Extended Abstracts of the 2018 International Conference on Solid State Devices and Materials, Tokyo, 2018, pp985-986

First-principles calculations of the effect of incorporating Hf atoms in AlON gate dielectrics of wide-bandgap-semiconductor power devices on the hole leakage current

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Abstract

In previous work, the hole leakage current has been observed in the AlON (aluminum oxynitride) gate dielectric of n-channel SiC MOSFET under the negative gate bias, which would present a serious reliability concern. We used first-principles calculations to investigate AlON dielectric films in detail. We found defect levels generated by N 2p orbitals in some AlON structures. These defect levels are the origin of the hole leakage current because they are near the top of the valence band. Moreover, we revealed that incorporating Hf atoms into AlON eliminates these defect levels, reducing the hole leakage current.

1. Introduction

Silicon carbide (SiC) and gallium nitride (GaN) are materials of interest for next-generation power-devices because they have superior physical properties to Si. For these devices, various gate dielectric materials, SiO_2, Al_2O_3, and HfO_2, have been reported in experiments. In particular, Al_2O_3 is a promising candidate owing to its large dielectric constant and bandgap [1-3]. It has been reported in previous studies that negative fixed charge is generated in Al_2O_3 gate dielectrics, leading to the deterioration in device reliability [4,5]. Kojima et al. reported that V_OV_{Al} complexes in Al_2O_3 are the origin of the negative fixed charge [6]. Moreover, the incorporation of N atoms into Al_2O_3 suppresses the formation of negatively charged V_OV_{Al} complexes [4-7].

In a recent study, Hosoi et al. found the hole leakage current in the AlON (aluminum oxynitride) gate dielectric of n-channel SiC MOSFET under the negative gate bias, which would present a serious reliability concern [8]. In addition, it has been reported that incorporating Hf atoms into AlON suppresses the hole leakage current [8]. However, the origin of the hole leakage current and the effect of the incorporation of Hf atoms are not well understood.

In this study, we performed first-principles calculations to investigate AlON and HfAlON dielectric films in detail.

2. Calculation methods and models

In our calculations, which included first principles molecular dynamics calculations (MD calculation), we optimized the atomic configurations and electronic structures using the VASP (Vienna ab initio simulation package) code [9-12], which is a first-principles calculation code based on density-functional theory [13]. We used the projector augmented wave potential [14] for interactions between the ion core and the valence electrons and the generalized gradient approximation by Perdew et al. [15] for the exchange-correlation potentials. The electronic wave functions were expanded in plane waves up to a kinetic energy of 500 eV. We used a 4×4×2 Monkhorst-Pack grid for the Brillouin zone integration. After optimization of the geometry, all the atomic forces were less than 5.0×10^{-2} eV/Å. Visualization for Electronic and Structural Analysis (VESTA) was used to draw the atomic configurations [16].

We first prepared a 2×2×1 supercell of α-Al_2O_3 containing 120 atoms. In this study, the amorphous Al_2O_3 was generated by first principles MD calculations. Initially, MD calculations were carried out for 10 femtosecond steps at a temperature of 6000 K. Second, we lowered the temperature to room temperature for 10 femtosecond steps. Third, we carried out structural optimization.

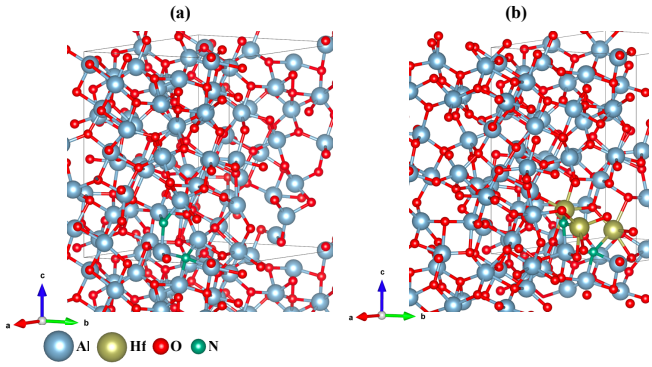

Fig. 1: The models of (a) AlON and (b)HfAlON. We constructed six AlON models and five HfAlON models.

3. Results and discussion

To construct the AlON models, we replaced three O atoms with two N atoms as shown in Fig. 1(a). We constructed six AlON models. Fig. 2 shows the band structures of these six models. In Fig. 2(a) and 2(b), we show defect levels near the top of the valence band. The defect levels are generated by the N 2p orbitals in the AlON models. These defect levels are the origin of the hole leakage current observed in the previous experiment [8] because they are near the top of the valence band.

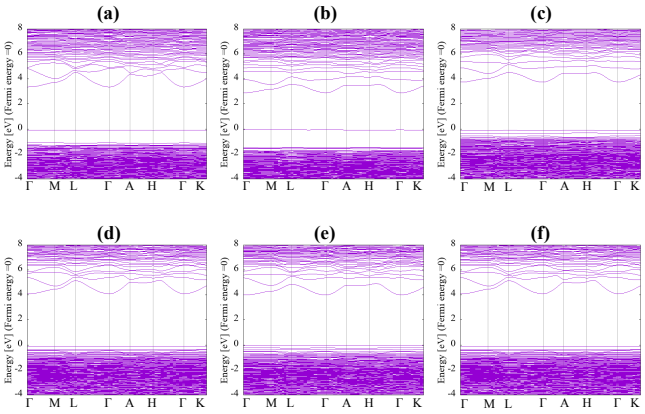

Fig. 2: Band structures of the six amorphous AlON models given in Fig. 1(a).

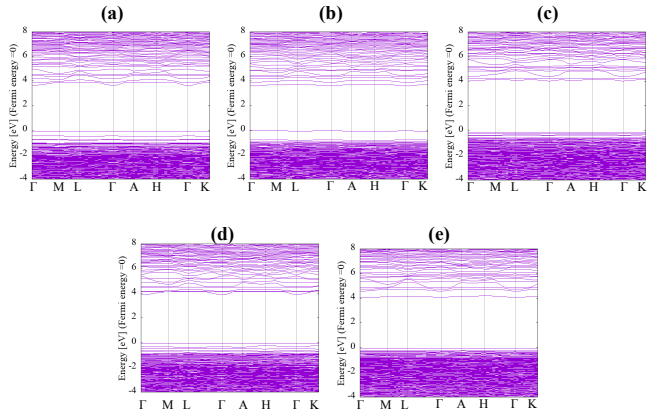

Fig. 3: Band structures of the five amorphous HfAlON models given in Fig. 1(b).

Further, we discuss the effects of incorporating Hf atoms in the AlON. To construct the HfAlON models, we replaced four Al atoms with three Hf atoms in AlON models as shown in Fig. 1(b). We constructed five HfAlON models. Fig. 3 shows the band structures of these five HfAlON models. We show the defect levels due to N 2p orbitals in Fig. 3(a) and 3(b). The total energies of the models for 3(a) and 3(b) are larger than that for model 3(c) by 3.45 and 0.28 eV, respectively. On the other hand, the total energies for models 3(d) and 3(e) are smaller than that for model 3(c) by 0.61 and 0.42 eV, respectively. Thus, the structures of models 3(c), 3(d), and 3(e) are more stable than the others. These results demonstrate that the defect levels are eliminated in the stable structures of the HfAlON models. This indicates that incorporating Hf atoms into AlON eliminates the defect levels generated by the N 2p orbitals, which is in a good agreement with the recent experiment [8].

4. Conclusions

In conclusion, we performed first-principles calculations to investigate the origin of the hole leakage current in the AlON gate dielectric of n-channel SiC MOSFET under the negative gate bias. As a result, we found that defect levels are generated by N 2p orbitals in some AlON structures. Because these are near the top of the valence band, they cause hole leakage current, which has been observed in previous work. Further, we considered the effect of incorporating Hf atoms into the AlON. Our calculations showed that incorporating Hf eliminates the defect levels, thus decreasing the hole leakage current.

Acknowledgements

This research is partly supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan, through its “Program for research and development of next-generation semiconductors to realize an energy-saving society", and the Council for Science, Technology, and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Next-generation power electronics” (funding agency: NEDO).

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