Invited Paper

Dynamic Monte Carlo Simulation for High Resolution Depth Profiling of Si/Ge Multilayer Film

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Dynamic Monte Carlo (DMC) simulation was carried out to see the transient effect of the primary reactive ion. The results of the DMC simulation, which takes into account both swelling and diffusion, describe the experimental results for the transient Si sputtering yield very well. We applied the DMC simulation to the depth profiling of Si/Ge multilayer films. In the SIMS depth profiling with 5.5keV O_2^+ ion beam, the etching rate of a Si layer is much slower than that of Ge layer because of the formation of SiO_2 layer during O_2^+ ion sputtering. In the AES depth profiling with 0.5keV Ar^+ ion beam and grazing incident angle, the etching rate of Si is almost the same as that of Ge, which is in good agreement with the DMC Simulation.

1. Introduction

With the continued scaling reduction in semiconductor devices, the depth resolution requirement from the semiconductor industry is already in the sub-nanometer range. Sputter depth profiling by secondary ion mass spectrometry (SIMS) and Auger electron spectroscopy (AES) have been widely used in semiconductor industries due to its high sensitivity and depth resolution. However, the depth resolution of conventional SIMS and AES using several keV ion beam sputtering is not good enough for the ultra shallow junctions. Recently, the low energy ion beams with oblique incident angles have been used to improve the depth resolution and to reduce the surface transient effect [1,2]. Even if we use low energy ions, the change in the sputtering yield in the pre-equilibrium region should be understood quantitatively for accurate depth profiling of shallow junctions and nanometer scale etching. Dynamic Monte Carlo (DMC) simulation complement experiments in the sense that they describe the detailed processes from a more fundamental viewpoint. In our previous works, the DMC method has been applied to the sputter depth profiling of AlAs/GaAs multilayered systems and delta-doped SiO_2 layer into Ta_2O_5 systems[3-5]. The simulation results described the AES depth profiling of AlAs/GaAs and SIMS depth profiling of the delta-doped SiO_2layers into Ta_2O_5 layers very well, but the primary ion effect was ignored in the previous simulation model. Therefore another scheme is necessary to apply it to reactive oxygen ion beam sputtering. We developed a DMC scheme for reactive ion sputtering, which takes into account the swelling and diffusion of implanted atoms as well as atomic mixing. The DMC simulation was also carried out to understand the transient processes from the initial stage to the steady state region for an amorphous Si surface with 500 eV O_2^+ ion beam sputtering. The simulation results describe the *in situ* MEIS experimental results for the in-depth composition profiles and the transient Si sputtering yield very well [6]. We applied the DMC simulation to the depth profiling of Si/Ge multilayer films because the depth profiling of Si-Ge systems is very important for the development of a new semiconductor devices. In the SIMS depth profiling with O_2^+ ion beam, the etching rate of a Si layer is much slower than that of Ge layer because of the formation of SiO_2 layer during O_2^+ ion sputtering. In the AES depth profiling with Ar^+ ion beam, the etching rate of Si is almost the same as that of Ge, which is in good agreement with the DMC simulation.

2. Model of Dynamic Monte Carlo Simulation

The Monte Carlo Simulation model for the interactions of energetic ions with solid is based on the elastic collision by binary encounter with randomly distributed target atoms and inelastic collision with electron gas using Ziegler-Biersack-Littmark(ZBL) potential and Lindhard's equation respectively[7]. Details of this program are seen in elsewhere[4,5]. Therefore, for the depth profiling, a newly introduced terms are described briefly. The effect of surface roughness is disregarded in these calculations. The interstitials and vacancies generated by collision cascade are distributed in pairs if the sputtered atoms are regarded as being sputtered only from the topmost atomic layer. These pairs migrate during collision cascade and the vacancies are eventually annihilated by recombination with interstitials or absorption into the sinks, e.g. surface, grain boundary, etc. Since the behavior of these interstitial atoms and vacancies is directly related to diffusion in sputtering and range of atomic mixing in a complicated manner, it is very difficult to describe the migration processes of these pairs accurately. In the present simulation, therefore, all the interstitial-vacancy pairs are assumed to be completely recombined in the mixing zone. The total number of atoms of each layer, therefore, remains constant so that the atomic density in each atomic layer keeps invariant during sputtering. Otherwise, the atomic density tends to increase by a knock-in effect as sputtering proceeds. The DMC scheme for reactive ion sputtering takes into account the swelling and diffusion of implanted atoms as well as atomic mixing. If the incident and scattered atoms have enough energy to overcome the surface binding energy, these atoms are sputtered. The surface binding energy for SiOx (O≤ x≤ 2) was obtained by the linear combination of the surface binding energy of SiO_2 and Si [8]. In the present calculation, the surface binding energies for SiO_2 and Si were 3.6 and 1.2 eV, respectively. To see the effect of diffusion, we moved 10% of O atoms in the two adjacent layers and 1% of O atoms from the next two adjacent layers. However, we assumed that if the ratio of O over Si in a layer was greater than 2, all the excess O atoms are moved into the right upper layer, which implies the onset of fast outward diffusion. Therefore the maximum oxygen concentration in DMC should be 67 at %, which correspond to SiO_2 formation. The number of pseudoatoms, representing one atomic layer, was 5000 in the present simulation. In this work, the DMC simulation has been applied to the calculation of concentration profile and sputtering yield changes for the Si surface bombarded with 500 eV O_2^+ ions at the transient state, which were compared with MEIS experimental results. We also applied the DMC simulation to the AES depth profiling of Si/Ge multilayer films.

3. Results and discussion

The change in the sputtering yield during the transient stages was calculated as a function of oxygen ion dose, and compared with the values measured by using MEIS with an amorphous Si layer grown on a clean Si(001) surface [9].

Figure 1 shows the change in the MEIS energy spectra of a 12 nm amorphous Si layer on Si(001) with sputtering. The as-grown 12 nm amorphous Si layer shows a uniform Si distribution throughout the whole layer. With O_2^+ ion bombardment, the Si peak intensity in the surface region decreased with a gradual formation of a surface oxide layer, and the O peak increased with increasing dosage from the beginning. An initial surface swelling was also observed due to the higher incorporation rate of the incident oxygen atoms, which can be deduced from the increase in the width of the Si peak in Fig. 1.

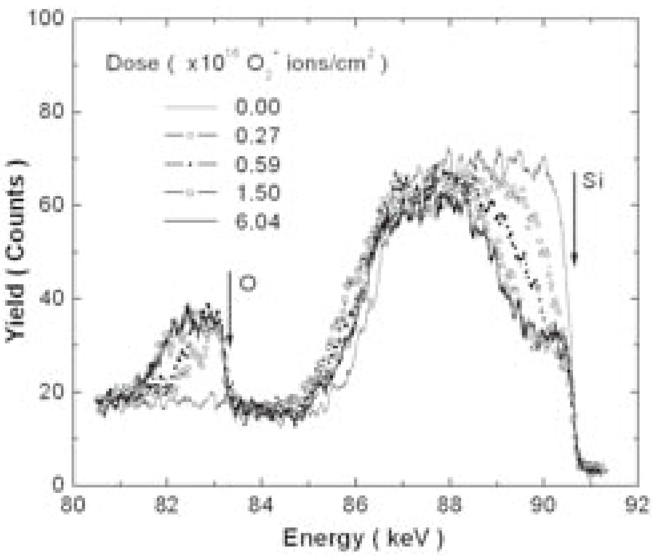


Figure 1. MEIS energy spectra for a 12 nm amorphous Si layer grown on Si(100) as a function of ion dose of 500 eV O_2^+ ion bombardment at surface normal incidence.

The total numbers of incorporated O atoms and ejected Si atoms, which were converted quantitatively from the Si and O peak areas of Fig. 1, are plotted in Fig. 2. The DMC results are also shown in Fig. 2 for comparison. The total number of incorporated oxygen atoms increased almost linearly during the transient stage, which shows that most of the incident atoms are implanted, and then it maintains a constant value at the steady state as described in the simulation model. The total number of the ejected Si atoms increased rapidly during the initial sputtering stage as the oxygen ion dose was increased, and thereafter it increased continually. The net change in the total number of atoms, which is related to the surface recession, is also shown in Fig. 2. The total number of incorporated-ejected atoms shows a negative value, indicating surface swelling. On the other hand, the number of incident oxygen at the initial stage of sputtering was less than that of implanted oxygen. The difference between the experimental results and DMC calculation for the total number of the incorporated oxygen atoms at the transient region is mainly due to oxygen flooding. Thereby, the transient dose in the experiment was reached faster than that in DMC simulation. Because of this fact, the oxygen flooding condition should be controlled very carefully for accurate and reproducible shallow SIMS depth profiling.

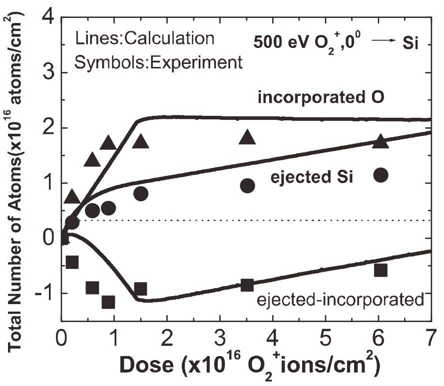


Figure 2. The total number of incorporated O (▲) and ejected Si (●) atoms in a Si surface as a function of ion dose of 500 eV O_2^+. The net change of the total number of atoms (■) is also shown.

The sputtering yield of Si can be calculated from the slope of the ejected Si atoms in Fig. 2 as shown in Fig. 3. The Si sputtering yield decreased very rapidly from 2.4 at the initial stage of the sputtering to less than 0.1 Si atoms per O_2 at the steady state. The surface recession depth was calculated from the difference between the original Si surface thickness and the thickness after sputtering. The negative value of the surface recession means surface swelling. The steady state was reached at 2.0 nm swelling at the ion dose of ~ 1.4×10^{16} O_2^+ions/cm^2, which corresponds to the 2.7 nm shifting to the thicker depth in SIMS depth profiling. This result shows that the depth scale in the shallow junction SIMS profiling, in the depth range of 10-30 nm, is seriously distorted and can only be corrected by quantitative measurement and DMC simulation of the sputtering yield change. The partial sputtering yield of Si and the surface recession at incident angle of 45° as a function of O_2^+ ion dose are shown in Fig. 4. The sputtering effect is more dominant than that of the surface swelling effect, therefore, the surface recession shows a positive value. The steady stage is reached after ~ 2.5×10^{16} O_2^+ ions/cm^2 ion doses, and the depth scale offset is about 1.3 nm. For the incident angle of 60°, the ion dose dependence of Si sputtering yield and the surface recession are shown in Fig. 5. The surface recession is almost linear and the transient effect decreases since the sputtering yield is very high and the accumulation effect is very low. The steady state is reached after ~1.5×10^{16} O_2^+ ions/cm^2 ion doses, and the depth scale offset is about1.0 nm. At surface normal incidence, the sputtering yield is very low and most of the incident atoms are accumulated on the surface. Therefore, the surface swelling by the accumulation of implanted reactive ions is more dominant than the surface etching by sputtering. Therefore, the transient effect becomes severe. On the contrary, at grazing incident angle, the sputtering yield is very high and the number of accumulated oxygen atoms is very small. Therefore, the surface swelling and the transient effects in the depth profiling using SIMS can be minimized. The DMC simulation was applied to the depth profiling of a multi-layered Ge/Si thin films. The Multi-layered Ge/Si thin films were grown by ion-beam sputter deposition (IBSD) as discussed elsewhere[10]. The target material was sputtered by a 1 keV Ar^+ ion beam produced by a Kaufmann type d.c. ion gun and was deposited on substrates at room temperature. The films were grown on 150 mm diameter Si wafers rotating with a speed of 30 rpm to improve the thickness uniformity. The film thickness was controlled by selection of the growth time. The

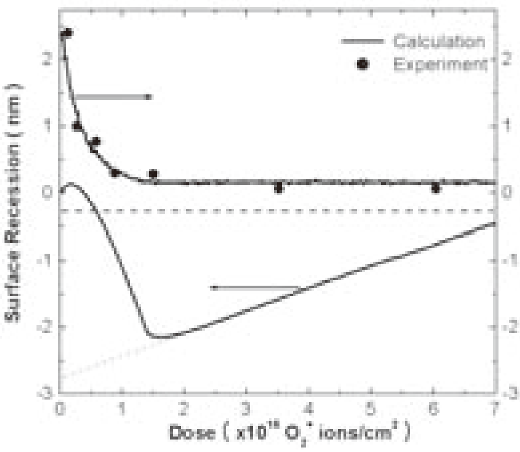


Figure 3. The sputtering yield of Si and the surface recession at surface normal incidence as a function of O_2^+ ion dose.

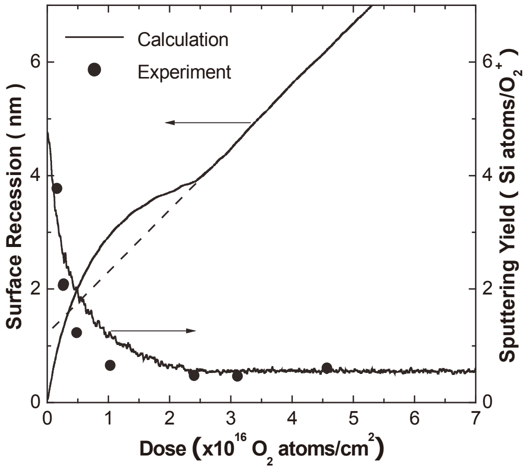


Figure 4. The sputtering yield of Si and the surface recession at incident angle of 45º as a function of O_2^+ ion dose.

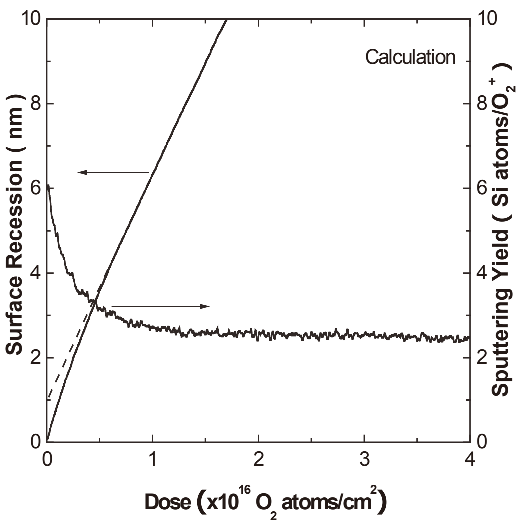


Figure 5. DMC simulation results of the Si sputtering yield and the surface recession at incident angle of 60º as a function of O_2^+ ion dose.

thickness of thin films was certified by high-resolution transmission electron microscopy (HR-TEM) measurement as shown in Fig.6. SIMS depth profile was performed on Cameca IMS-4f using ion energies of 10.5keV with O_2^+ ion species and bias voltage of 4.5 kV. The SIMS depth profile of a Si/Ge multi-layered thin film is shown in Fig. 7. The etching rate of a Si layer is much slower than that of Ge layer because of the formation of SiO_2 layer during O_2^+ ion sputtering. The DMC simulation results obtained from sputtering yield for SiO_2/Ge and SiO_2/GeO multi-layered thin films are also shown in Fig. 7. As can be seen in figure, the simulation results for SiO_2/Ge multi-layered thin film is in good agreement with the experimental results from the view point of the etching rate. It means that Si layer becomes oxidation, but Ge layer does not react with oxygen during O_2^+ ion sputtering. Actually it was confirmed that Ge layer does not form oxidation state at steady state during O_2^+ ion sputtering by means of XPS and high resolution RBS experiment, which is not shown here. In the case of O_2^+ ion bombardment, the surface was fully or partially oxidized by incorporated oxygen atoms, However, in the case of Ar^+ ion bombardment, the implanted Ar atoms are more easily re-sputtered into the vacuum. After 500 eV Ar ion bombarding on Si surface, the maximum atomic concentration of Ar is ~ 6 at% at a depth of ~2 nm for normal incidence but is not detected for the grazing incidence angle of 80°. Details on the in-depth distribution of Ar atoms can be seen in elsewhere [11]. When the low energy Ar ion beam at grazing incident angle was utilized

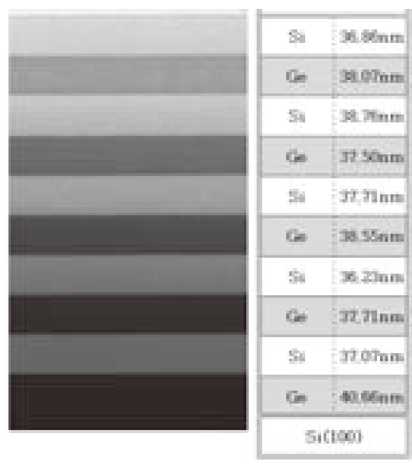
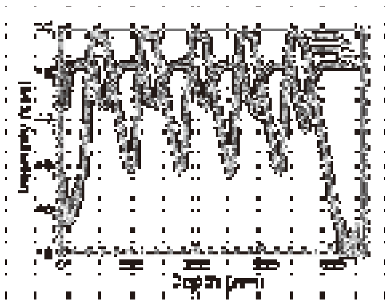
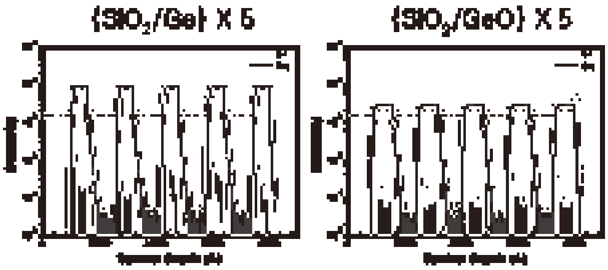


Figure 6. The thickness of multi-layered Si/Ge thin film certified with TEM experiment.



(a) Experiment Result

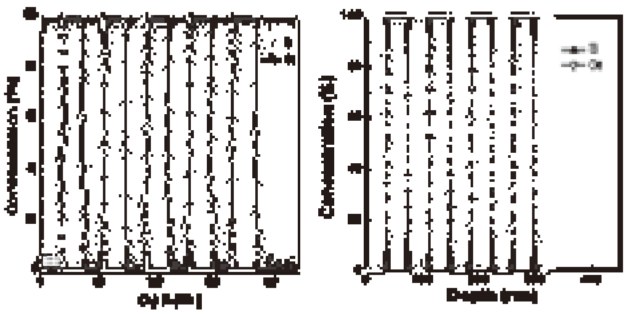


(b) Simulation Result

Figure 7. SIMS depth profiling of Si/Ge multi-layered thin film.

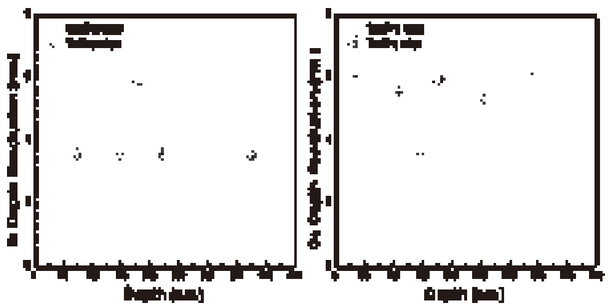
in the sputter depth profiling, the surface swelling and the transient effects in the depth profiling can be minimized. The AES depth profiling of the Si/Ge multilayer was performed with the PHI-700 nano-probe by using 500 eV Ar^+ ion beam sputtering at the incident angle of 75 degree from surface normal. The primary electron beam energy for AES measurement was 10keV and the beam current was 10nA. The Ge MNN and Si LMM peak intensity was used to measure the depth profiling. The Zala-rotation mode was used to minimize the surface roughness effect in depth profiling. Depth profiling is shown in fig. 8 together with the DMC simulation result for comparison. As can be seen in figure, the depth profiling of muti-layered thin film does not have any degradation in each layers of the multi-layered thin films and the etching rate of a Si layer is almost same as that of Ge layer, which is in good agreement with the experimental results.

For comparing the simulation results with experimental results in more detail, the leading edge growth and the trailing edge decay length of multi-layered thin films were obtained with exponential function as commonly done in depth profiling. The results are shown in fig.9. The depth resolution of the simulation is better then that

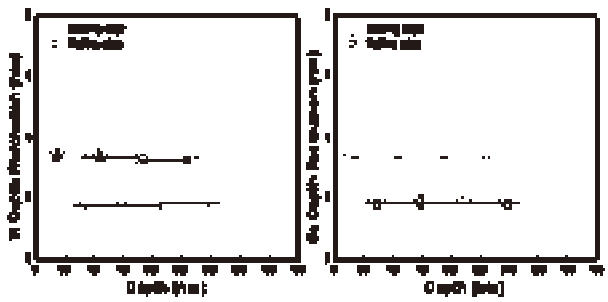


(a) Experiment Result (b) Simulation Result

Figure 8 AES depth profiling of Si/Ge multi-layered thin film



(a) (b)



(c) (d)

Fig. 9. Depth resolution of Si layer on Ge layer (a) and Ge layer on Si layer (b) in experiment, and Si layer on Ge layer (c) and Ge layer on Si layer (d) in simulation.

of the experimental results, since the simulation model does not include mainly the roughness, but generally the simulation is in quite good agreement with the experiment. It is of interest to note that the leading edge growth length is larger than the trailing edge decay length in each Si layers, but vise versa in each Ge layer, which is in contrast to other generally observed cases. Another interesting thing is that the depth resolution of Ge layer on Si layer is better than that of Si layer on Ge layer from the viewpoint of the leading edge growth length. It can be explained in terms of the atomic mixing effect. The low energy Ar ion beam at the grazing incident angle could be useful to achieve the high depth resolution without any serious transient effects.

4. Conclusions

The DMC simulation is based on the surface swelling owing to the accumulation of implanted oxygen atoms in the partially oxidized layers and fast out-diffusion of oxygen atoms towards the surface in the fully oxidized layer. The simulation and experimental results show that the transient sputtering effect can be minimized using grazing incidence. In the SIMS depth profiling with O_2^+ ion beam, the etching rate of a Si layer is much slower than that of Ge layer because of the formation of SiO_2 layer during O_2^+ ion sputtering. In the AES depth profiling with Ar^+ ion beam, the etching rate of Si is almost the same as that of Ge, which is in good agreement with the DMC Simulation. The low energy ion beam at the grazing incident angle should be utilized to achieve the high depth resolution

5. Acknowledgment

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6. References

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