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## **Molecular Dynamics and Monte-Carlo Simulation of Sputtering and Mixing by Ion Irradiation**

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### Abstract

Molecular dynamics (MD) and Monte-Carlo (MC) simulations of low-energy (<500eV) Ar ion irradiation on Si substrates were performed in order to investigate the mixing and sputtering effects. Both MD and MC simulation show similar results in sputtering yield, depth profile of projectile and mixing of substrate. For these incident energies, the depth of the mixed region is determined by the implant range of incident ions. For example, when the incident energy is 500eV, the Ar ions reach a depth of 40Å so that the Si atoms that reside shallower than 40Å are fully mixed at an ion dose of about  $5.0 \times 10^{16}$  atoms/cm<sup>2</sup>. The resolution of secondary ion mass spectrometry (SIMS) was also studied. It was found that the resolution of SIMS depends on the depth of mixing, which depends in turn on the implant range of the probe ions. This is because the mixing of substrate atoms occurs more frequently than sputtering, so that the information about the depth profile in the mixing region is disturbed.

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Keywords =Molecular dynamics simulation, Monte-Carlo simulation, SIMS resolution, ion mixing, sputtering

### Introduction

Secondary ion mass spectrometry (SIMS) is a useful technique to measure the depth profile of components in target materials [1]. Improving the resolution of SIMS analysis is required more and more recently because of the rapidly shrinking design rules in LSI fabrication. It is considered that the resolution of SIMS depends on the incident energy. In the collisional process of the probe atom, the incident atom induces a large number of collisions, so that the original distribution of substrate atoms is disturbed. With increasing incident energy, the disturbance of the original coordinates in the target becomes more frequent, and this causes a decrease in SIMS resolution. To perform high-resolution SIMS, it is necessary to use low-energy probe ions. However, as the incident energy decreases, it becomes difficult to obtain a sputtering yield which is sufficiently high for measurements. Therefore, the proper energy of the probe atom should be selected according to the required resolution. In this paper, the collisional processes of Ar atoms onto Si(001) substrate are simulated with both molecular dynamics (MD) and Monte-Carlo (MC) methods. The sputtering yield and the disturbance of delta-doped layer are compared. From these results, the dependence of SIMS resolution on the incident energy of probe ions will be discussed.

### Simulation details

In order to examine the mixing effects by ion beam irradiation, both molecular

dynamics (MD) and Monte-Carlo (MC) simulations of Ar ions impacting on Si substrates were performed. For MD simulation, the Stillinger-Weber model potential [2] was applied to the interaction between Si atoms and the Ziegler-Biersak-Littmark (ZBL) model potential [3] was applied to Si and Ar atoms. The ZBL model was also used in the TRIM calculation. The cut-off radius of Si-Ar interaction was set to 3.1Å, which corresponds to the mean bond length of Ar-Ar (in f.c.c. structure) and Si-Si (in diamond). A Si(001) substrate, which consists of 2048 Si atoms and has the dimensions of 20Å×20Å×90Å, was prepared as the target material. In the simulation, 500 Ar atoms were radiated on the substrate sequentially every 770fs with the impact point selected randomly on each impact. After irradiation with 500 Ar atoms, the corresponding dose of Ar ions was calculated to be  $1.25 \times 10^{16}$  atoms/cm<sup>2</sup>. The substrate temperature was kept at 300°C by applying the Langevin dynamics method to the half bottom part of the substrate.

The MC simulations were also performed using the TRIM Dynamics (T-DYN) code [4, 5], which is based on TC (TRIM-CASCADE) [6] and was improved to be able to follow all recoil atoms, primary knock-on atoms and secondary knock-on atoms in the same way as it would follow the incident ions. The target substrate has an area of  $1 \times 10^5$  Å<sup>2</sup> and a depth of 250Å. The parameters describing substrate property are set to:  $E_b$  (binding energy) = 2eV,  $E_{sb}$  (surface binding energy) = 3eV and  $E_d$  (displacement energy) = 3eV.

In both cases of MD and T-DYN simulation, Ar ions were radiated at normal incidence to the surface with energies of 100, 200 and 500eV. Si marker layers with thickness 2.5Å, which corresponds to two mono-layers of Si(001), were positioned at depths of 0Å, 10Å, 20Å and 40Å. The evolution of the mean depth and the deviation of each marker layer were examined in order to discuss the mixing effect by ion irradiation. The sputtered depth and the number of sputtered marker atoms provide the SIMS profile. From these SIMS profiles, the energy dependence of the SIMS resolution could be discussed.

### Results and discussion

Fig. 1 shows the energy dependence of the sputtering yield of Ar ions to Si(001) substrate calculated by both MD and T-DYN. For incident energies below 1keV, the sputtering yield rapidly decreases as the incident energy decreases. Fig. 2 shows the distribution of incident Ar ions by MD (Fig. 2a) and T-DYN (Fig. 2b). The mean implant depth and the deviation in each simulation are given in parentheses in the legends of Figs. 2a and 2b. From Fig. 1 and Fig. 2, both T-DYN and MD show similar sputtering yields and implant profiles in the incident energy range of 100eV to 500eV. These results indicate that the substrate property parameters for T-DYN are confirmed for these low energy ion impacts.

The evolution of the Si marker layer was investigated using the MD and MC methods. Fig. 3 shows snapshots of mixing by Ar ion with 500eV calculated by MD simulation. The atoms in the marker layer at 0Å, 20Å and 40Å are indicated as large circles and other substrate Si atoms are represented by small dots. On the other hand, the results by T-DYN calculations at 500eV Ar ion irradiation with an atomic dose of  $1.0 \times 10^{15}$  atoms/cm<sup>2</sup> (Fig. 4a) and  $1.0 \times 10^{16}$  atoms/cm<sup>2</sup> (Fig. 4b) are shown in Fig. 4. It is shown in both MD and T-DYN calculation that, as the ion dose increases, the surface marker at 0Å expands to a deeper region in the substrate, whereas the layer at 20Å expands isotropically, and the deeper layer at 40Å moves towards the surface to a

shallower region. At ion doses above  $1.0 \times 10^{16}$  atoms/cm<sup>2</sup>, these three markers show a similar profile in shape and the distribution of marker atoms is close to that of incident Ar atoms shown in Fig. 2.

Fig. 5 shows the dose dependence of the mean depth of each marker layer calculated by both MD and MC. The thick lines indicate the results by T-DYN calculation and symbols and error-bars are those obtained by MD calculation. The upper figures show the results with the dose ranging from 0 to  $1.4 \times 10^{16}$  atoms/cm<sup>2</sup>, and the lower ones show doses ranging to  $1.0 \times 10^{17}$  atoms/cm<sup>2</sup>. The transition of the surface level is calculated from the sputtering yield and is shown as thin lines. Both MD and T-DYN results show similar profiles for all marker layers. In the case of the irradiation with 100 and 200eV, the marker layer at 40Å does not extend, which is different from the case of 500eV. As the ion irradiation proceeds, the mean depth of each marker layer converges to the mean implant depth of the incident Ar atoms. Fig. 2 and 5 indicates close correlations between the implant depth and the mixing region. In the case of 200eV Ar ion irradiation, for example, the marker at 40Å moves rapidly towards the surface when the atomic dose is above  $3.0 \times 10^{16}$  atoms/cm<sup>2</sup>. This is because, as the sputtering proceeds, the depth of the marker at 40Å becomes more and more shallow. The sputtered depth at  $3.0 \times 10^{16}$  atoms/cm<sup>2</sup> is calculated to be 8.2Å, and thus the thickness of the mixing region could be estimated to be about 30Å ( $\approx 40\text{Å} - 8.2\text{Å}$ ). This thickness corresponds to the implant range of Ar ions with 200eV, which in turn is calculated to be 28.1Å by the formula ( $15.5\text{Å}$  (mean depth) +  $2 \times 6.3\text{Å}$  (the deviation)). These results suggest that, with these low-energy ion implantations, the mixing of the implant region occurs faster than surface sputtering.

From the sputtering yield and the number of sputtered marker atoms, T-DYN simulations provide the SIMS response functions for the delta-doped marker layer. Fig. 6 shows the SIMS response functions by Ar ions accelerated with 100, 200 and 500eV. In all figures the dashed and dotted lines indicate the responses from the markers at 20Å and 40Å, respectively. The solid-thick line is the sum of the two response lines in each figure, and is expected to represent a SIMS profile in real experiments. In any case, the signal from the marker at 20Å is detected at a lower dose than that expected from the sputtering yield, because of mixing of the surface region. In the case of 500eV, the signal from 40Å is also detected at the sputter depth of 3Å. This result means that both marker layers are mixed fully, as shown in Figs. 3, 4 and 5. As the incidence energy decreases, the penetration depth and the thickness of the mixed region are reduced. In the cases of 100 and 200eV of incident energy, the total signal shows two peaks, which can be divided into 2 different signals. Comparing the profiles at these incident energies, the signal from 20Å starts to increase at the sputtered depth of 0Å in both cases, whereas the signal from 40Å is detected at 14Å for 100eV and at 8Å for 200eV. This result indicates that the thickness of the mixing layer is 26Å for 100eV and 32Å for 200eV, which agrees with the results shown in Fig. 5. It is assumed that the resolution of SIMS measurement equals the thickness of mixing depth and also the implant range of probe ions.

### Conclusions

The evolutions of marker layers in a Si substrate by sequential Ar ion radiations were investigated using the MD and MC methods. Both types of simulation show results consistent with each other in regard with sputtering yield, implant profile and mixing phenomena. At an incident energy of 500eV, the surface region shallower than 40Å is

mixed, so that the marker layer at 20Å extends itself isotropically, whereas the marker at 40Å goes up to a shallower region. The SIMS resolution depends on the depth of the mixed region and therefore depends on the incident energy of probe ion. From the T-DYN calculation, it was found that the energy of 200eV, at which the Ar probe ion gives about 30Å of implant and mixing range, is the highest energy to resolve the marker separated with 20Å by SIMS analysis. As the incident energy decreases, the implant and mixing ranges are reduced, and the resolution is expected to improve further.

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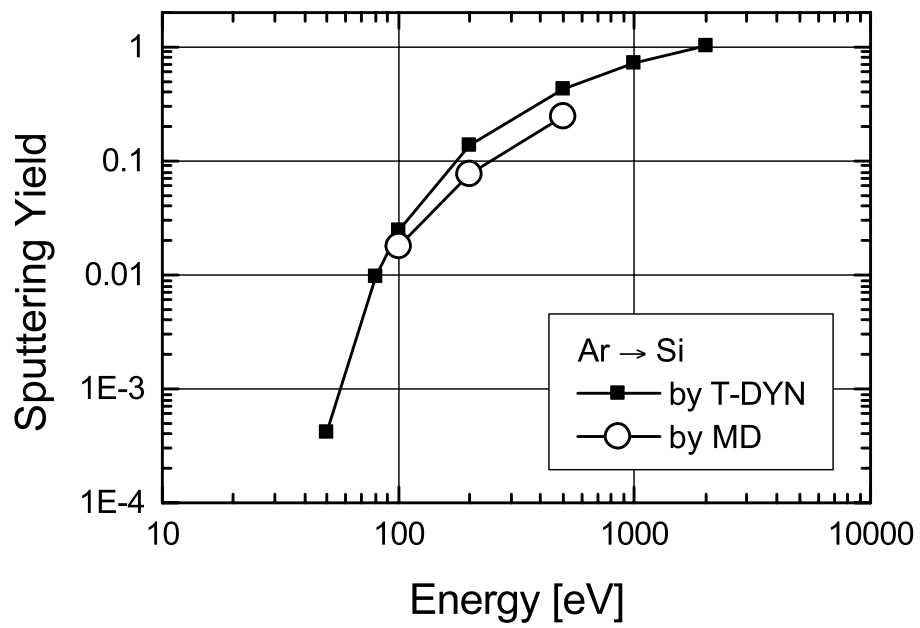


Fig. 1: Incident energy dependence of Si sputtering yield calculated by MD and T-DYN.

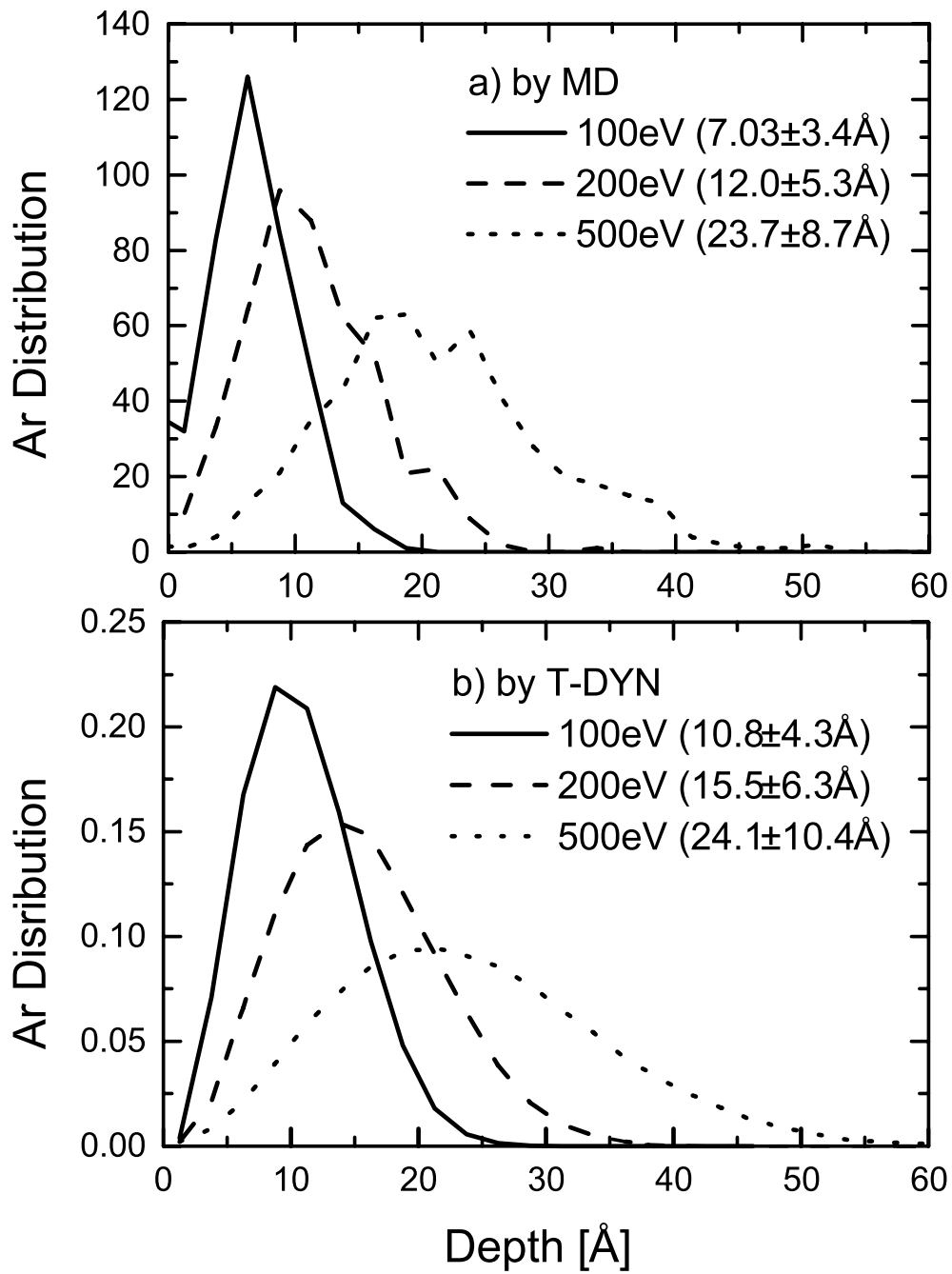


Fig. 2: Depth profile of implanted Ar ions calculated by MD (upper, a) and T-DYN (lower, b)

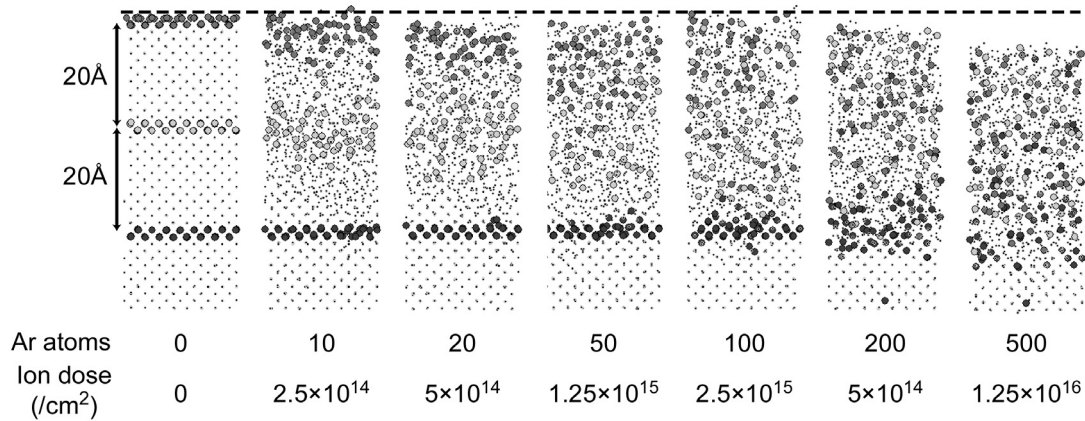


Fig. 3: Snapshots of the mixing of Si substrate by Ar irradiation with 500eV/atom, calculated by MD. Large circles represent the marker Si atoms, which are initially positioned at 0Å, 20Å and 40Å

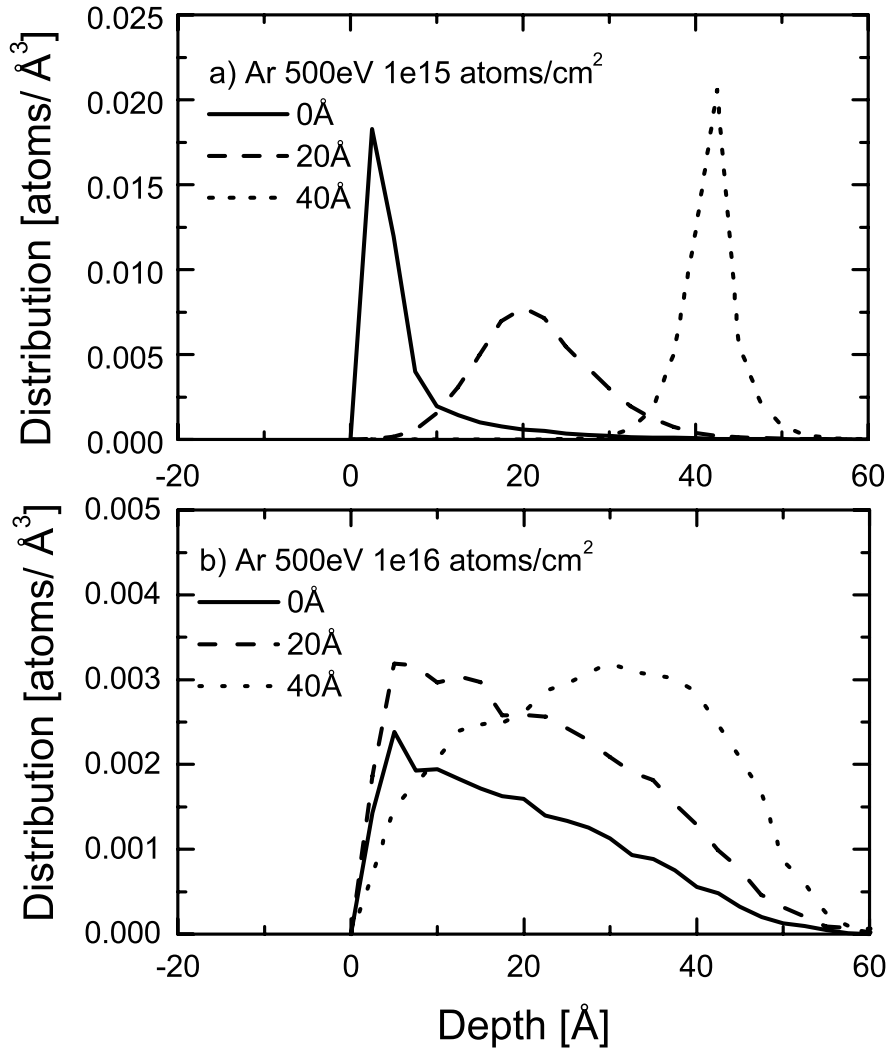


Fig. 4: Distribution of marker atoms calculated by T-DYN. The incident energy is 500eV and the atomic dose is (a)  $1.0 \times 10^{15}/\text{cm}^2$  and (b)  $1.0 \times 10^{16}/\text{cm}^2$ .



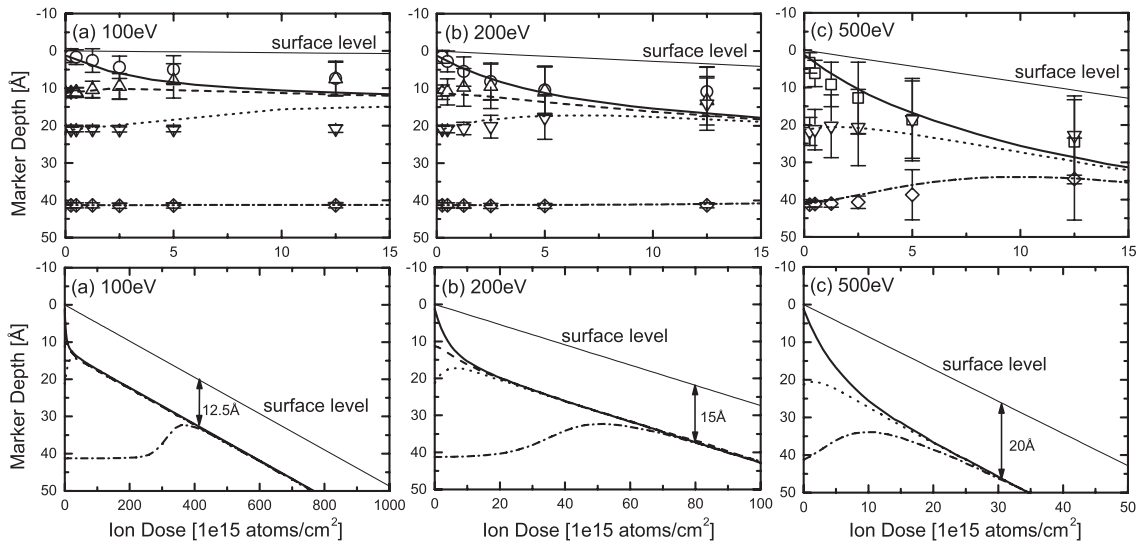


Fig. 5: Ion dose dependence of the mean depth of marker atoms with sequential Ar impacts with (a) 100eV, (b) 200eV and (c) 500eV. Lines and symbols represent the results by T-DYN and MD, respectively. The dose dependence of the sputtered depth is shown with thin line.

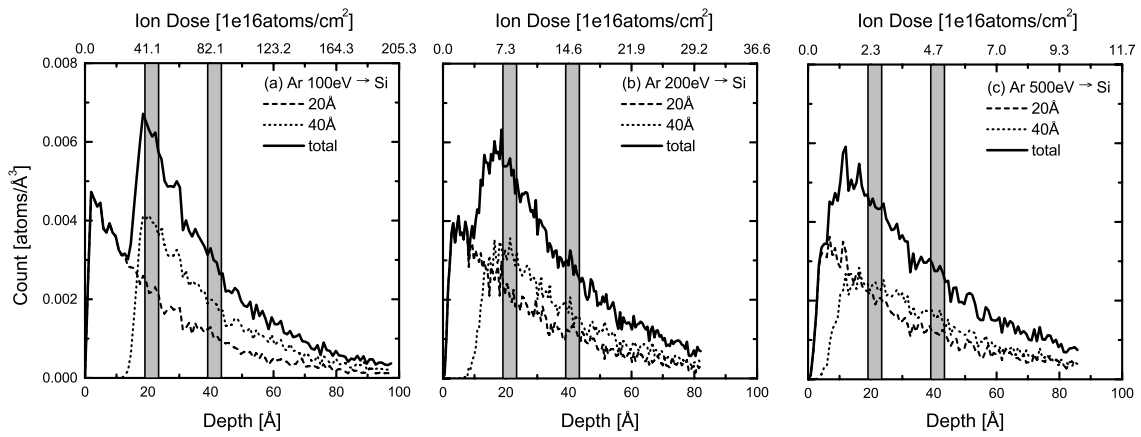


Fig. 6: SIMS response profile of two marker layers calculated by T-DYN. The incident energy is (a) 100eV, (b) 200eV and (c) 500eV.