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First Principles Study of the effect of Hydrogen Annealing effects on SiC MOSFETs

Kenta Chokawa[1] and Kenji Shiraishi[1,2]

[1] Graduate School of Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8603, Japan

Phone: +81-52-789-2715 E-mail: chokawa@fluid.cse.nagoya-u.ac.jp

[2] Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya, Aichi 464-8603, Japan

Abstract

The interface of 4H-SiC MOSFETs has many defects and these introduce states that are a problem for high performance devices. In order to improve device performance, post oxidation annealing in H_2 gas has been performed. Although, this has been found to be very effective for improving the performance of Si MOSFETs, it does not improve the interface of 4H-SiC MOSFETs. In this study, we investigated the effect of H_2 annealing and the difference between this for Si MOSFETs and 4H-SiC MOSFETs. Si vacancies at the Si(111) interface can be terminated by H atoms at high annealing temperatures. In the case of the 4H-SiC(0001) interface, H atoms cannot terminate the defects at high temperature. Thus, H_2 annealing cannot improve the 4H-SiC MOSFETs whereas it can improve Si MOSFETs. On the other hand, C vacancies can be terminated by N atoms by annealing in nitrogen, and these atoms remain even at high temperature. Therefore, the annealing of 4H-SiC MOSFETs should include nitrogen in order to improve device performance.

1. Introduction

The wide bandgap and high thermal conductivity of 4H-SiC makes it a promising material for the next generation of electronic power devices. It is expected that 4H-SiC metal-oxide-semiconductor field-effect–transistors (MOSFET) will be able to operate at high temperature and at high voltage with low energy consumption. In addition to these advantages, a SiO_2 dielectric film can be formed in SiC by thermal oxidation at high temperature, so 4H-SiC MOSFETs can be constructed using the SiC/SiO_2 interface. However, the 4H-SiC/SiO_2 interface formed by thermal oxidation has many defects resulting in poor device performance and reliability. Of the many defect structures, Si (V_{Si}) and C (V_C) vacancies have been studied as the origin of this oiir performance, and there have been some attempts to improve the characteristics at the interface by post oxidation annealing (POA). POA has also been used for Si MOSFETs, and H_2 annealing reduced the number of defect states introduced at the Si/SiO interface by thermal oxidation [1]. This is also effective for 4H-SiC MOSFETs, but not all the defect states are removed [2]. To further improve 4H-SiC MOSFETs, it is expected that POA will play an important role, so we need to understand the effect of H_2 annealing on 4H-SiC MOSFETs. In this study, we examined termination of the vacancies by H_2 gas using first principles calculations based on the density functional theory.

2. Method and Models

All calculations were performed using VASP code [3]. We assumed a (0001)/SiO_2 interface for the 4H-SiC MOSFETs and prepared a 4H-SiC (0001) 3×3 surface slab model (Fig. 1(a)). We also prepared a Si (111) 3×3 surface slab model to compare the results. These models have 16 atomic layers with 144 atoms, and the atoms in the topmost and bottommost layer are terminated by H atoms.

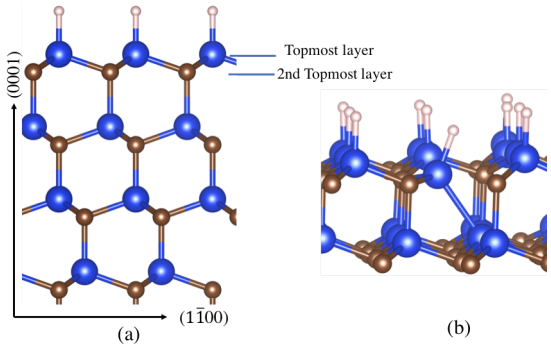


Fig. 1. The calculation model of 4H-SiC (0001) interface. (a) A side view of the 4H-SiC model and (b) the C vacancy model. The large blue, small brown and small white spheres represent the Si atoms, C atoms and H atoms, respectively.

To introduce a V_C at the 4H-SiC(0001) interface, we remove one C atom from the 2nd topmost layer, and the resulting structure has one Si-Si dimer and two Si dangling bonds (Fig. 1(b)). The V_{Si} at the Si(111) interface is constructed in the same way and resulting structure also has a Si-Si dimer structure and two Si dangling bonds.

We terminated the dangling bonds of each model by H atoms to simulate the H_2 annealing, and, in order to assess the stability of the termination, we calculated the adsorption energy (E_{ad}) using the following equations,

$$E_{ad} = E_{term} - [E_{vac} + nE_H(T,P)], \quad (1)$$

$$E_H(T,P) = E_H + \mu_H(T,P), \quad (2)$$

where E_{term} and E_{vac} are the total energies of the H atom terminated and vacancy models, respectively, n is the number of H atoms, and E_H and $\mu_H(T,P)$ are the total energy and chemical potential of the H atoms, respectively. E_H is set to half the total energy of the H_2 molecule. We used a statistical-mechanical approach to calculate the temperature and partial pressure dependence of the chemical potential as follows [6],

$$\mu_{\mathrm{H}}(T,P) = -k_{\mathrm{B}}T \ln\left(\frac{gk_{\mathrm{B}}T}{p} \times \zeta_{\mathrm{trans}}\zeta_{\mathrm{rot}}\zeta_{\mathrm{vibr}}\right), \quad (3)$$

$$\zeta_{\mathrm{trans}} = (2\pi m k_{\mathrm{B}}T/h^2)^{3/2}, \quad (4)$$

$$\zeta_{\mathrm{rot}} = 1/(\pi\sigma)\{8\pi^3(I_{\mathrm{A}}I_{\mathrm{B}}I_{\mathrm{C}})^{1/n}k_{\mathrm{B}}T/h^2\}^{n/2}, \quad (5)$$

$$\zeta_{\mathrm{vibr}} = \prod_{i=1}^{3N-3-n}\{1-\exp(-h\nu_i/k_{\mathrm{B}}T)\}^{-1}, \quad (6)$$

where ζ_{trans}, ζ_{rot} and ζ_{vibr} are the partition functions for the translational, rotational and vibrational motions, respectively. Here, k_{B} is Boltzmann's constant, T is the temperature, g is the degree of degeneracy of the electron energy level, p is the partial pressure of the particles, m is the mass of each particle, h is Planck's constant, σ is the symmetric factor, I is the moment of inertia, n is the degree of freedom of the rotation, N is the number of atoms in the particle, and ν is the frequency.

3. Results

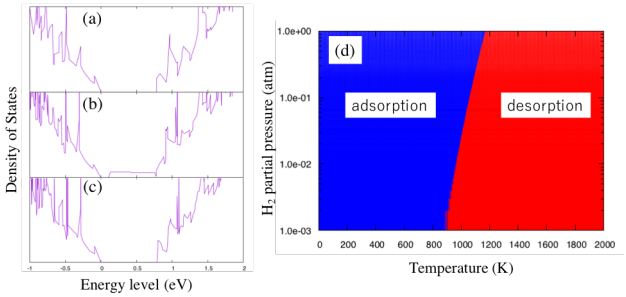


Fig. 2. The density of states of (a) Si(111) interface model, (b) Si vacancy model and (c) H terminated model. The valence band maximum is set to 0.0eV. (d) H atom adsorption conditions for Si vacancies at the Si(111) interface.

First, we inserted two H atoms for a V_{Si} at the Si(111) interface so that the resulting structure had no dangling bonds. The termination is written as follows,

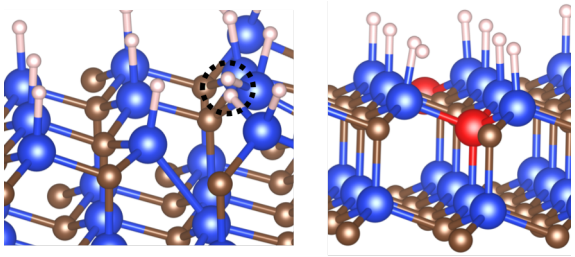
$$\mathrm{Si(Si\ vacancy)} + \mathrm{H_2} \rightarrow \mathrm{Si(H\ termination)}. \quad (7)$$

The Si dangling bonds have states in the bandgap, but these disappear when terminated with H atoms (Fig. 2(a)-(c)). Then, we calculated the adsorption energy for H termination and determined the conditions for which the dangling bonds can or cannot be terminated (Fig. 2(d)). As a result, H termination is possible at 1000K with P=0.1atm, which are typical experimental conditions. However, these termination conditions are different from those given in a previous report in which silicon vacancies at the $Si(100)/SiO_2$ interface were studied [5]. In our model, the interface is terminated by H atoms only, so stress relaxation by structural optimization is easier, resulting in a larger energy gain than in the previous work, which is considered to be the reason for the difference.

Secondly, we terminated the V_C at the 4H-SiC(0001) interface by H atoms as follows,

$$\mathrm{SiC(C\ vacancy)} + \mathrm{H_2} \rightarrow \mathrm{SiC(H\ termination)}. \quad (8)$$

The resultant structure keeps the Si-Si dimer structure and forms two Si-H bonds (Fig. 3(a)). As a result, defect states due to the Si dangling bonds disappear after H termination (Fig. 4(a)-(c)). Then, we calculated the adsorption energy and this shows that H_2 annealing is effective at room temperature (Fig. 4(e)). However, by considering the experimental conditions, which are above 1400K, H_2 annealing cannot remove the defect states. This is the reason why H_2 annealing cannot improve the interfacial states of 4H-SiC MOSFETs.



(a) (b)

Fig. 3. (a) The H termination model and (b) the N termination model of C vacancies at the 4H-SiC(0001) interface. The large blue, small brown, large red and small white spheres represent the Si, C, N and H atoms, respectively. The circled H atoms are those adsorbed H atoms by annealing.

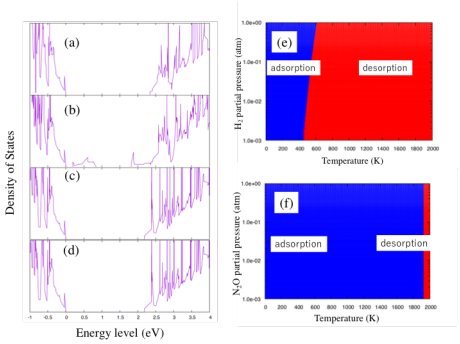


Fig. 4. The density of states of (a) 4H-SiC(0001) interface model, (b) C vacancy model, (c) H terminated model and (d) N termination model. The valence band maximum is set to 0.0eV. (e) H atom adsorption condition and (f) N atom adsorption condition for C vacancy at 4H-SiC(0001) interface.

In the above calculation, we clarified that H_2 annealing cannot terminate the V_C at the 4H-SiC(0001) interface. There are some reports that indicate that the interfacial characteristics can be improved by annealing with N atoms (NO, N_2O). Therefore, we investigated the possibility of termination by N atoms. We inserted N atoms and performed structural optimization; consequently, the Si-Si dimer is broken and a Si_4-N structure is formed at the interface (Fig. 3(b)), which is the same structure obtained by substituting C atoms by N atoms in SiC. Thus, the Si dangling bonds and their defect states disappear from the bandgap (Fig. 4(d)). Then, we calculated the adsorption energy assuming annealing by N_2O molecules as follows,

$$\mathrm{SiC(C\ vacancy)} + \mathrm{N_2O} \rightarrow \mathrm{SiC(N\ termination)} + \mathrm{NO}. \quad (9)$$

We set the partial pressures of the N_2O molecules and the NO molecules to be the same. The adsorption energy shows that annealing using N_2O is effective for C vacancies even at high temperatures above 1400K (Fig.4(b)). Therefore, annealing with N atoms is important for improving the interfacial characteristics of 4H-SiC MOSFETs.

4. Conclusion

We studied the termination of vacancies at Si(111) and 4H-SiC(0001) interfaces. We clarified that H_2 annealing is effective for Si MOSFETs, but cannot terminate C vacancies at the 4H-SiC MOSFET interface. This is the reason why H_2 annealing is insufficient for 4H-SiC. H atoms can terminate Si dangling bonds at room temperature, but are desorbed at high temperatures above 500K. However, when C vacancies at the 4H-SiC(0001) interface are terminated by N atoms, they are not desorbed even at high temperature and can therefore remove the defect states from the bandgap. Therefore, H_2 annealing is not realistic for 4H-SiC MOSFETs, but annealing with N atoms should be performed in order to improve the interfacial characteristics.

References

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