3D Modeling of Sputter Process with Monte Carlo Method

Yongchan Ban and Taeyoung Won

Research Institute of Semiconductor and Thin Film Technology
School of Electrical and Computer Engineering, Inha University,
253 Yonghyun-Dong, Nam-Ku, Inchun, 402-751, KOREA
Tel: +82.32.860.7436 Fax: +82.32.862.1350
E-mail: ycban@hsel.emde.inha.ac.kr

Abstract

In this paper, a rigorous three-dimensional Monte Carlo calculation to simulate the sputter yield as a function of the incident ion energy and the incident angle as well as the atomic ejection distribution of the target is presented. The sputter yield of the target atom (Al and Cu) has been calculated for the different species of the incident atoms with the incident energy range of 10eV ~ 10KeV, which coincides with the previously reported experimental results.

1. Introduction

Since sputtering is a versatile and flexible method for the efficient deposition of a wide variety of materials, it has been widely used in semiconductor industries. In order to obtain an optimum sputtering condition for the VLSI process, we have to employ a physics-based model rather than using an analytic approach. Currently, there are a couple of numerical methods available for the simulation of sputtering process. One is the binary collision approximation (BCA) and the other is the molecular dynamics (MD) model. In this work, the BCA approach was chosen for the development of the sputtering simulator because the MD approach requires excessive CPU time in spite of its inherent accuracy. In this paper, a three-dimensional Monte Carlo calculation of the sputter yield with varying the energy and the angle of the incident ion is reported, which coincides with the experimental data [1].

2. Model of the Sputter Process

In Figure 1 is shown the schematic diagram describing the steps of the Monte Carlo calculation for the sputtering yield employed in the study. The species of the incident ion, the bombarding energy, and the incident angle should be provided at the input stage of the calculation. The material parameters are provided in the internal library of the simulator. The trajectories of the incident ions and the recoiled atoms are monitored during their slowing-down processes by comparing their energy with the predetermined lattice binding energy. The loss of energy of the particles was assumed to be due to the nuclear and electronic stopping process [2]. Since the nuclear and electronic stopping processes are assumed to have no correlation, the particles undergoing the nuclear collisions will lose discrete amount of energy, while the atoms under the electronic interactions will lose the continuous amount of energy.

Figure 2 shows the schematic diagram of the cascade process of the collision [3]. The primary knock-on atom (PKA) is represented by the label I, which is automatically augmented by 1 after each subsequent collision, whereas the secondary knock-on atom (SKA) succeeds the label index of the primary knock-on atom (PKA). In addition, if the current PKA is sputtered out of the target or the remaining energy of the PKA is less than the binding energy, the final recoiled atom will be regarded as new PKA with the label index of I. This new PKA will experience the recoil process in a similar manner to the previous PKA. When the label index I is equal to zero, the PKA means the ion repeating the above process.

3. Simulation Results

In Figure 3 are shown the calculated sputter yield distributions of the target atoms as a function of the incident energy in the case of normal incidence of argon and hydrogen, respectively. The solid line denotes the calculation and the experimental data are exhibited with triangles for comparison. As shown in Figure 3, the sputter yield increases with incident energy until the maximum yield is obtained. The incident energy of the heavy ion (Ar) for the maximum sputter yield is about 10KeV, while the maximum sputter yield is obtained for the incident hydrogen atom with energy of less than 1KeV. The reason for this reduction of the sputter yield seems to be due to the fact that the electronic energy loss which isn't happen a scattering event is larger than the nuclear energy loss while the mean flight path increases simultaneously in proportion to the amount of the incident energy. The calculated sputter yield shown in Figure 3 (c) and (d) appears comparatively low and the reason for this seems like the transferred energy to the target atom is relatively small in the case of the light ion such as hydrogen.

In Figure 4 is shown the sputter yield distribution of the target atoms as a function of the different incident angles for the Ar ion with fixed incident energy of 1KeV. As shown in Figure 4, the sputter yield increases with angle of incidence and seems to have the maximum value in the range of 60 ~ 80 degree, while it decreases rapidly for the larger angle due to the reflection of incident ions. Angular distributions of sputtered particles are interfaced with the deposition and etching simulator for the calculation of etching rate in the plasma chamber. Figure 5 shows the three-dimensional angular distributions of the sputtered particles. The X-Y plane represents a surface of sputter target. Figure 5 (a) and (b) reveals that the sputter yield in the direction normal to the surface seems to be negligible and have azimuthal symmetry. In the meanwhile, the number of sputtered atom will be relatively appreciable in the direction normal to the surface when the incident angle is around 60 degree.

4. Conclusions

A three-dimensional Monte Carlo calculation for the sputter process is reported in this paper. We calculated the sputter yield as a function of the incident ion energy and the incident angle, and simulated the atomic ejection distribution of the target. The sputter yield of the target atom (Al and Cu) has been calculated for the different species of the incident atoms with the incident energy range of 10eV ~ 10KeV, which coincides with the previously reported experimental results.

5. References

[1] Y. Yamamura et. al, "Energy Dependence of Ion-sputtering Yields from Monatomic Solids at Normal Incidence," Atomic Data and Nuclear Tables, vol. 62, pp.149, 1996.

[2] J. F. Ziegler et. al, "The Stopping and Range of Ions in Solids," vol. 1, New-York, Pergamon, 1985.

[3] J. P. Biersack, "Sputtering Studies with the Monte Carlo Program TRIM.SP," Appl. Phys. A 34, pp.73, 1984

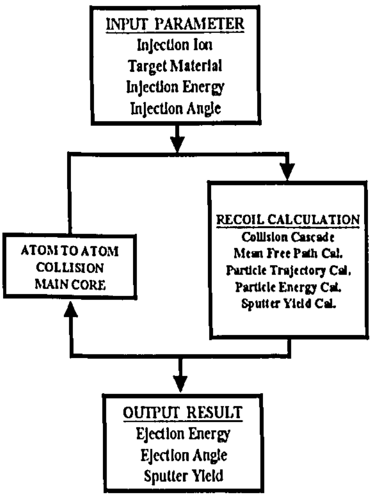


Figure 1: Calculation flow of the sputter simulation: The parameter of the ion and the target are set in input stage. Thereafter the atomic trajectory is calculated and a collision cascade is processed.

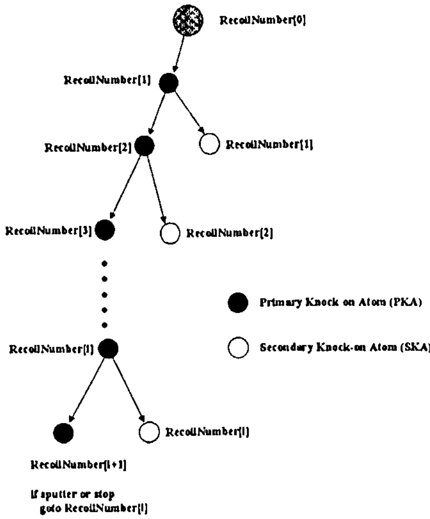
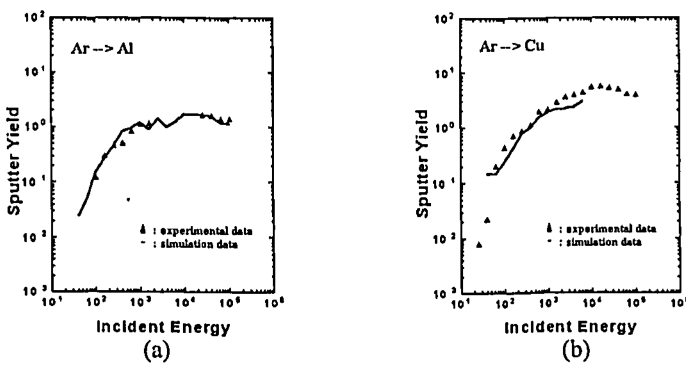


Figure 2: The schematic diagram of the collision cascade process shows that the primary knock-on atom marked by black circle(PKA) successively collides with the secondary knock-on atom marked by white circle(SKA) in the target.



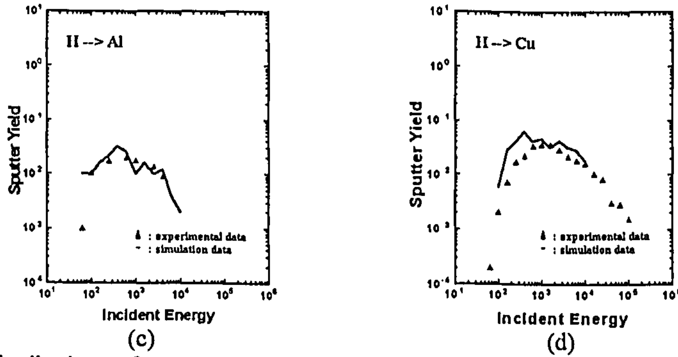


Figure 3: Distributions of sputter yield as a function of the incident energy [eV] of Ar, H at normal incidence. The incident energy of the heavy ion (Ar) for the maximum sputter yield is about 10KeV(a)(b), while the maximum sputter yield is obtained for the incident hydrogen atom with energy of less than 1KeV(c)(d).

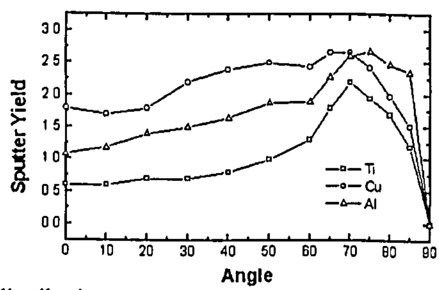


Figure 4: Sputter yield distributions as a function of the incident angle [degree] of Ar ion at 1KeV. The sputter yield increases with angle of incidence and seems to have the maximum value in the range of 60 ~ 80 degree, while it decreases rapidly for the larger angle due to the reflection of incident ions.

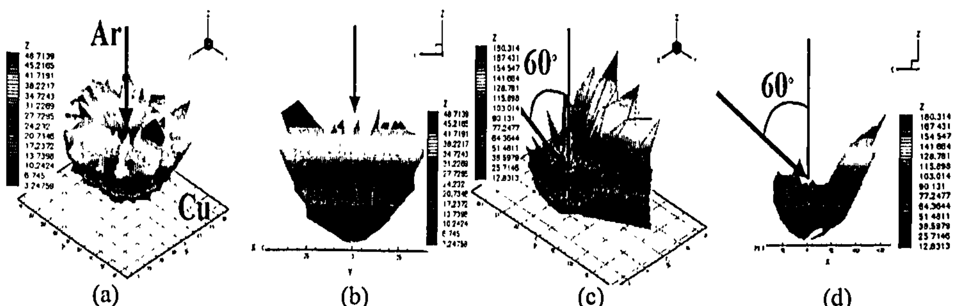


Figure 5: The bird's eyes view of three-dimensional angular distributions of target atoms for Ar ion with fixed incident energy of 1KeV: Figure (a) and (b) reveals that the sputter yield in the direction normal to the surface seems to be negligible and have azimuthal symmetry. In the meanwhile, the number of sputtered atom is relatively appreciable in the direction normal to the surface when the incident angle is around 60 degree.