 \times 10^{28} \text{ s}^{-2}$ and $q = -1.8 \times 10^{28} \text{ s}^{-2}$), Eqs.(4) and (5) are written as

$$\Omega_x - \omega_0 = -3.42 \times 10^{-4} \sigma_x \quad (15)$$

and

$$\Omega_z - \omega_0 = -20.5 \times 10^{-4} \sigma_x \quad (16)$$

The coefficient -3.42×10^{-4} in Eq.(15) is smaller than a half of the coefficient -7.75×10^{-4} in Eq.(8) although Eq.(16) agrees well with Eqs.(9) and (10). Using the values in Ref. 5 (i.e. $p = -1.683 \times 10^{28} \text{ s}^{-2}$ and $q = -2.630 \times 10^{28} \text{ s}^{-2}$), Eqs.(4) and (5) are written as

$$\Omega_x - \omega_0 = -3.44 \times 10^{-4} \sigma_x \quad (17)$$

and

$$\Omega_z - \omega_0 = -30.4 \times 10^{-4} \sigma_x \quad (18)$$

Both Eqs.(17) and (18) are very different from Eqs.(8) and (9). Thus, the result in Ref.(4) agrees best with our result for uniaxial stress along the [100] direction. In the same way, it is found that the result in Ref.(4) also agrees best with our result for biaxial stress isotropic in the (001) plane.

4. Analysis Using a Method Neglecting Thermal Vibration

Molecular dynamics simulation contains the effect of thermal vibration. In this section, using the Tersoff potential⁽⁶⁾ and a method neglecting thermal vibration, we calculate the Raman frequency ω_0 in the absence of stress and the conversion coefficients p and q .

In the computation cell shown in Fig. 1, we apply a very small relative displacement for the optical phonon with the wave number of zero to each pair of atoms i and j whose binding vectors are $(a/4, a/4, a/4)$, where a is the lattice constant. The spring constant that is related with the Raman frequency ω_0 is calculated by dividing the force needed for applying this displacement by the value of this displacement. Using the value of this spring constant, the Raman frequency is obtained as $\omega_0 = 534.56 \text{ cm}^{-1}$. This value agrees well with the known value 520 cm^{-1} ⁽³⁾⁻⁽⁵⁾ and our result 494.2 cm^{-1} from molecular dynamics simulation. By applying the uniaxial strain in the [100] direction, the spring constants in the [100] and [001] direction are changed into values different from the spring constant in the absence of strain. The conversion coefficients p and q are obtained as $p = -3.2 \times 10^{28} \text{ s}^{-2}$ and $q = -2.4 \times 10^{28} \text{ s}^{-2}$ by using the changes in the spring constant in the [100] and [001] directions. The results are almost independent of the strain (Fig. 13). The values of the conversion coefficients, shown in Fig. 13, are of the same order as those obtained with

Fig. 13 Relationships between strain ϵ_x and coefficients p and q neglecting thermal vibration

molecular dynamics simulation (i.e., $p = -1.4 \times 10^{28} \text{ s}^{-2}$ and $q = -1.8 \times 10^{28} \text{ s}^{-2}$). Therefore, we can roughly estimate p and q by using the method that neglects thermal vibration. However, thermal vibration must be taken into account in order to calculate p and q more precisely. As shown in Sections 3.1 and 3.2, molecular dynamics simulation, which contains the effect of thermal vibration, is useful for precisely calculating p and q .

5. Summary

The effect of stress on the Raman frequencies of crystalline silicon are studied by using molecular dynamics simulation, both for uniaxial stress along the [100] direction and for biaxial stress which is isotropic in the (001) plane. We calculated the conversion coefficients which are needed for converting the shifts of Raman frequencies into stress. The results are as follows.

(1) The tensile stress causes the Raman frequencies to decrease. The values of the conversion coefficients p and q , which describe the changes in the spring constant due to strain in the [100] and [001] directions, respectively, are obtained as $p = -1.4 \times 10^{28} \text{ s}^{-2}$ and $q = -1.8 \times 10^{28} \text{ s}^{-2}$ both for the uniaxial and biaxial stress. These values agree well with the experimental values obtained by Chandrasekhar et al.⁽⁴⁾ (i.e., $p = -1.43 \times 10^{28} \text{ s}^{-2}$ and $q = -1.89 \times 10^{28} \text{ s}^{-2}$). The conversion coefficients can be roughly estimated using a method that neglects thermal vibration.

(2) The obtained relationship between the uniaxial stress and the Raman frequency for vibration in the [001] direction agrees well with the experimental result we obtained using microscopic Raman spectroscopy.

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