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NO Annealing Simulation of 4H-SiC/SiO_2 by Charge-Transfer Type Molecular Dynamics

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Abstract. We have developed a new interatomic potential of Si-O-C-N with newly added N for classical molecular dynamics simulation of NO annealing at 4H-SiC/SiO_2 interface. By adjusting the potential parameters to reproduce the material properties obtained from first-principles calculations for various kinds of structures, the accuracy of the potential has improved well enough to reproduce the formation of Si_3N termination at the 4H-SiC/SiO_2 interface during NO annealing. We have also observed that the defects with C=C double bonds have been modified into C-N bonds, which is supposed to be the decomposition process of residual C atoms in the NO annealing of 4H-SiC/SiO_2.

Introduction

Silicon carbide (SiC) has attracted great attention because of its potentially superior properties to Si in terms of high-voltage and high-temperature power device application [1]. The performance of 4H-SiC metal oxide semiconductor field-effect transistors (MOSFETs), however, has been limited by the low channel mobility and the threshold voltage instability, which is primarily caused by large amount of interface traps (D_{it}) and/or near interface traps (NITs) [2]. Interface nitridation by nitric oxide (NO) annealing has been widely used to reduce the D_{it} and NITs, while its microscopic mechanism is still under discussion.

Classical molecular dynamics (MD) simulation is one of the effective ways to analyze the mechanism of defect passivation by NO annealing on the atomic scale. However, there was no interatomic potential which could reproduce the atomic structure of 4H-SiC/SiO_2 interface. Recently, thermal oxidation process at the 4H-SiC/SiO_2 interface has been demonstrated in classical MD simulations with a charge-transfer-type interatomic potential [3]. The precisely-fitted interatomic potential parameters have enabled us to reproduce the orientation-dependent reaction barriers and the formation of residual C defects with C=C double bonds, whose interactions with NO are crucially important for understanding the microscopic role of NO annealing. In this paper, we developed the interatomic potential of Si-O-C-N with newly added N in order to reproduce the kinetics of NO annealing at 4H-SiC/SiO_2 interface.

Methods

We utilized a hybrid charge-transfer-type interatomic potential based on the Tersoff potential. The function form of the potential is the same as described in Ref. [4]. In order to treat NO annealing at the 4H-SiC/SiO_2 interface, a potential consisting of Si, O, C, and N is needed. Since the potential consisting of Si, O, and C has been established in previous studies [3], we added N to the potential. For this purpose, we created structures for N-containing systems (N, N-Si, N-O, N-C, N-Si-O, N-Si-C, N-O-C) whose atomic situations, such as bond angle and coordination number, are expected to emerge and actually emerged during the simulation of 4H-SiC/SiO_2 interface. The target systems include crystals, molecules, interfaces, and surfaces; typical structures are shown in Fig.1. The

interatomic potential parameters were adjusted to reproduce the material properties such as cohesive energy, atomic force, and lattice constants, obtained from first principles calculations.

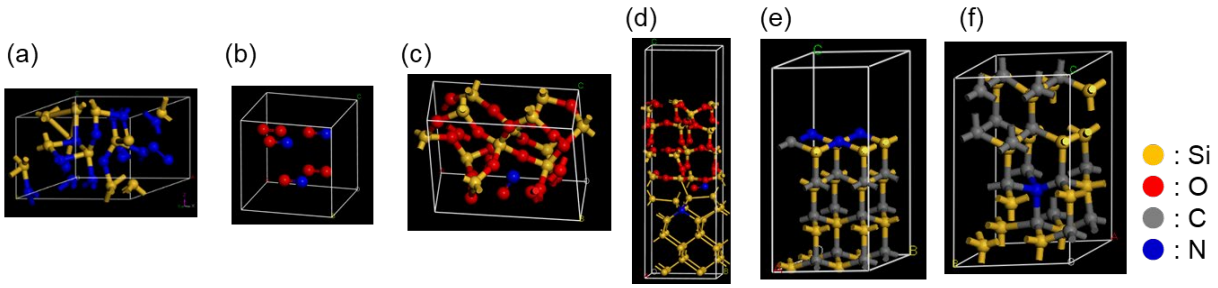

Fig. 1 Typical fitted structures that are expected to emerge on NO annealing process in SiC/SiO_2 interface: (a) Si_3N_4 crystal, (b) NO and O_2 molecules, (c) a NO molecule in SiO_2, (d) a NO molecule in Si/SiO_2 interface, (e) SiC surface terminated by N, and (f) SiC crystal with N substituted for C. Yellow, red, grey, and blue circles represent Si, O, C, and N atoms, respectively.

The first-principles calculations were carried out with the plane wave code Quantum ESPRESSO [5], using ultra-soft pseudopotentials and generalized gradient approximation for electron exchange and correlation. The cutoff energy was set to 680 eV and the k-space mesh was set below $0.07A^{-1}$ for each structure.

In the NO annealing simulation, we utilized classical MD simulation with the LAMMPS package [6]. The time step was set to 0.5 fs. The model of 4H-SiC/SiO_2 interface was prepared according to ref. [3]. Briefly, in order to relax the interface between SiC and SiO_2, the initial SiO_2 layer and the top surface of the SiC layer were annealed at 5000 K and then at 2000 K for 1 ps each. Even when the 4H-SiC/SiO_2 interface model was fabricated by oxidizing the top surface of the SiC layer with O_2 molecules, NO annealing simulations described below yielded the qualitatively identical interface structures, confirming that this short-time interface relaxation does not affect the present results. NO molecules were introduced into the SiO_2 at a fixed density of 1 molecule/nm^3 and the positions of the molecules were randomly selected from a region 1.8 Å away from all existing atoms. After 1 ps of MD simulation in the NVT ensemble, unreacted NO molecules as well as CO and CO_2 molecules produced by decomposition of SiC or residual C in SiO_2 were forcibly excluded, going back to the introduction of new NO molecules.

Results and Discussion

We first fitted the interatomic potential parameters for N-containing systems. Figures 2(a) and 2(b) display the comparisons of cohesive energies and atomic forces respectively between first-principles calculations and the developed interatomic potential of N-Si-O. Our interatomic potential well reproduced the cohesive energies within the range of 0.5 eV for most of the structures. The correlation coefficient in atomic force is 0.88, which is comparable to the previous study for Si-O-C [3]. The other pairs of potentials (N, N-Si, N-O, N-C, N-Si-O, N-Si-C, N-O-C) also reproduced the results of first-principles calculations. The total number of structures used for the fittings amounted to more than 11,000. These fittings provided a set of parameters necessary to simulate NO annealing at the 4H-SiC/SiO_2 interface.

Before the introduction of NO molecules, we performed interface relaxation. Figures 3(a) and 3(b) show the results of interface relaxation for the 4H-SiC($000\bar{1}$) and (0001) surfaces, respectively. In both models, the interface became amorphous and C atoms on the SiC surface formed residual C defects in SiO_2, which include C=C double bonds and are known as the possible origin of D_{it}.

At the same time, the SiC surfaces have orientation-dependent bonds with the amorphous layers: the topmost C layer bonded with Si or residual C in SiO_2 at the 4H-SiC($000\bar{1}$) surface, while the topmost Si layer bonded with residual C atoms and O atoms in SiO_2 at the 4H-SiC(0001) surface. Such crystal orientation dependence is consistent with the experimental study [7, 8].

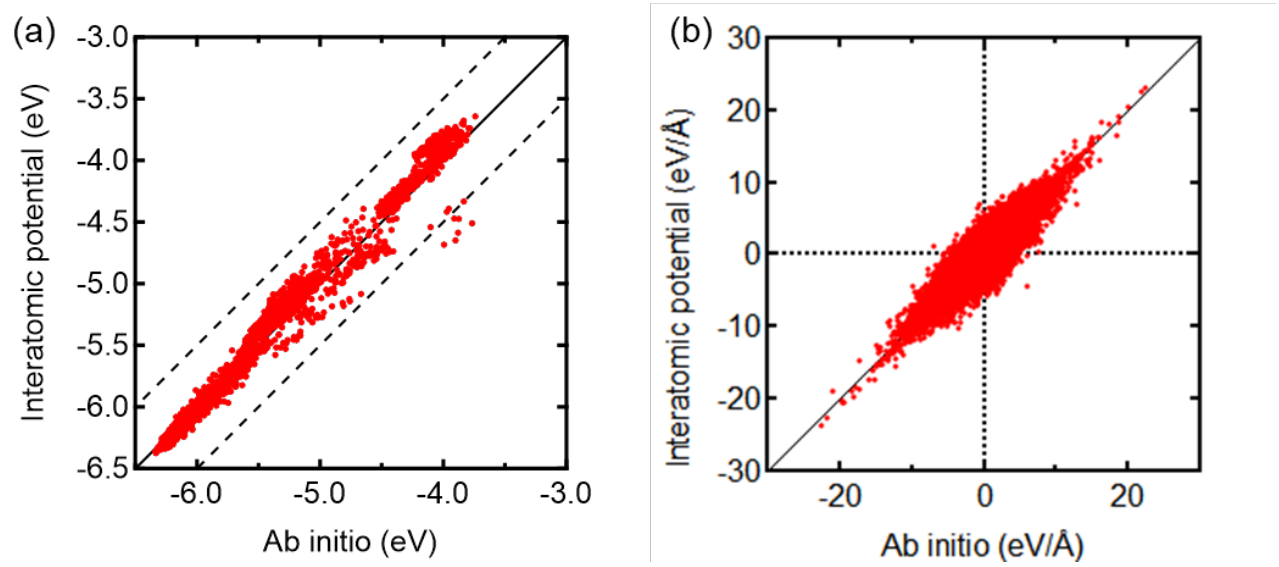

Fig. 2. (a) Cohesive energy and (b) atomic force comparison between first-principles calculation and interatomic potential for Si-O-N system.

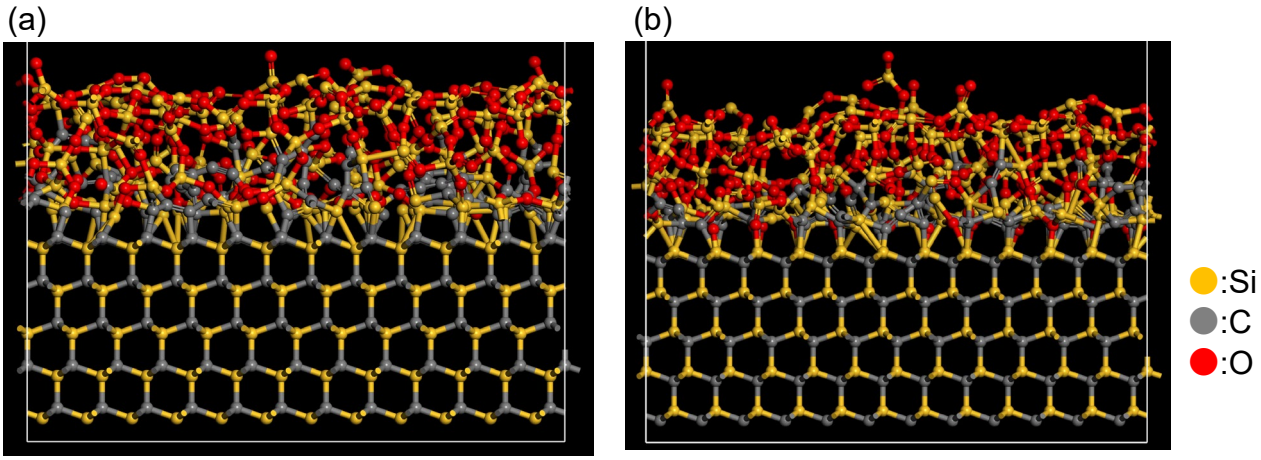

Fig. 3. Cross sections of (a) 4H-SiC(000$\bar{1}$)/SiO_2 and (b) 4H-SiC(0001)/SiO_2 annealed at 5000 K and then at 2000 K before introduction of NO molecules. Yellow, red, and grey circles represent Si, O, and C, respectively.

We performed NO annealing for the relaxed 4H-SiC/SiO_2 interface structures. Figures 4(a) and 4(b) show the cross sections of 4H-SiC(000$\bar{1}$)/SiO_2 and 4H-SiC(0001)/SiO_2 respectively calculated at 1600 K for 400 ps with NO molecules, where N atoms were incorporated near the interfaces. O and N atoms were aligned above Si atoms at the 4H-SiC(0001)/SiO_2 surface, while relatively disordered bonds were formed at the 4H-SiC(000$\bar{1}$)/SiO_2 interface. In addition, N substituted for C at the 4H-SiC(000$\bar{1}$) surface and formed a three-coordinated structure with Si as shown in the bottom panel of Fig.4 (a). This Si_3N termination is qualitatively consistent with the experimental observation [9], suggesting that our interatomic potential is fitted enough to reproduce the dangling bond termination at the 4H-SiC/SiO_2 interface by NO. We also observed that as the amount of gas introduced was reduced, the interfacial structure formed more slowly, but the resulting structure was the same. This confirms that the annealing time has little effect on the simulation results.

Furthermore, C-N defects, which have bonds between C and N, were formed on the SiO_2 region, implying that the bonding state of C=C defects are modified by reaction with NO. Since the Si-N bonds are reported to be dominant by X-ray photoelectron spectroscopy [10], the observed C-N defects are supposed to be one of the intermediate defects in the decomposition process of residual C

defects in NO annealing. Analysis of these defects would lead to better understanding of NO annealing process in 4H-SiC MOSFETs.

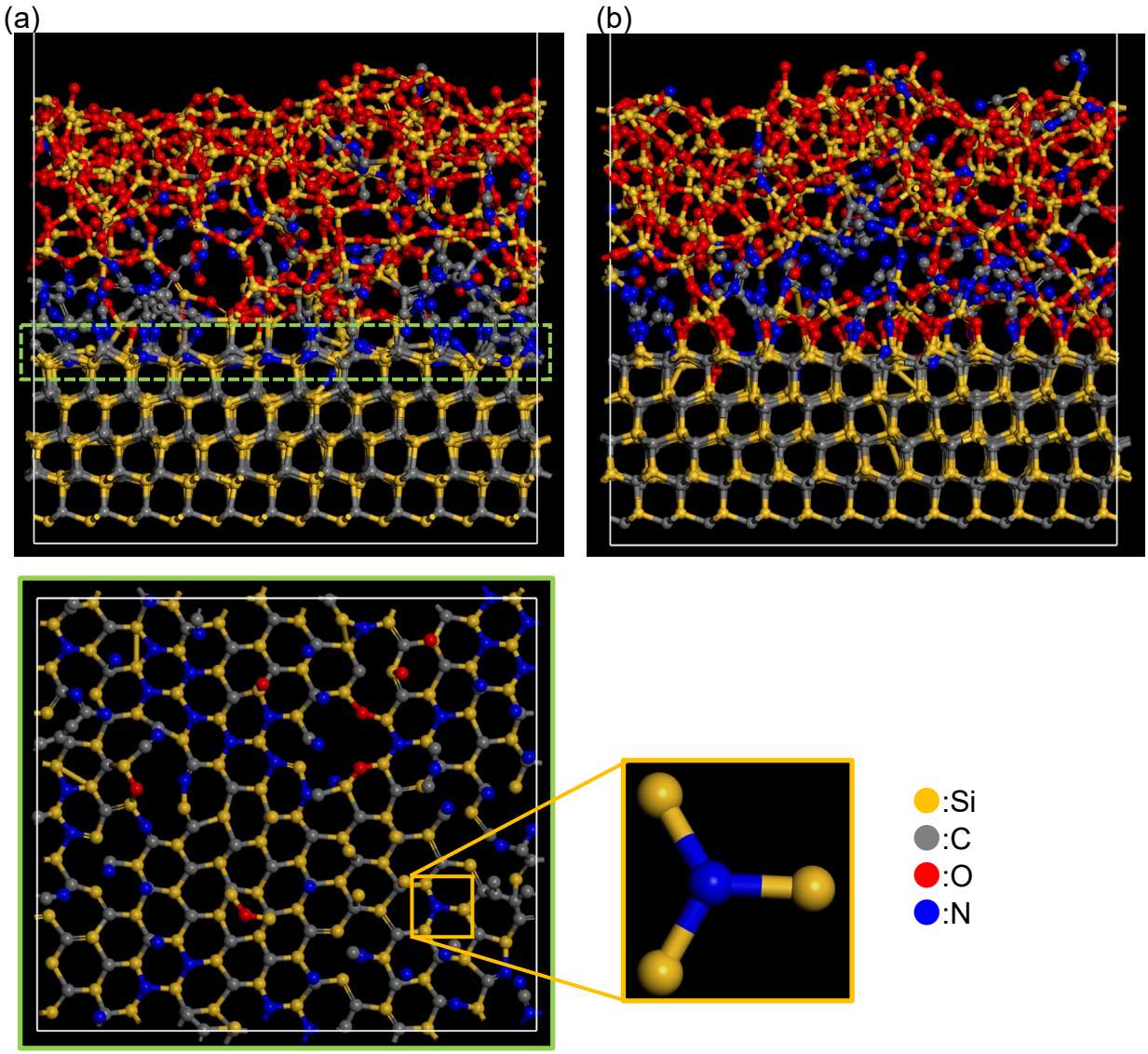

Fig. 4. Cross sections of (a) 4H-SiC(000$\bar{1}$)/SiO_2 (top panel) and (b) 4H-SiC(0001)/SiO_2 calculated at 1600 K for 400 ps with NO molecules. The bottom panel of (a) is the top view of the 4H-SiC(000$\bar{1}$)/SiO_2 interface area enclosed by a green broken line in Fig. 3(a). Yellow, red, grey, and blue circles represent Si, O, C, and N atoms, respectively.

Summary

In this work, we have developed the new interatomic potential consisting of Si, O, C, and N for NO annealing simulation of large-scale 4H-SiC/SiO_2. We adjusted the potential parameters to reproduce materials properties obtained by first-principles calculations for more than 11,000 structures. The fitted potential have reproduced the formation of Si_3N interface termination during NO annealing, where C=C defects were modified into C-N defects. Analysis of these defects would lead to better understanding of NO annealing process in 4H-SiC MOSFETs.

References

[1] T. Kimoto, Material science and device physics in SiC technology for high-voltage power devices, Jpn, J. Appl. Phys. 54 (2015) 040103.

[2] T. Kimoto, and H. Watanabe, Defect engineering in SiC technology for high-voltage power devices, Appl. Phys. Express 13 (2020) 120101.

[3] S. Takamoto, T. Yamasaki, T. Ohno, C. Kaneta, A. Hatano, and S. Izumi, Elucidation of the atomic-scale mechanism of the anisotropic oxidation rate of 4H-SiC between the (0001) Si-face and (000$\bar{1}$) C-face by using a new Si-O-C interatomic potential, J. Appl. Phys. 123 (2018) 185303.

[4] S. Takamoto, T. Yamasaki, J. Nara, T. Ohno, C. Kaneta, A. Hatano, and S. Izumi, Atomistic mechanism of graphene growth on a SiC substrate: Large-scale molecular dynamics simulations based on a new charge-transfer bond-order type potential, Phys. Rev. B 97 (2018) 125411.

[5] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G.L. Chiarotti, M. Cococcioni, I. Dabo, QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter 21 (2009) 395502.

[6] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J. Comput. Phys. 117 (1995) 1-19.

[7] X. Zhu, H.D. Lee, T. Feng, A.C. Ahyi, D. Mastrogiovanni, A. Wan, E. Garfunkel, J.R. Williams, T. Gustafsson, and L.C. Feldman, Structure and stoichiometry of (0001) 4H-SiC/oxide interface, Appl. Phys. Lett. 97 (2010) 071908.

[8] H. Watanabe, T. Hosoi, T. Kirino, Y. Kagei, Y. Uenishi, A. Chanthaphan, A. Yoshigoe, Y. Teraoka, and T. Shimura, Synchrotron x-ray photoelectron spectroscopy study on thermally grown SiO2/4H-SiC(0001) interface and its correlation with electrical properties, Appl. Phys. Lett. 99 (2011) 021907.

[9] D. Mori, Y. Oyama, T. Hirose, T. Muro, and F. Matsui, Local structural determination of N at SiO_2/SiC(000$\bar{1}$) interfaces by photoelectron diffraction, Appl. Phys. Lett. 111 (2017) 201603.

[10] K. Moges, M. Sometani, T. Hosoi, T. Shimura, S. Harada, and H. Watanabe, Sub-nanometer-scale depth profiling of nitrogen atoms in SiO_2/4H-SiC structures treated with NO annealing, Appl. Phys. Express 11 (2018) 101303.