First-Principles Study on Shape Degradation during Oxidation Process for Three-Dimensional Structure Devices

Yuji Yajima[1], Kenji Shiraishi[2,3,7], Tetsuo Endoh[4,5,7], and Hiroyuki Kageshima[1,6,7]

[1]Interdisciplinary Graduate School of Science and Engineering, Shimane Univ., Matsue 690-8504, Japan, [2]Graduate School of Engineering, Nagoya Univ., Nagoya 464-8603, Japan, [3]IMaSS, Nagoya Univ., Nagoya 464-8603, Japan, [4]Graduate School of Engineering, Tohoku Univ., Sendai 980-8579, Japan, [5]CIES, Tohoku Univ., Sendai 980-0845, Japan, [6]Graduate School of Natural Science and Technology, Shimane Univ., Matsue 690-8504, Japan, [7]JST-ACCEL, Sendai, 980-0845, Japan

E-mail: s179630@matsu.shimane-u.ac.jp

Abstract

The shape degradation during oxidation process for three-dimensional structure devices is investigated. For this purpose, the effect of emitted Si in the oxide is studied based on the first-principles molecular dynamics. It is found that the Si diffusion is enhanced as the pressure increases. Because large compressive stress is induced in the interfacial oxide for the oxidation of three-dimensional Si structure, this means that the Si diffusion is enhanced and causes the shape degradation. Based on the results, it is proposed that an oxidation process that induces smaller stress, such as wet or pyrogenic oxidation, is needed to prevent shape degradation.

1. Introduction

Recent technological progress in silicon (Si) integration devices demands researches on the fine control of three-dimensional (3D) device structures, such as the vertical body channel-metal oxide semiconductor field effect transistor (Vertical BC-MOSFET), which has a vertical Si pillar as the channel (Fig. 1) [1]. In fabricating this device, however, it is known that the shape of Si pillar is significantly degraded after the thermal oxidation process to form the gate insulator (Fig. 2) [2]. In our previous studies, we have revealed that the origin of this degradation is the Si emission from the interface into the oxide during the oxidation process [2-6].

In this contribution, we focus on the effect of large compressive stress accumulated in the interfacial oxide during oxidizing the Si pillar (Fig. 3). By extending our previous study [7], we theoretically study the effect of stress on the Si diffusion in oxide using the first-principles molecular dynamics.

2. Calculation method

We perform the first principles molecular dynamics calculation using the code, VASP [8]. We employ the density functional of local density approximation (LDA) and the pseudopotential method. The energy cut off for the plane-wave expansion is 400 eV (about 30 Ry), and the k-point is set to the Γ point. A supercell including 24 SiO_2 is adopted for the unit cell for the defect-free pristine case. Since the oxide with the emitted Si can be regarded as Si-rich SiO_x, we remove O atom from the pristine supercell and shrink the volume size to obtain system conditions with various pressures. Hereafter, the emitted Si in the oxide is also called as SiO according to our previous study comparing with the experimental results [7]. The details of the calculation method are similar to our previous study [7].

3. Results and discussion

First, we show the self-diffusion coefficient of silicon (D_{Si}) as the function of pressure (P) in Fig. 4. Here, N_{VO} is the number of removed oxygen atoms. Figure shows pressure dependence of D_{Si} by N_{VO}. Under every condition, D_{Si} is suppressed in high pressures. However, in low pressures, D_{Si} increases and has a local maximum only for N_{VO} ranged from 0 to 12. Increase of D_{Si} for $N_{VO} = 0$ is consistent with previous report [9]. Next, we fit the

calculated D_{Si} by the Lorentz type function as following:

$$D_{Si} = c \frac{b/\pi}{(P-a)^2 + b^2}. \qquad (1)$$

The fitting results are shown in Fig. 5. And we fit the obtained parameter a, b and $\log c$ by the parabolic functions of N_{VO} as following:

$$a = a_0 + a_1 N_{VO} + a_2 N_{VO}^2, \qquad (2)$$
$$b = b_0 + b_1 N_{VO} + b_2 N_{VO}^2, \qquad (3)$$
$$\log c = (\log c)_0 + (\log c)_1 N_{VO} + (\log c)_2 N_{VO}^2. \qquad (4)$$

The fitting results are shown in Fig. 6 and Table 1. To clarify SiO diffusion, we expand D_{Si} as

$$D_{Si} \sim \exp A_0 + (\exp A_0) A_1 V_{24SiO2} C_{SiO}$$
$$= D_{Si(th)}^{SD} + D_{SiO}^{SD}/C_{SiO}^0 C_{SiO}. \qquad (5)$$

Here, V_{24SiO2} is the volume of 24 SiO_2, C_{SiO} is the concentration of SiO, $D_{Si(th)}^{SD}$ is the thermal diffusion coefficient, D_{SiO}^{SD} is the SiO diffusion coefficient and C_{SiO}^0 is the solubility of SiO in the oxide. The final form of Eq. (5) is same as the equation proposed by Uematsu et al. [10]. Using Eqs. (1) and (5), we obtain A_0 and A_1 as the functions of P as following:

$$A_0 = (\log c)_0 + \log b_0 - \log \pi - \log((P-a)^2 + b_0^2), \qquad (6)$$
$$A_1 = (\log c)_1 + b_1/b_0$$
$$+ (2(P-a_0)a_1 - 2b_0 b_1)/((P-a_0)^2 + b_0^2). \qquad (7)$$

Then, using A_0 and A_1, $D_{Si(th)}^{SD}$ and D_{SiO}^{SD}/C_{SiO}^0 are expressed as

$$D_{Si(th)}^{SD} = \exp A_0, \qquad (8)$$
$$D_{SiO}^{SD}/C_{SiO}^0 = (\exp A_0) A_1 V_{24SiO2}. \qquad (9)$$

We show D_{SiO}^{SD}/C_{SiO}^0 as the function of pressure in Fig. 7. This figure shows that the effect of SiO on the Si diffusion in oxide is enhanced by the pressure. We also confirm that $D_{Si(th)}^{SD}$ is also enhanced by the pressure. This means that the Si diffusion in oxide is strongly accelerated by the pressure.

Since SiO is the emitted Si, these results indicate that the emitted Si for the pillar oxidation enhances the Si diffusion in oxide more than for the planar oxidation because of the higher compressive stress accumulation. For the pillar oxidation, it has been already revealed that the compressive stress enhances the rate of Si emission [5], and that the geometry enhances the diffusion of emitted Si in oxide [2]. Combining these results, we can conclude that the Si diffusion in oxide should be highly enhanced for the pillar oxidation.

4. Conclusions

We find that the effect of emitted Si on the Si diffusion in oxide is enhanced as the pressure increases. This means that the shape degradation is pronounced in the pillar oxidation. Some oxidation process that induces smaller strain, such as wet or pyrogenic oxidation, is needed to prevent the shape degradation.
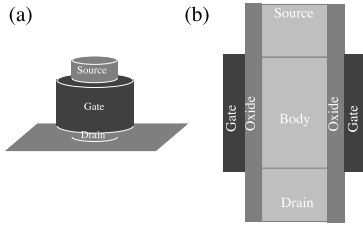
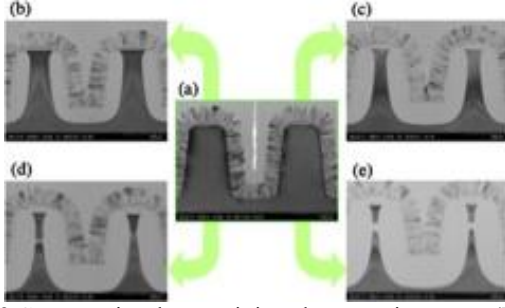Fig. 1 Schematics of the device structure of vertical BC-MOSFET. [6]

Fig. 2 Cross sectional transmitting electron microscopy (TEM) images of the thermal oxidation of Si pillar. [2]
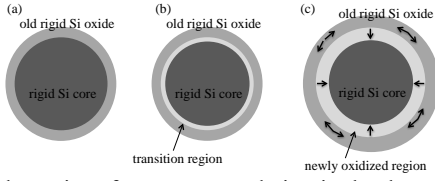

Fig. 3 Schematics of stress accumulation in the thermal oxidation of Si pillar. [6]
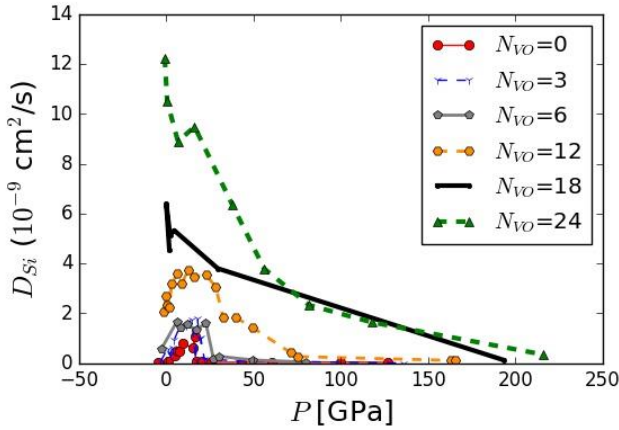

Fig. 4 D_{Si} as the function of pressure for various N_{VO}.

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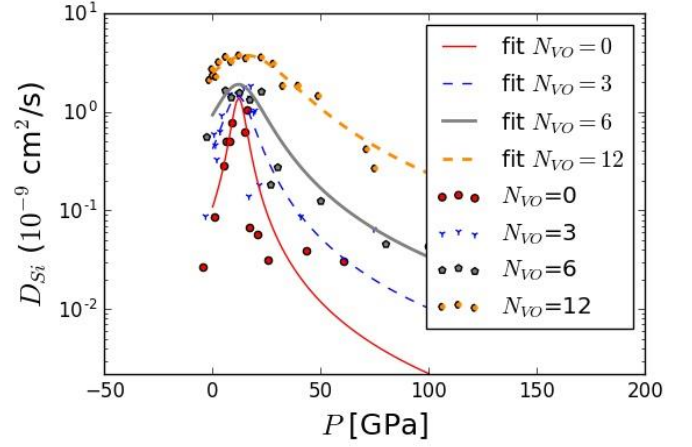[7] Y. Yajima et al, Jpn. J. Appl. Phys. **57**, 06KD01 (2018).
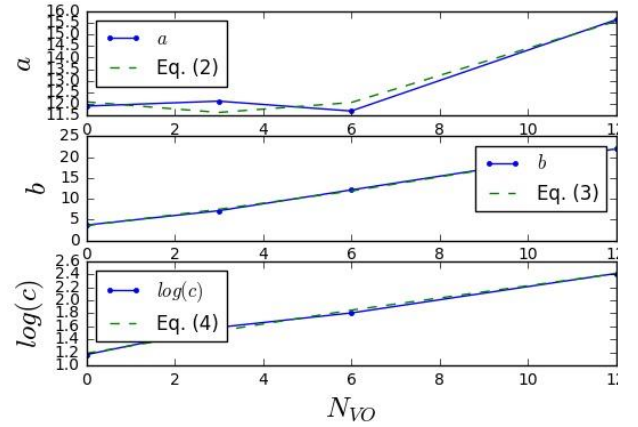

Fig. 5 D_{Si} and fitting results by Eq. (1).

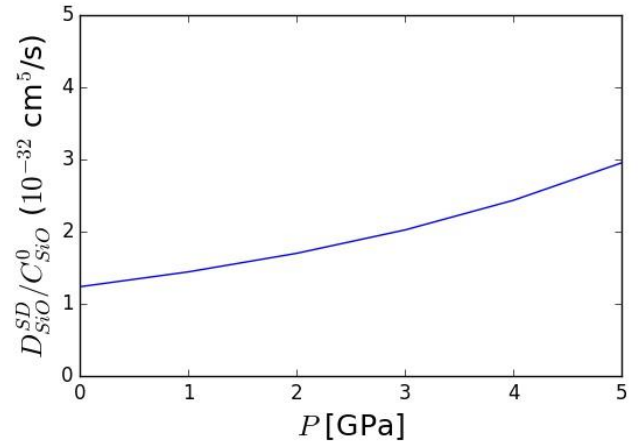Fig. 6 a, b, $\log c$, and fitting results by Eqs. (2), (3) and (4).

Fig. 7 D_{SiO}^{SD}/C_{SiO}^{0} as the function of pressure.

Table 1 Fitting results by Eqs. (2), (3) and (4).

a_0	12.088	b_0	3.5403	$(\log c)_0$	1.1835
a_1	−0.3004	b_1	1.2302	$(\log c)_1$	0.119
a_2	0.0492	b_2	0.00258	$(\log c)_2$	−0.0014

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