Emission Trajectory Calculation of Ions from the Shave-off Cross Section for Realization of 3D Shave-off Method*

Yuto Takagi†
School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
and
Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

So-Hee Kang, Kohei Matsumura, and Takeki Azuma
Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

Bunbunoshin Tomiyasu and 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

(Received 12 January 2018; Accepted 16 June 2018; Published 14 July 2018)

Secondary ion mass spectrometry can analyze all elements and has high versatility. In our laboratory, we have established a method of sputtering the whole sample from the side by using partial primary beam called Shave-off method, which increases spatial resolution and eliminates an effect originated by surface roughness. Furthermore, designing the ion optics that can enlarge and converge the emitted secondary ions from the cross section of the micro sample on the detector, high-precision three-dimensional distribution data with surface resolution of several nanometer level and depth direction resolution of several tens of nanometer level can be obtained at high speed. However, the secondary ions trajectory and the ion aberration caused by the lens in the Shave-off condition have not been verified. In this study, we have constructed a simulation of calculating the trajectory of emitted ions from the Shave-off cross section. It is expected that the simulation will be of great help and powerful tool for future development. [DOI: 10.1380/ejssnt.2018.324]

Keywords: Secondary ion; Mass spectrometry; Ion trajectory; Lens; Focused ion beam

I. INTRODUCTION

Observation and measurement inside the solid samples are required for design and evaluation in high technology fields such as advanced batteries, carbon fibers, electrical and electronic information engineering technologies, and biomaterials [1]. Conventional analysis methods, for example, X-ray CT method can obtain three-dimensional image in a short time, but the spatial resolution is not sufficient due to the limited X-ray focusing diameter to micrometer order. One of CT methods, TEM-CT method has a high spatial resolution but cannot analyze translucent samples. Although confocal microscope is also often used, spatial resolution depends on the wavelength used in measurement, and samples without light transmission cannot be measured.

On the other hand, secondary ion mass spectrometry (SIMS) is highly sensitive method due to its destructive analysis and can be applied to all elements measurement. It is highly versatile as an analytical method. Owing to its high sensitivity, SIMS has been used to analyze the distribution of dopants in semiconductors [2], the elemental distribution of active materials in electrodes of batteries [3] and environmental particles such as PM2.5 [4]. Also, it has been used to analyze invaluable samples such as the particles brought from the asteroid, Itokawa by Hayabusa [5, 6]. However, its resolution depends on the primary beam diameter and there is a problem that as we analyze to inside of the samples, the spatial resolution decreases due to its surface roughness and mixing effect caused by collision cascade.

In our laboratory, a method of sputtering the whole sample from the side by using partial primary beam called Shave-off method have been established, which increases spatial resolution and eliminates an effect originated by surface roughness [7, 8]. Now, 1D and 2D Shave-off method has been established [9–12]. In the Shave-off

* This paper was presented at the 11th International Symposium on Atomic Level Characterizations for New Materials and Devices '17, Aqua Kanai Beach Resort, Kanai, Hawaii, USA, December 3-8, 2017.
† Corresponding author: takagi@icl.t.u-tokyo.ac.jp

FIG. 1. FIB-SIMS apparatus.
SIMS apparatus, using Mattauch-Herzog double focusing mass spectrometer (Fig. 1), different mass ions can be all focused on the same plane. Only horizontal axis of the detector is used for mass analysis. Therefore, installing 2D detector which can detect mass-to-charge ratio \((m/z)\) and the sample depth profile simultaneously, and applying enlargement and convergence of emitted secondary ions on the detector, 3D Shave-off method will have been established. This 2D detector can detect the range from a certain \(m/z\) to twice its value and the value can be determined by changing the magnetic field intensity under the condition that acceleration voltage of secondary ions is fixed. After the novel detector installed, measuring the emission angular distribution of the secondary ion from the Shave-off cross-section and designing the ion optical system, 3D Shave-off method that 3D composition data with resolution of less than several tens of nanometer can be obtained at high speed will be developed.

II. SIMULATION

In this study, to design the novel ion optics for 3D Shave-off SIMS method, secondary ion trajectory simulation was constructed. It is necessary to estimate about how the spread in the depth direction is in the present ion optics situation and what trajectory of the ions emitted from the Shave-off cross-section like to be. It is also necessary to evaluate the ion aberration by the lens, and the potential of the secondary ion transport system from the ion extrusion electrode.

A. Simulation construction

To investigate the ion trajectories emitted from the sample, ion optics for simulation have been constructed by using Autodesk Inventor (Professional 2018, Autodesk) and SIMION (SIMION Ver. 8.1, Scientific Instrument Services). SIMION\textsuperscript{R} is widely used for ion optics designs and simulations (Fig. 2). Design conditions are shown in Table I.

![SIMION image](image)

FIG. 2. SIMION\textsuperscript{R} image.

![Electrostatic analyzer](image)

FIG. 3. Confirmation of double focus on the simulation: Ions; \(^{1}\text{H}^{+}, ^{84}\text{Kr}^{+}\). Initial energy; 5 keV ± 10 eV. Electrostatic analyzer inner; −250.5 V, outer; 250.5 V. Magnetic analyzer; 1 T.

![Mattauch-Herzog double focus](image)

FIG. 4. Mattauch-Herzog double focus replicated on this simulation.

<table>
<thead>
<tr>
<th>TABLE I. Design Conditions.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actual</td>
</tr>
<tr>
<td>Main slit height</td>
</tr>
<tr>
<td>width</td>
</tr>
<tr>
<td>(\alpha) slit height</td>
</tr>
<tr>
<td>width</td>
</tr>
<tr>
<td>(\beta) slit height</td>
</tr>
<tr>
<td>width</td>
</tr>
<tr>
<td>Main-slit–(\alpha)-slit distance</td>
</tr>
<tr>
<td>Electric analyzer</td>
</tr>
<tr>
<td>Magnetic analyzer</td>
</tr>
</tbody>
</table>
FIG. 5. Secondary ion trajectory calculation: Ions; $^{12}\text{C}^+$, $^{28}\text{Si}^+$, $^{56}\text{Fe}^+$. Initial energy; 1–100 eV. Repeller electrode; 5.11 kV. Sample voltage; 5 kV. Electrostatic analyzer inner; –250.5 V, outer; 250.5 V. Magnetic analyzer; 1 T.

FIG. 6. Intensity of secondary ions from quasi-shave-off section as a function of emission angle (experimentally measured).

B. Double focus

First, we confirmed that each ion was focused on the detector. From the center of the main slit, when the half apex angle was 3° with respect to the optical axis direction (Fig. 3), the convergence points of each ion was calculated. In this calculation, widths of all slits were designed with 10 mm.

Since all the elements from hydrogen to krypton were aligned almost in a straight line, it could be confirmed that the double focus condition was satisfied (Fig. 4). The $z$ value of emission point coordinate is set as zero.

C. Calculation of the ion trajectory

Secondary ions are released from the sample plane of approximately 87° under the Shave-off condition [13] and they are emitted strongly in the direction of approximately 30°. Therefore, the detection positions of ions when the emission angle was changed from the same point on the sample was calculated, and the defocus degree of the image by the emission angle was evaluated. And initial energy distribution effect on the image was also verified. In this calculation (Fig. 5), widths of all slits are fixed to the maximum value, 10 mm.

FIG. 7. Ions ($^{12}\text{C}^+$, $^{28}\text{Si}^+$, $^{56}\text{Fe}^+$) detection position dependence on emission angle ($z = 0$ is optical axis).

FIG. 8. Emission angle 30° ion ($^{28}\text{Si}^+$) detection position dependence on its initial energy.

III. RESULTS AND DISCUSSION

In our laboratory, the measurement experiments with a quasi-Shave-off section using a sample with nearly vertical tilt gave suggestion that the maximum of emission ions intensity is 30° in angle (Fig. 6). Therefore, the ions emitted from around 30° are needed to be measured efficiently in Shave-off condition.

As the secondary ion emission angle became larger, the detection position value of depth ($z$) also became larger although they were emitted from the same point of the sample surface (Fig. 7). In addition, in this simulation, the deviation of the detection position due to the release angle is calculated with wider slits than the slits used in actual measurement. Since the mass resolution is determined by the ratio of the slit width $d$ to the electric field rotation radius $S$ ($S = 200$ mm), $S/d$, the values of mass to charge ratio are blurred with the slit width set to about 10 mm. However, in this condition, the deviation of the mass-to-charge ratio is about less than 0.1 $m/z$. There-
Therefore, it does not have a critical influence on the mass resolution under the condition in actual measurement. In order to further improve the resolution in the depth direction, it is necessary to construct a lens or optics to reduce the effects of $z$ direction defocus. In this study, the emission point was symmetric center of the ion optical axis. Therefore, when the secondary ions emitted far from the axis, the distribution would be bigger.

On the other hand, initial energy distribution had effect on not only depth direction value but also mass axis value (Fig. 8). However, because initial energy of secondary ions is not more than 30 eV [14], energy distribution effect on mass direction image is not so large.

From these result, first of all, it is necessary to deal with angular distribution effects. To efficiently transport secondary ions even under Shave-off conditions, it is considered effective to tilt the incident angle of primary ions by $30^\circ$ so that secondary ions are emitted to the analyzer optical axis direction, in addition, to install slits which can decrease the effect of angular distribution. The effect of initial energy distribution on detection position is the next step.

IV. CONCLUSIONS

We have constructed a simulation method to calculate the ion trajectories emitted from sample surface. This simulation revealed the emission angle critically effected on the ion images on the detection. When designing the lenses, this method is a powerful tool. In constructing the secondary ion optical transport system taking into consideration the features of these Shave-off methods, it is expected that the simulation construction and results of this study will be of great help for future development. On the base of simulation and calculation, and measurement, by designing the magnifying cylindrical lens system that enlarges the secondary ions generated from the micro sample cross section only in the depth direction ($z$) and converge them on the detector (Fig. 9), 3D Shave-off method will be achieved.

ACKNOWLEDGMENTS

This work was supported by JSPS KAKENHI Grant Number 16H03814.


