Extended Abstracts of the 2009 International Conference on Solid State Devices and Materials, Sendai, 2009, pp320-321

Atomistic Modeling of GeO_2/Ge and SiO_2/Si Interface Structures

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1. Introduction

Ge CMOS has been of increasing interest as a promising candidate for future electronic device over the scaling limit of Si technology, because of the intrinsically higher carrier mobility of Ge than that of Si. However, realizing a good GeO_2/Ge interface is one of the most critical issues for establishing Ge MOS technology because the volatilization of Ge monoxide (GeO) occurs and the quality of the GeO_2/Ge interface tends to deteriorate during thermal oxidation processes. Recently, it has been found that this problem is overcome by employing a cap layer [1] or transforming the Ge oxides to Ge oxynaitrides (GeO_xN_y) [2]. In addition, it has been reported that the interface trap density (D_{it}) value can be reduced with an increase in the oxidation temperature as long as GeO volatilization does not occur [3, 4]. These reports provide us a bright prospect for realizing Ge CMOS.

As researches for establishing Ge CMOS technology proceed, it is more necessary to understand the atomistic picture of GeO_2/Ge interface accurately and in detail. In addition, it is extremely meaningful to compare with the properties of SiO_2/Si interface which has been well studied in previous works, and to extract differences and similarities between the two interface structures. In this work, we performed large-scale molecular dynamics (MD) simulations on GeO_2/Ge interface structure by using newly developed interatomic potential function for Ge, O mixed systems. We modeled also an SiO_2/Si model with almost the same size as the GeO_2/Ge to compare both interface structures.

2. Interatomic potential for Ge, O mixed systems

In our previous works, we developed an interatomic potential function for Si, O mixed systems [5]. This potential function is an extended version of the Stillinger-Weber potential for pure Si systems [6], which comprises of two- and three-body potential energy terms. All potential parameters are determined so as to reproduce *ab initio* molecular orbital calculations of small clusters. In this work, we applied the same approach to develop the interatomic potential function for Ge, O mixed systems.

On the whole, binding energies and distortion energies of bond angles in the Ge, O systems is weaker than those in the Si, O systems, except the Ge-O-Ge bridging oxygen angle. As shown in Figure 1, Ge-O-Ge angle is found to be harder than Si-O-Si angle by the *ab initio* calculation, and has a narrower equilibrium angle of 133° than that of Si-O-Si of 144°.

3. Building SiO_2/Si(001) and GeO_2/Ge(001) model

Building the SiO_2/Si and GeO_2/Ge interface structure is started from the preparation of a single-crystal Si(001) and Ge(001) substrate, respectively. In case of SiO_2/Si, the initial structure is (001)-terminated Si model (5200 atoms) of 5.43 nm thick in [001] and 4.34 nm long in [100] and [010]. In case of GeO_2/Ge, the initial structure is (001)-terminated Ge model (5200 atoms) of 5.65 nm thick in [001] and 4.52 nm long in [100] and [010]. In this calculation, two-dimensional periodic boundary condition is adopted in parallel directions to the surface, hence the structures is allowed to make a free volume expansion only in the surface normal direction.

Next, an SiO_2 and a GeO_2 films are formed by inserting O atoms layer by layer into the Si-Si bonds and Ge-Ge bonds from the surface, respectively. After one layer of O atoms are inserted, the whole structure is relaxed by MD simulation adopting our interatomic potentials.

Figure 2(a) and (b) shows the SiO_2/Si(001) and GeO_2/Ge(001) structure obtained after the oxidation 17 layers, respectively. The thickness of the SiO_2 film is about 4.3 nm and that of GeO_2 film is about 4.9 nm.

4. Results and discussion

Figure 3(a) and (b) show bridging oxygen bond angle distributions in the SiO_2 and GeO_2 films obtained in this calculation. In case of the SiO_2 films, the peak of the Si-O-Si angle distribution shifted toward a small angle from the equilibrium angle of 144°. On the other hand, the peak of the Ge-O-Ge angle distribution coincided with the equilibrium angle of 133°. In addition, the width of the peak in the Ge-O-Ge distribution was narrower than that in the Si-O-Si distribution. These results show that the oxidation-induced strain in the GeO_2 films is smaller than that in the SiO_2 films.

Figure 4 shows the stress profile in the SiO_2 and GeO_2 films. The value of the stress is the mean value of the in-plane component of stress at given depth in the oxide film. This result suggests that the GeO_2 film model was more relaxed than the SiO_2 film model. Combined with the bond angle distribution, it is concluded that the oxidation-induced strain was weaker than in the GeO_2 film than in the SiO_2 film.

Figure 5 shows binding defects appeared in the SiO_2 and GeO_2 films. Small spheres show atoms with dangling bonds in the oxide films. The total number of defects was

larger in the SiO_2 films than in the GeO_2 films. In addition, the density of defects corresponding to P_b center at the interface was estimated to be $7.0\times10^{13}cm^{-2}$ and $2.5\times10^{13}cm^{-2}$, respectively. Thus the density of the interfacial defects of GeO_2/Ge structure was lower than that of SiO_2/Si.

These results indicate that the GeO_2/Ge interface structure has superior interfacial properties to the SiO_2/Si interface structure, in terms of the oxide stress and defect density. This is qualitatively agreeing with the recent experimental results [3], the minimum D_{it} value lower than $10^{11}cm^{-2}eV^{-1}$ could be obtained for GeO_2/Ge MOS interface fabricated by direct oxidation of Ge substrates. The reason for the superiority of GeO_2 film is attributed to the following two facts. (1) The binding energies and distortion energies of bond angles in the Ge, O systems is weaker than those in the Si, O systems on the whole. (2) GeO_2 film has a smaller lattice mismatch with the substrate than the SiO_2 film because the equilibrium angle of the Ge-O-Ge bridging oxygen bond is smaller than that of the Si-O-Si bond.

5. Conclusions

We developed new interatomic potential function for Ge, O mixed systems by extending an existing potential function for Si, O mixed systems, and performed a series of MD simulations of GeO_2/Ge interface structure. It was found that the oxidation-induced strain was weaker than in the GeO_2 film model than in the SiO_2 film model. Furthermore, the defect density at the GeO_2/Ge interface was lower than at the SiO_2/Si interface. These calculation results show that the GeO_2/Ge interface structure can be more excellent interface than the SiO_2/Si interface.

Acknowledgements

We acknowledge supports from Grant-in-Aid for Young Scientists (A) Grant No. 19686005. Grant-in-Aid Scientific Research (B) Grant No. 20360023.

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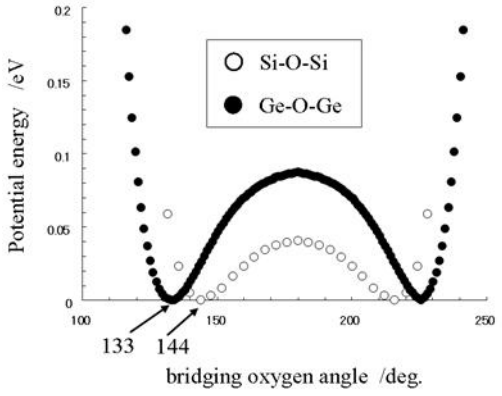

Fig. 1 Structural energy vs Si-O-Si and Ge-O-Ge angle

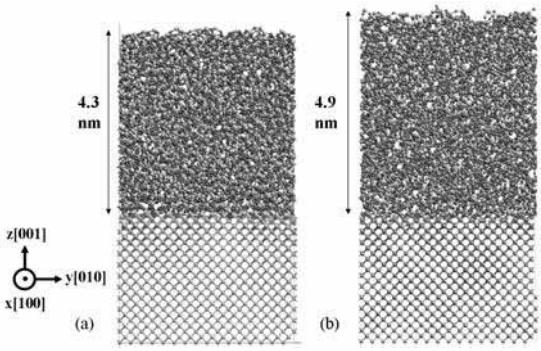

Fig. 2 (a) SiO_2/Si and GeO_2/Ge structure models.

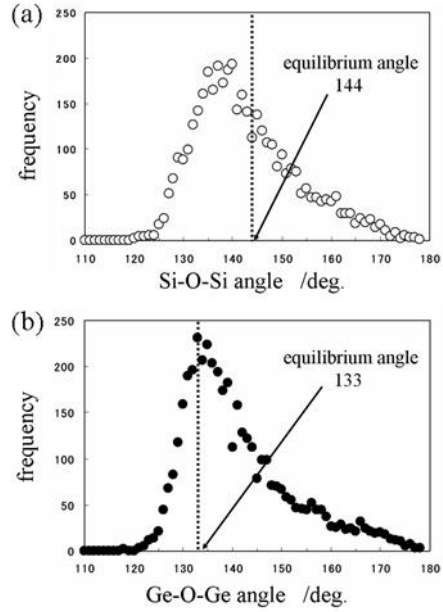

Fig. 3 (a) Si-O-Si and (b) Ge-O-Ge bond angle distribution

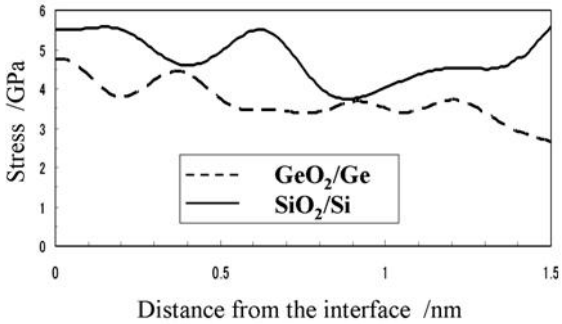

Fig. 4 Stress profile within the SiO_2 and GeO_2 films.

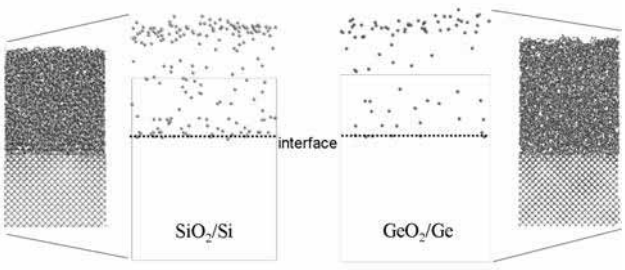

Fig. 5 Defects within the SiO_2 film and GeO_2 film.