Prediction of SiO_2 sputtering yield using Molecular Dynamics Simulation

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Abstract-**The surface of processed wafers during the plasma etching process is exposed to the shower of relatively high energy particles, and the surface reaction that evaporates the upper surface layer is induced by the collision. The evolution of surface profile during plasma etching needs to be known in order to control the fine details of features of semiconductor devices. The process is a complex combination of following factors such as incident particle's kinetic energy, incident angle and substrate conditions. In this study, we performed molecular dynamics simulations of Ar^+ ion bombarding SiO_2 substrate and observed the sputtering yield as the incident angle and energy changes. Our primary goal is to verify the process as the reliable source of microscopic sputtering yield data. We inserted 10 ps of relaxation right after each bombardment so that the concentrated heat to diffuse into the bulk region and it gave us similar results to a previous study,[1] and observed the surface evolution during the process. These effort predicted different sputtering yield from previous study, but the overall patterns of reaction product trajectories were similar.**

I. Introduction

The surface profile change during plasma etching process is the most popular procedure to create sub micron level of fine features on semiconductor surface. As the device size shrinks the importance of the fine controlling the surface features increased, and the prediction of the surface profile evolution under a certain process condition becomes more important ever. Our approach is one of the efforts to devise a molecular dynamics simulation strategy to supply microscopic level of sputtering yield as an input for further surface evolution simulation as a function of incident ions' kinetic energy and incident angle. We will first describe the model, and differences of the simulation procedure from other previous studies. Conclusion will include the comparison of results.

II. System Description And Simulation Methodology

The system we are focusing on is composed of clean SiO_2 substrate bombarded by Ar^+ ion which can be observed in certain conditions of Ar-O_2 plasma process. Molecular dynamics simulation which uses Verlet algorithm with neighbor lists based on linked cell scheme [2] was used to deal with this system using Feuston et al.'s SiO_2 potential [3]. It is also assumed that there is no surface polymer layer formation during the etching process and sputtering is primarily due to physical mechanism. Any inclusion of polymer layer is still considered difficult since the interatomic potential suitable for polymer layer, and the structure or density of the polymer layer is not available [4].

The simulation uses a slab of SiO_2 placed in a simulation cell that has periodic boundary condition applied to x direction and y direction only. The slab is made up of 16 unit cells (4 each in x and y directions) and 12 layers of them were stacked to the z direction. This system is about 60 Å tall and the position of atoms located at the lowest height were fixed to keep the system from rotating or drifting during bombardment. 5-Å-thick layers right above the fixed atoms were linked to a heat

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bath at 300 K so that the whole slab can release thermal energy generated from ion bombardment.

The previous study done by Graves group [1] uses a relatively abrupt quenching method after some relaxation period of 1 ps or so, but we tried to use milder way of cooling down the system since we believe that the system could have some slower process of surface re-structuring which might affect surface property. Therefore, the bombardment interval after each collision was chosen so that the temperature of the surface region can slowly return to the original temperature by heat conduction to the bulk part of the slab mimicked by heat bath.

In order to achieve this effect, we carried out a series of bombardment simulation at 100 eV Ar^+ ion with different SiO_2 slab thickness.

The number of layers in z direction was carefully chosen by examining the cooling curves of the slabs that closely imitates an ion bombardment simulation with 100 Å thick system which covers 40 unit cell depth in z direction. We used it as the reference system and tried to find the smallest system whose temperature change pattern after bombardment closely imitates that of the reference system. The system was monitored for each 5 Å thick region during the after-bombardment cooling period, and the cooling curves of 12-unit-cell-thick system showed no significant difference from the reference system. We also found that the surface region returned to the original temperature of 300 K after about 10 ps has passed conducting thermal energy to the bottom heat bath layers. Therefore, after each bombardment, the substrate is allowed to relax for 10 ps.

Most of the sputtering event occurs within the first a few ps period, and this extra relaxation time allows the thermal energy to change the morphology of the substrate.

This relatively long relaxation time was employed since the similar previous study resulted in underestimated sputter yield values and they concluded that its reason seemed to be the inaccuracy of the potential functions used. [1] We believed that the reason could also be the rapid quenching and tried to verify the effect with longer relaxation time that leads the surface atoms to cool down slower and rearrange themselves. The overall simulation flow is, thus, as if Fig. 1.

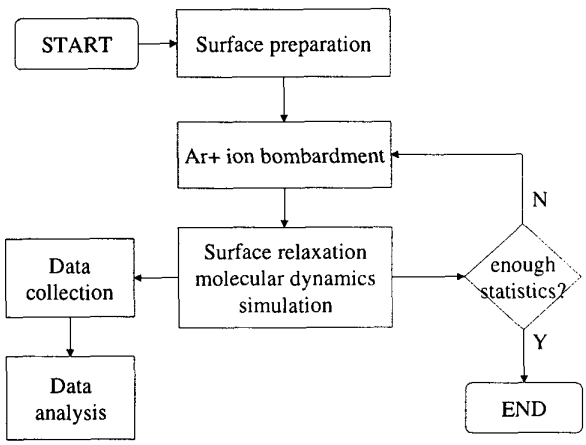

Fig. 1. The flow chart of bombardment simulation.

We varied the incident Ar^+ ion's energy from 30 eV to 300 eV with the incident angle of 15, 30, 45, 60, 67, 75, 85°. The ion first hits the surface and then heats up the surface as well as internal region of the substrate. The initial structure of the system was from a perfect crystal, and it was relaxed at 300 K for 100 ps exposing (100) surface to the z direction.

During the relaxation due to the abrupt bond breakage, the surface region is rearranging itself although the accurate structure could not presumably obtained. (See the leftmost column in Fig. 2.) The surface region was locally heated to very high temperature right after each bombardment process and then rapidly cooled transferring heat to the bottom heat bath layers, which eventually changed the morphology of the whole part of the system amorphous after 200 bombardments. This was a universal feature irrespective of the incident particles' kinetic energy and incident angle, and only the system with larger than 75° of incident

angle were able to preserve certain amount of crystal-like substrate near heat bath region at the bottom.

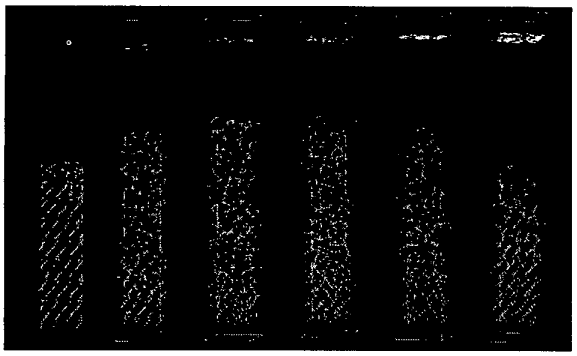

Fig 2. The change of substrate morphology after 200 ion bombardments
[from left, before bombardment, 15, 30, 45, 60, 75°]

III. RESULTS

The data obtained are about the reflection of Ar^+ ion, implanted Ar^+ ion and sputtered substrate atoms. The reflection angle distribution and direction as well as sputtering product statistics was collected as in other previous study [1].

The two main results of this study are summarized in Fig 3 and Fig 4. These are directly useful result necessary to predict the surface profile evolution prediction to be used in surface evolution simulation scheme currently under development.

Fig 3. depicts a simple principle, that is, "a vertical dive is necessary to hold the bombarding ion on the surface", and the higher the incident ion energy the better the particle sticks to the surface at least in this small window of energy range.

Apparently, as the incident ion's energy gets higher the sputtering yield is larger as was shown in Fig 4., which is qualitatively similar to the previous study [1]. The curves show peaks at near 67° of incident angle, but the peak can be shifted slightly for different incident energy. This tendency is also similarly observed in a similar study carried out by Liu et al. [5]. Although they used EAM potential function for Cu substrate, the overall sputtering yield function exhibits a similar pattern with slightly different peak position.

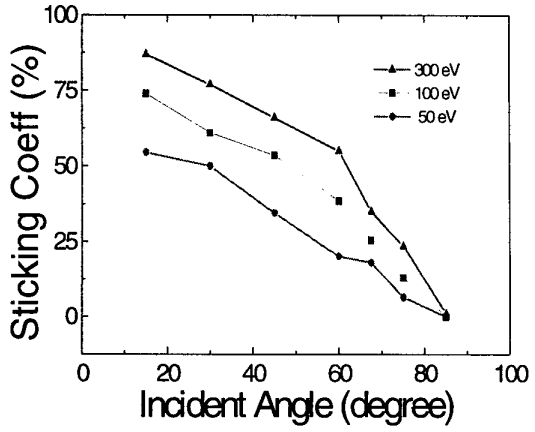

Fig 3. Sticking coefficient of Ar^+ ion bombarded with 50, 100, 300 eV of kinetic energy to SiO_2 (100) surface

We also found that our sputter yield value is quite small compared to the previous results at a comparable incident energy level [1]. We believe this is because we have allowed the surface to rearrange during the relaxation process for 10 ps with relatively slow cooling using the bottom heat bath layer, which allows formation of more stable configuration on the surface compared to the case with relatively abrupt cooling process employed in the other study in [1]. This difference may not be very important in a qualitative sense and more precise study should be carried out to clarify this issue. However, we can expect that the absolute dry etching rate as well as the relative rate as a function of particles' incident kinetic energy, and angle must also take the surface rearrangement due to the heat cycles into account. This is due to the fact that the surface structure stability is a very important factor for the binding energy of surface atoms and it is directly related to the sputter yield function.

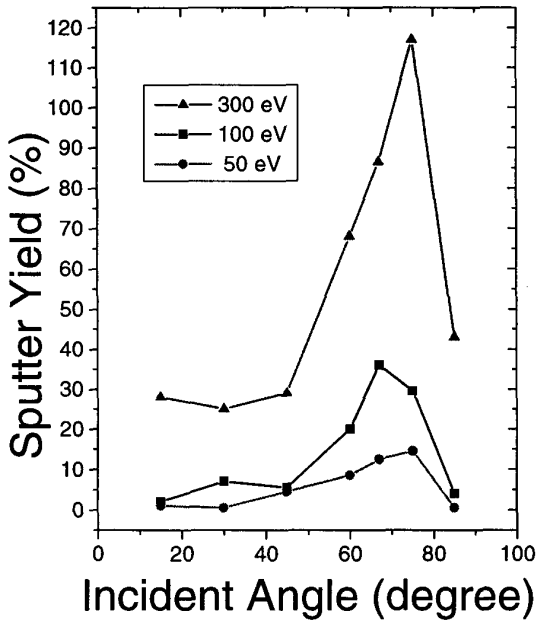

Fig 4. Sputter yield of Ar+ ion bombarded to SiO2 surface at 50, 100, 300 eV.

Future study should make sure that the systems reach a stage where the statistics of sputtered atoms and reflected atoms get convergent. We were not able to fully confirm this due to the amount of time the sputtering simulation needed. Previous study proclaimed that convergence was achieved by analyzing the surface structure [1]. However, we believe the convergence of the statistics can be more convincing although we could not carry out the full length of simulation to achieve rigorous convergence due to the fact that our simulation cell is much larger and the time of simulation being longer to finish the convergence test in time than previous studies [1]. It will be possible to improve the situation by employing dual time step molecular dynamics simulation and parallel processing.

IV. Conclusion

We have shown that a more mild approach to dissipate the heat generated by ion bombardment during molecular dynamics simulation could affect the sputter yield greatly by comparing with previous study. Since sputter yield can be obtained from molecular dynamics simulation, and can be directly used as valuable raw data to predict the surface evolution during plasma etching, it will be possible to predict more precisely how the surface evolves as a function of time during the etching process. It will be possible to design a process by fully exploiting this capability of construct delicate sub micron structures by carrying out simulation before hand. Therefore the fine adjustments in molecular dynamics simulation seems to have significant impact in the further development of surface evolution simulation studies.

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