Study on Sputtering Mechanism of Shave-off Profiling*

Makiko Fujii†
Institute of Industrial Science, The University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8505, Japan

Masashi Nojima
Research Institute of Science and Technology, Tokyo University of Science, 2641 Yamazaki, Noda, Chiba 278-8510, Japan

Masanori Owari
Institute of Industrial Science, The University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8505, Japan and Environmental Science Center, the University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

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Shave-off profiling with nano-beam SIMS achieves the highly precise depth profiling with nanometer-scaled depth resolution by utilizing FIB micro-machining process to provide depth profile. This method is very unique depth profiling for acquiring a depth profile by shave-off scanning mode (A fast horizontal sweep of FIB is combined with the very slow vertical sweep). Shave-off profiling has its own features; absolute depth scale, pin point depth profiling and application for rough surface and/or hetero interface. However, the discussion of the sputtering mechanism in shave-off profiling is still insufficient because shave-off scanning mode has distinctive position of the primary ion beam against the sample. In this study, we discussed the difference of sputtering mechanism between shave-off scan and conventional raster scan from the view point of sputtered atom yields of experimental results and calculation results. In addition, the molecular dynamics (MD) simulation under shave-off condition is improved in order to visualize the sputtering mechanism of shave-off profiling. As a result, ‘shave-off sputtered atom yield’ is rather high compared to conventional sputtered atom yield according to distinctive sputtering mechanism of shave-off scanning mode. [DOI: 10.1380/ejssnt.2011.386]

Keywords: Secondary ion mass spectroscopy; Sputtering; Ion bombardment; Ion-solid interactions; Molecular dynamics; Shave-off profiling

I. INTRODUCTION

In recent years, the establishment of local part analysis in a limited area is aspired for semiconductor and electronic device industry. We have been developing shave-off profiling with the nano-beam secondary ion mass spectrometer (nano-beam SIMS), one of the powerful methods that can be applied for analyzing such materials and devices [1]. Shave-off profiling achieves the highly precise depth profiling with nanometer-scaled depth resolution by utilizing a Focused Ion Beam (FIB) micro-machining process to provide depth profile. In our previous studies, we obtained highly precise depth profiles of real-world samples [2–4]. In addition, shave-off scanning mode has been applied for low damage section processing to realize the highly accurate three-dimensional microanalysis [5].

However, the discussion of sputtering mechanism in shave-off profiling is still insufficient because shave-off scanning mode has distinctive position of primary ion beam against sample. In this study, we investigate the difference of sputtering mechanism between shave-off scan and conventional raster scan from the view point of sputtered atom yield using experimental results and calculation results.

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†Corresponding author: m-fujii@iis.u-tokyo.ac.jp

II. EXPERIMENTAL

A. Sputtered atom yield

The sputtered atom yield is generally assumed as the number of the sputtered atoms against the number of the irradiated primary ions, or for practical reasons it can be expressed in \( \mu \text{g} / \mu \text{C} \). The relation between the atomic sputtering efficiency and the practical unit is specifically written in elsewhere [6]. There are two conventional methods widely used to determine the sputtered atom yield. One is the experimental method that uses some kinds of

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FIG. 1: Schematic image of shave-off scan mode.
FIG. 2: The image of atomic initial position after equilibration. The pink sphere represents Ga ion moving toward the surface with 24 keV of kinetic energy. The purple spheres represent Al atoms temperature-controlled at 0 K. The blue spheres represent Al at 300 K. The light blue spheres represent Al atoms with no temperature control.

TABLE I: Estimated depth resolution of obtained shave-off profiles.

| Composition of Sample | Target Ion | Al⁺ | Si⁺ |
|-----------------------|-----------|-----|-----|
| Depth Resolution      | 1.0 nm/s  | 29  | 48  |
|                       | 4.0 nm/s  | 24  | 34  |

On the other hand, 'shave-off sputtered atom yield', we newly proposed, is essentially different from the general sputtered atom yield because of the distinctive position of primary ion beam against sample. 'Shave-off sputtered atom yield' relies on the elemental composition of only Z direction of the sample. Because the FIB is moving into depth direction at the constant speed and the sample is completely shaved off, the difference of sputtered atom yield of individual atoms composing the sample is needless to consider in the shave-off profiling. Therefore, only one 'shave-off sputtered atom yield' can be determined at every sample even if the sample is compound or mixture. In addition, it is unnecessary to estimate the sputtered volume using total amount of beam current. The other is the computer calculation method, i.e. Monte-Carlo simulation [7].

In this study, we estimate the 'shave-off sputtered atom yield' by combining the experimental and new calculation methods following below.

B. Shave-off profiling

Shave-off profiling with nano-beam SIMS has been developed for nano-dimensional analysis [9]. Primary ions of this apparatus are field-emitted Ga⁺ focused ion beam (Ga-FIB) with 30 keV accelerated energy and about 35 pA beam current. The beam diameter is about 40 nm in FWHM in this condition. The mass analyzer is a modified Mattaugh-Herzog type originally equipped with a spark source mass spectograph (JEOL JMS01BM).

In order to obtain the amount of beam exposure to sample, the measurements with different scanning speed were carried out. The relationship between beam exposure and scanning speed was explained in detail elsewhere [10]. Here, shave-off parameter $\alpha$ is considered briefly. $\alpha$ is a parameter indicating a position of intensity profile of primary ion beam where the sample is shaved off completely. In other words, $\alpha$ expresses the amount of beam exposing to sample in the unit time. This value can be determined from the depth resolution of experimental profiles obtained by changing the scan speed toward depth direction.

The samples were multi-layer thin film (Al 1 µm / SiO₂ 0.8 µm / Si Substrate). They were prepared using FIB micro-machining technique. The size of the thinned sample was 6.5 µm in width, 1 µm in thickness and 6 µm in height. A protection film of carbon of about 0.3 µm thickness was deposited on the sidewall of the sample in order to protect the sample from damage by the long tail of FIB during the shave-off profiling.
TABLE II: Comparison of sputtered atom yields in shave-off scan mode and conventional raster scan mode.

| Material | Sputtered Atom Yield \([\mu m^3/nC]\) |
|----------|----------------------------------------|
|          | Shave-off Method | Average of experimental method \([6]\) | Computer Calculation Method (SRIM) \([6]\) |
| Al       | 0.38            | 0.29                                    | 0.44                                    |
| Si       | 0.90            | 0.24                                    | 0.35                                    |

C. Estimation of ‘shave-off sputtered atom yield’

In our previous work, the intensity profile of FIB, as the primary ion beam of nano-beam SIMS apparatus, was estimated by simulation method \([10]\). The estimated intensity profile of our FIB under the practical experimental condition was the convolution of Gaussian 30 nm FWHM with Lorenzian 15 nm FWHM. The amount of beam exposure to sample was calculated using this intensity profile of the beam. Then the value of \(\alpha\) was determined by depth resolution of the obtained shave-off profiles. The volume of the sputtered sample during the shave-off profiling was determined clearly as mentioned above. Specifically, the shaved off volume of the thinned sample prepared using FIB micro-machining technique is equal with the volume of the sputtered sample. Then, the ‘shave-off sputtered atom yield’ was estimated using these values.

D. Molecular dynamics simulation under shave-off condition

Molecular Dynamics (MD) simulation is widely used to demonstrate the interaction between incoming particle and surface \([11]\). In this study, for visualizing the sputtering mechanism under shave-off condition, MD simulation was performed. Al (110) substrate, which consists of 3456 atoms, was prepared as the sample. Figure 2 shows the atomic initial positions. Ga ion with energy of 24 keV was radiated to the sample after sufficient equilibration. The velocities of Ga into \(X\) and \(Y\) direction were determined according to Maxwellian distribution with 300 K. In order to demonstrate shave-off condition, periodic boundary condition was only used in \(Y\) direction. In addition, temperature-controlled layers were set as shown in Fig. 2 to prevent from overheat. Morse potential was applied to the interaction of Al-Al and Al-Ga. Coulomb potential was also applied to between Al and Ga atoms. The impact point was selected randomly within the range of two atomic layer of \(X\) direction of the sample. In order to obtain the tendency about sputtering, we ran the calculation with 100 different aiming points and observed sputtered surface for 65.3 fs after bombardment.

III. RESULTS AND DISCUSSION

Figures 3(A) and (B) show the leading edges of obtained shave-off profiles of Al\(^{+}\) and Si\(^{+}\), respectively. In order to estimate the value of \(\alpha\), the measurements were carried out under scanning speed toward depth direction of 1.0 nm/s and 4.0 nm/s. Under the condition of fast scan speed, large amount of beam exposure in the unit time is needed to sputter the sample completely. Therefore, the value of \(\alpha\) becomes smaller, or draws near to the center of beam. At the same time, the influence of the long tail of FIB becomes smaller and the depth resolution becomes higher. The estimated depth resolutions are listed in Table I. The estimated ‘shave-off sputtered atom yield’ is shown in Table II. The sputtered atom yields of Al and Si in conventional raster scan determined using both experimental and calculation method by Mulders et al. \([6]\] are also listed in Table II. These results indicate that the ‘shave-off sputtered atom yield’ is, on the whole, high compared with general sputtered atom yield. This might be explained by the edge effect. In the shave-off condition, a surface of the sample was shaved off completely by the beam and the ‘new’ surface with the high sputtering rate is generated simultaneously. However, in general, the sputtered atom yield slightly changes with the tilt angle and they have a possibility to interchange. On the other hand, it was indicated that the value of ‘shave-off sputtered atom yield’ has different tendency against conventional value between Al and Si. This result suggests that shave-off scan has different sputtering mechanism from that of conventional raster scan. Figure 4 shows the result of MD simulation indicating 45.3 fs after Ga irradiation demonstrated using MD simulation.

TABLE III: Result of MD calculation. The average number of sputtered atoms obtained by 100 different aiming points.

| The number of ejected atoms \([atoms/ion]\) | X-Y surface | Y-Z section | Total   |
|------------------------------------------|-------------|-------------|---------|
| 1.36                                     | 1.90        | 3.26        |         |
that the sputtered atoms were ejected from both \(X-Y\) surface and \(Y-Z\) section. Table III shows the number of the sputtered atoms ejected from \(X-Y\) surface and \(Y-Z\) section obtained by the MD calculation with 100 different aiming points. This result indicates that the ejection from \(Y-Z\) section has a little superiority to that from \(X-Y\) surface. Moreover, the estimated sputtered atom yield of 3.26 atoms/ion can be calculated to 0.34 \(\mu\)m\(^3\)/nC. It accords well with the experimental result.

**IV. CONCLUSIONS**

In order to discuss the difference of sputtering mechanism between shave-off scan mode and conventional raster scan mode, we estimated the ‘shave-off sputtered atom yield’ using new method combining experimental and calculation method. Then, we compared estimated ‘shave-off sputtered atom yield’ with the conventional sputtered atom yield. In addition, MD simulation was improved to be applied to shave-off scanning mode to confirm that the sputtering occurred in both the surface and shaved off section. As a result, ‘shave-off sputtered atom yield’ is rather high compared to conventional sputtered atom yield according to distinctive sputtering mechanism of shave-off scanning mode.

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