Simulation of Secondary Ion Mass Spectrometry for Steep Dopant Distribution Profiling

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Abstract – This paper describes Monte Carlo simulations of Secondary Ion Mass Spectrometry (SIMS) depth profiling for steep dopant distribution to evaluate quantitative differences between the measured and actual profiles. SIMS measurement data for steep dopant distribution profiles inherently show some broadening due to, for instance, recoiling effects. The simulation procedure was based on a binary-collision approximation Monte Carlo ion implantation simulation with consideration of density modification and surface recession. Calculation of secondary emission-count reproduced actual SIMS measurement profiles quite well. With a help of a statistical enhancement technique, a resolution function can be calculated for retrieving an actual profile from the measured one with the deconvolution method.

I. INTRODUCTION

Secondary ion mass spectrometry (SIMS) is one of the most commonly used techniques for dopant profiling. Recent device structure requires critical impurity distributions which are not only shallow but also steep. Moreover, modern process simulators have been continuously improved by modification of their process models such as ion implantation and dopant diffusion models. Accuracy of such simulators and simulation model parameters have often been checked and been extracted by comparing them with SIMS data. It is very important to keep in mind that the SIMS limited depth resolution plays a major role in the analysis of shallow and/or steep dopant distribution profiles. This paper describes Monte Carlo simulations of SIMS depth profiling for steep dopant distribution to evaluate quantitative differences between the measured and actual profiles.

II. MODELING

Figure 1 shows our experimental data for the two types of different SIMS measurements for one of the low-energy arsenic implantation profile.

Since the modern SIMS instruments avoid the signal from the crater edge[1], the most important factors for the depth-resolution deterioration are the inherent knock-on effects, i.e., the relocation of the impurity atoms. Previous Monte Carlo sputtering simulations, such as the TRIM.SP[2], are not suitable for this purpose because the atoms which are not energetic enough for ejecting from the surface are often neglected. We have therefore extended our own Monte Carlo ion-implantation simulation code[3] to calculate all recoiled atoms in the collision cascade and calculate secondary atom ejection from the sputtered surface. Furthermore, dynamic changes of the atom density and surface position were also taken into account. Calculations were performed in one-dimension. The actual SIMS

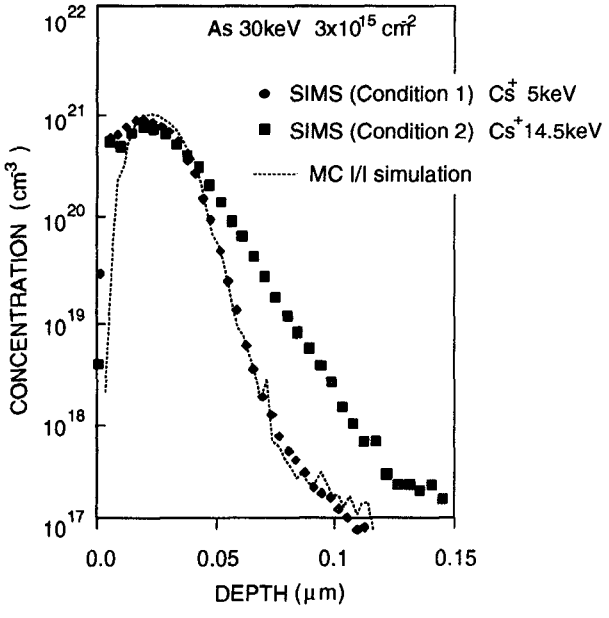

Fig. 1: Experimental arsenic distribution profile data for the two different types of the SIMS measurement conditions. The dashed line shows the calculation result of the MC ion implantation simulation.

Table 1: Different SIMS measurement conditions. (Quadrupole: PHI-6650, Magnetic-sector: CAMECA-ims-3f).

	Condition 1	Condition 2
SIMS	Quadrupole	Magnetic-sector
Primary ion	Cs^+	Cs^+
Energy	5.0keV	14.5keV
Incident angle	60°	24.5°
Ion flux	$5.4 \times 10^{15} cm^{-2}/sec$	$1 \times 10^{15} cm^{-2}/sec$
Sputtering rate	0.6nm/sec	0.58nm/sec

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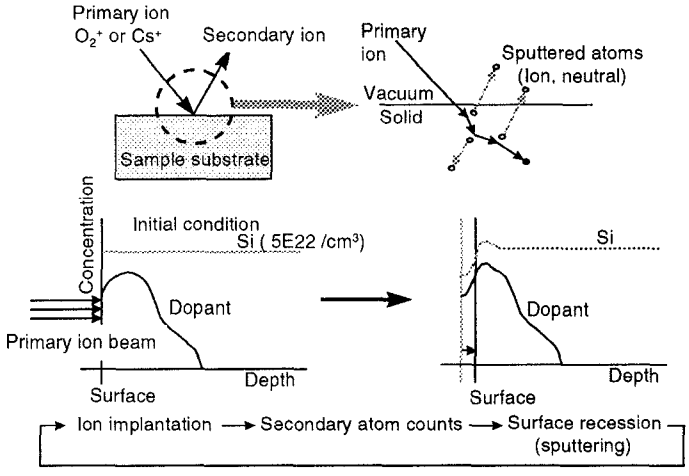

Fig. 2: SIMS simulation procedure.

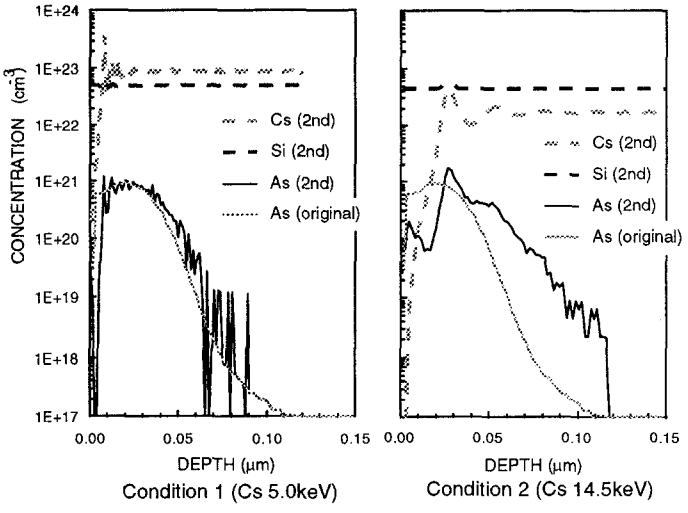

Fig. 3: Calculation results for secondary atom concentration of SIMS measurement. The calculation result of condition 2 shows unexpected oscillation.

measurement time period was divided into small time steps Δt. In each time step the primary ion (Cs^+ or O_2^+) implantation was calculated considering full recoil cascade and the secondary atom ejection from the surface. The energy value of 12.5eV was used for the recoil atom threshold. A recombination radius was introduced for the pair of recoil cascade atom and vacancy to avoid producing unrealistic super-dense region near the silicon substrate surface. The numbers of the secondary atoms correspond to the actual SIMS measurement data. Then, the substrate composition and density changes were recorded and surface position was moved according to the given sputter rate. These procedures were iterated until the calculation depth reached its desired value.

III. RESULTS AND DISCUSSION

A. SIMS simulation

A starting original profile was chosen as the quadrupole SIMS data which agree with the MC ion implantation simulation result (Fig. 1). The quadrupole SIMS (condition 1 in Table 1) data gave a good depth resolution and the SIMS simulation could reproduce the data quite well. In the case of the Cs^+ 14.5keV (condition 2), however, calculated Cs and Si atomic density profiles in the early stage were far from the equilibrium as shown in Fig. 3. This is due to the constant sputter-rate assumption in this calculation scheme. Therefore, the pre-calculation was performed until the system reaches its steady-state. Then, for the impurity distribution profiling, this quasi-steady state density profiles were used for the initial condition of the substrate to obtain the smooth secondary atom profiles for the impurity distributions as shown in Fig. 4.

In this case, the calculated profile shows an artificial shift due to the skipping of detailed initial nonequilibrium state calculation. The shift, however, could be estimated by converting the initially assumed Cs^+ dose amount in the substrate to the depth scale by using the sputter-rate and the primary beam current. The shift amount is somewhat changed by the surface roughness treatment in this calculation.

The resulting calculation profiles could reproduce the Cs^+ 14.5keV SIMS measurements (condition 2) quite well for the as-implanted arsenic profile (Fig. 5(a)). The SIMS measurement for the different type of the profile such as the profile after diffusion could also be reproduced by the calculation as shown in Fig. 5(b). Since this simulation is based on the Monte Carlo

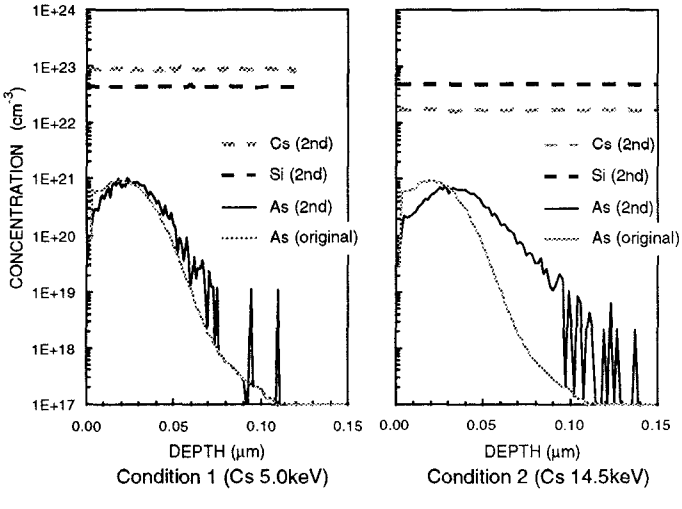

Fig. 4: Calculation results for secondary atom concentration of SIMS measurement using quasi-steady-state initial conditions. Smooth profiles were obtained for both SIMS conditions (except for the Monte Carlo statistical noise).

method, a large amount of the calculation time is necessary. For example, in the case of Fig. 4, the calculation time for the condition 1 was 1312 seconds, for the condition 2 was 4548 seconds, by using the 8 processor units of the parallel computer called Cenju-3(NEC). Moreover, due to the limited sampling ion numbers, the calculated profiles have some noise in the tail region as shown in Fig.4. Therefore, an efficient statistical enhancement technique was applied to the calculation procedure to obtain smooth and wide range solutions without significant computation time increase as described in the next section.

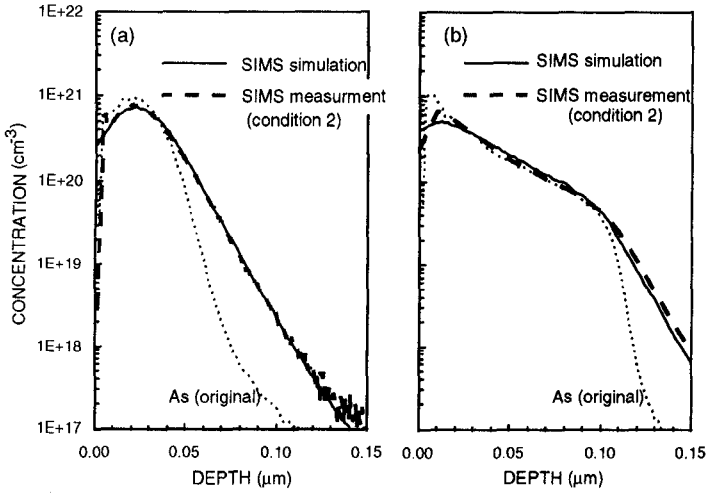

Fig. 5: Comparison between calculated secondary atom counts and actual SIMS measurement data. Calculation data were shifted toward the surface according to the quasi-steady state initial condition. (a) Profiles after ion implantation. (b) Profiles after diffusion (850℃, 4 hours). A statistical enhancement technique was applied for the SIMS simulation.

B. Statistical enhancement and resolution function

One of the important objectives of the SIMS simulation is to retrieve a true profile from a measured one. This could be achieved if one could obtain an appropriate resolution function $R(x)$ of the SIMS system.

The resolution function was calculated by performing the SIMS simulation for the virtual delta-dope layer. A statistical enhancement technique for this calculation was developed using the observation in which the low concentration impurity does not have any significant effect on the silicon and primary ion profiles in the substrate. The probability of the collision event for impurity atoms was statistically enhanced by the local atomic composition ratio of the impurity atom in the substrate where the sampling-ion weight was reduced by the reciprocal composition ratio. The resulting secondary ion count profiles became sufficiently smooth as shown in the Fig.6 at the expense of only 2.8 times larger computation time. Without this

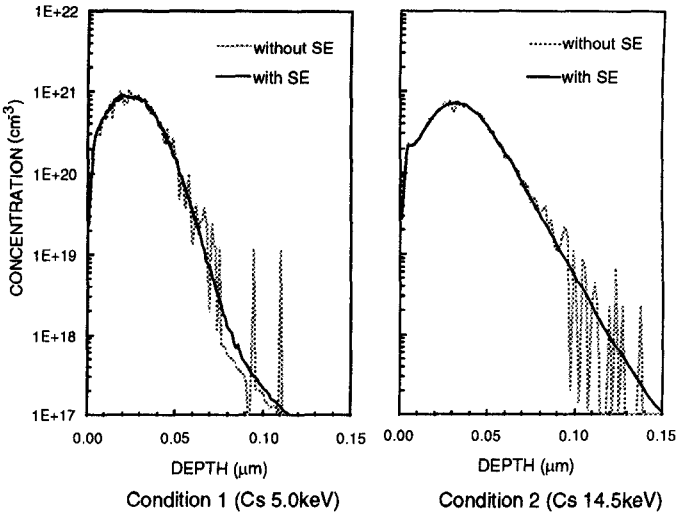

Fig. 6: Calculation results of the secondary atom counts with/without a statistical enhancement (SE) technique.

statistical enhancement technique, it is almost impractical to calculate the SIMS profiling response for a delta-dope distribution profile with limited sampling numbers. Fig. 8 shows the calculation result for the SIMS profiling response for the arsenic virtual delta-dope distribution with the statistical enhancement technique. Smooth shape and sufficient dynamic range were obtained within a reasonable computation time. Calculated resolution function tail region can be approximated by the exponential decay function $\exp(-x/L)$. The decay length L was found to be approximately 10.5nm for the case of Fig. 8.

When this result was used as the resolution function $R(x)$, an approximated true profile $C_{true}(x)$ could be retrieved by the deconvolution of the integral (1)[4]:

$$I(x) = \int_{-\infty}^{\infty} C_{true}(\xi) R(x - \xi) d\xi \qquad (1)$$

where $I(x)$ represents the SIMS measured profile. Several methods have been proposed for this deconvolution of the con-

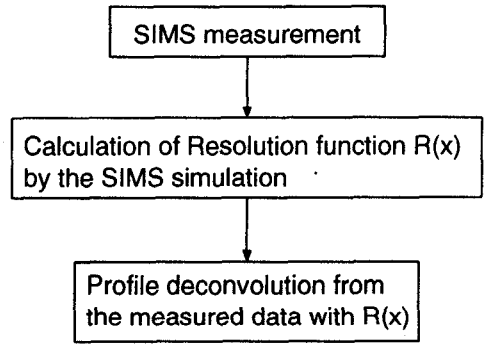

Fig. 7: Procedure for the profile retrieve by deconvolution with calculated resolution function.

volution integral (1). For example, if the SIMS measurement profile was smooth enough, a simple iteration (2)[5] would have become convenient approach.

$$C^n(x) = C^{n-1}(x) + I(x) - \int_{-\infty}^{\infty} C^{n-1}(\xi)R(x-\xi)d\xi \quad (2)$$

where, n represents iteration-stage number. Fig. 9 shows the deconvolution result for the implanted arsenic SIMS measurement profile of condition 2. In this cases, the SIMS measurement profile was noisy and needed to be smoothed out prior to the deconvolution procedure. The deconvolved profile in Fig. 9 shows still some noise in the tail region. The maximizing entropy concept[6] might play a better role for avoiding such a noise and smoothing error.

This procedure shown in Fig.7 is useful for the correct analysis of diffusion amount in the SIMS data for critical doping profiles where the dopant distributions are steep and/or shallow such as the doping-super-lattice experiments for the transient enhanced diffusion characterization.

IV. CONCLUSION

Based on the Monte Carlo atomic full-cascade collision calculation, SIMS profiling simulation was performed for characterizing steep dopant distribution profiles. The results are useful in evaluating appropriate conditions for the SIMS measurement and to improve the pre-existing SIMS measurement data by the deconvolution with the resolution function which can be calculated by using this simulation.

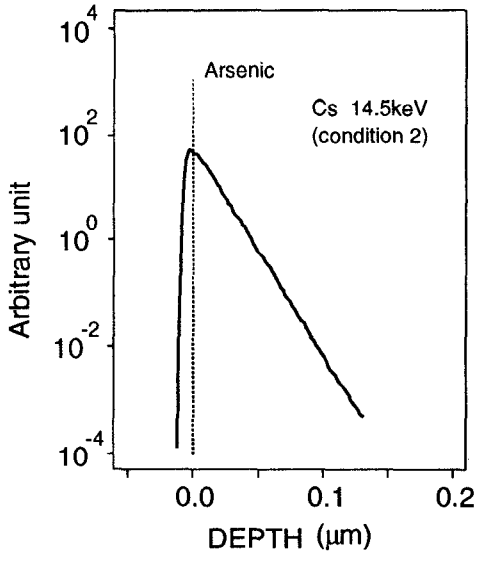

Fig. 8: SIMS simulation result for the virtual delta dope profile. Thick solid line: calculated resolution function. Broken line: initial delta dope profile. Dopant: Arsenic. SIMS condition 2. A statistical enhancement technique was applied to obtain a smooth and wide-range profile with a reasonable computation time (about 1 hour by Cenju-3(NEC) using 16 processor units.)

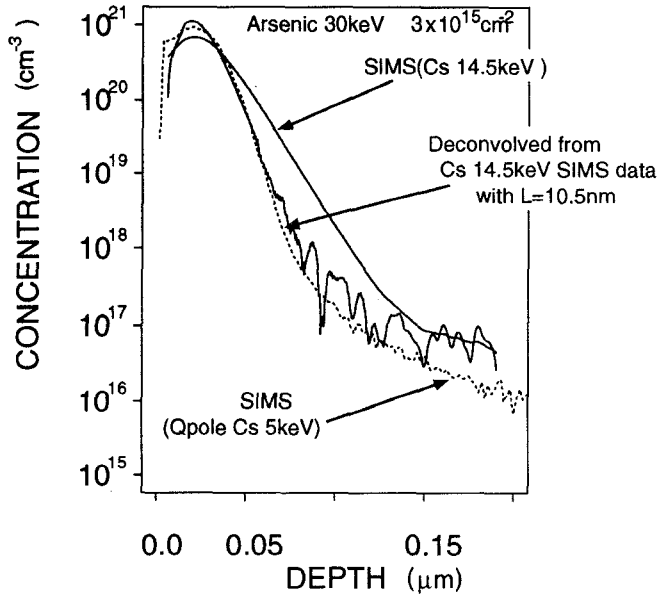

Fig. 9: Deconvolution results for the SIMS measurement data of the implanted arsenic distribution profile.

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