Toward a scanning atom probe - computer simulation of electric field -

Osamu Nishikawa *, Masahiro Kimoto

Department of Electronics, Kanazawa Institute of Technology, 7-1 Ohtigaoka, Nonoiichi, Kanazawa-South, Ishikawa 921, Japan

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Abstract

Development of a new atom probe (AP) named "scanning atom probe (SAP)" is proposed. The SAP consists of a funnel-shaped micro-extraction electrode and a thin flat plate grooved or micro-photoetched in a checkerboard pattern, shaping up many micro tips. The extraction electrode scans over the grooved sample surface and stands still above a particular tip forming a minute field emission or field ion microscope with a high field area well confined in a small space between the tip and the electrode. The field distribution in the confined space depends on many factors, setting the configuration and arrangement of the tip and electrode. Accordingly, the field distribution in the confined space is computed in order to find the optimum tip and electrode configuration, and the relative position of them. Variation of the field strength with tip-electrode distances, cone angles of the tip, and the configuration of the electrode, are discussed.

1. Introduction

In a conventional field ion microscope (FIM) [1] an a few mm long single sharp tip faces a nearby grounded electrode and phosphor screen about 10 cm away. Application of a positive high voltage, 3-30 kV, to the tip with the tip radius of 100 to 1000 Å generates an extremely high field, 3-6 V/Å, above the hemispherical surface of the tip apex. When the field strength is high enough, "field-ionized" gas atoms project an FIM image of the tip apex on the screen with atomically high resolution. At higher fields, surface atoms at the tip apex are removed in an orderly fashion as positively charged ions by a peculiar phenomenon called "field evaporation" [1]. This suggests that one can directly observe the atomic arrangement on the apex hemisphere with the FIM and mass-analyze individual evaporated ions with a mass analyzer attached to the FIM: the combined instrument of an FIM and a mass-analyzer is called the atom probe (AP) [1,2].

Since the AP is an ultimate micro-mass-analyzer, it has been utilized in the microanalysis of various materials such as metals, semiconductors, and conductive polymers and ceramics [2-6]. However, it has also been realized that the AP application is intrinsically limited because the sample needs to be a sharp tip and the analyzed area is an extremely small hemispherical tip apex.

Furthermore, the fabrication of a sharp tip is another problem. Although the preparation process of tips from a fine metal wire is well develop-
opend and relatively easy, the tip making from a
metal block or a semiconductor wafer is still fairly
complicated. A hopelessly difficult case is to fab-
ricate a tip with a specified spot of a specimen at
the apex or a tip with a multi-layer structure
grown on a wafer at the tip end.
In order to break through these difficulties a
new AP named "scanning atom probe (SAP)" is
proposed. A specimen of the SAP is a thin plate
which is grooved in a checkerboard pattern form-
ing many tips. A funnel-shaped micro-extraction
electrode scans over the specimen and forms a
minute field emission or field ion microscope
when the electrode is positioned above one of the
tips. Then, the high field generated by a bias
voltage applied to the electrode or the specimen
is confined to a small space between the elec-
trode and the specific tip.
In this study the feasibility of developing the
SAP was examined by computing the field distri-
bution between a tip and an extraction electrode
for various tip lengths, cone angles of the tips,
and the position and configuration of the elec-
trode.

Fig. 1. Schematics of a grooved specimen.

2. Scanning atom probe

Unique features of the SAP are a flat speci-
men and a micro-extraction electrode. The speci-
men plate is grooved or micro-photoetched in a
checkerboard pattern forming many sharp spikes
or tips. The assumed depth of the grooves is
several to a few tens of microns and the spaces
between the tips are tens to hundreds of microns,
Fig. 1. The funnel-shaped extraction electrode
scans over the grooved specimen surface and
stands still above a particular tip, Fig. 2. Since the
diameter of the open hole at the end of the
extraction electrode can be made as small as a
few to ten microns, the high field is well confined
in a small space between the tip and the elec-
trode when a negative or positive bias voltage is
applied to the sample or the electrode. Then, the

Fig. 2. Schematics of the extraction electrode and a tip formed
by grooving.

Fig. 3. Schematics indicating parameters to calculate the field
distribution in the space between the electrode and the tip.
conventional field emission microscope (FEM) [7,8] and an FIM. Detection of individual evaporated ions by a mass-analyzer makes the FIM serve as the SAP.

3. Computation of field distribution

The confinement of the field depends on many factors setting the configuration and arrangement of the tip and electrode. The most effective factor is the tip–electrode gap; the narrower the gap, the smaller the high field space and the lower the bias voltage. However, care must be taken to avoid field emission from the open end of the electrode when the SAP is operated as an FIM because a high-density emission current from the electrode may damage the tip apex. Thus, the highest field strength on the electrode surface should be less than one tenth of that of the tip apex.

Accordingly, the field distribution in the confined space was computed in order to find the optimum tip and electrode configuration by vary-

Table 1
Variation of field strengths at the tip apex and the electrode end

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<th>φ (Å)</th>
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Fig. No. indicates the number of the figure shown in this report. Tip radius r = 1000 Å, h: tip length, d: height difference between the tip apex and the electrode end, θ: cone angle of the tip, φ: diameter of the open hole at the electrode end, cone angles and end curvatures of the electrode are α₁, α₂ and R, respectively. E₁ and E₂ are the field strengths (V/Å) at the tip apex and the electrode end for V = 10 kV, respectively, and Eᵣ = E₁/E₂.
angles and end curvatures of the electrode $\alpha_1$, $\alpha_2$ and $R$, respectively, Fig. 3. Since the tip–electrode assembly is symmetric around the tip axis, cylindrical coordinates were employed to calculate the electric potential $V$. Then, Laplace's differential equation was transferred to difference equations and the $r$–$z$ space was divided into $M \times N$ sections to compute the potentials at each $i$–$j$th crossing point $V_{ij}$, Fig. 4. In the present calculation $M$ and $N$ were 800 and 1600, respectively. The calculation of a field distribution with a Macintosh Quadra 950 took 10 to 40 h, depending on initial setting.

4. Field strength and field distribution

An intuitive estimate of the field strength suggests the field strength at the tip apex, $E_t$, increases with decreasing $r$ and $\theta$, and increasing

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![Image](image.png)

**Fig. 5.** Variation of $E_t$, $E_r$, and $E_z$ with $d$, $\theta = 30^\circ$.

![Image](image.png)

**Fig. 6.** Equipotential and field lines around the tip and the electrode. $r = 1000 \ \AA$, $h = 3.2 \ \mu m$, $\theta = 20^\circ$, $d = 0$, $\phi = 2.4 \ \mu m$, $\alpha_1 = 30^\circ$, $\alpha_2 = 35^\circ$ and $R = 6000 \ \AA$. $E_t$ and $E_z$ for $V = 10 \ kV$ are 8.02 and 0.74 $V/\AA$, respectively, and $E_t = 10.8$. The potential difference between two equipotential lines $\Delta V$ is 200 $V$.  

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Similarly, the field strength at the end of the electrode $E_e$ decreases with increasing $\phi$, $d$ and $R$. Accordingly, the ratio of the field strengths, $E_r = E_t/E_e$, should increase with decreasing $r$ and $\theta$, and with increasing $h$, $\phi$, $d$ and $R$. However, the confinement of the high field in a small space between the tip apex and the electrode requires small $\phi$, $d$ and $R$, and large $\theta$, which is favorable for fabricating the tips by grooving.

The calculated values of $E_t$, $E_e$ and $E_r$ for the tip bias voltage $V_t = 10$ kV and $r = 1000$ Å are listed in Table 1 for various $h$, $\theta$, $d$, $\phi$ and $R$. The variation ranges of $E_t$, $E_e$ and $E_r$ at $V_t = 10$ kV are rather narrow, from 8.1 to 4.5 V/Å, from 1.48 to 0.51 V/Å and from 12.3 to 4.1, respectively, for the variation of $h$ from 2.2 to 6.4 μ, $\theta$ from 20° to 90°, $d$ from $-0.5$ to 1.0 μ, $\phi$ from 2.4 to 4.8 μ and $R$ from 6000 to 9000 Å. As presumed, $E_t$ increases as the electrode approaches the tip, but $E_r$ rather stays constant because $E_e$ also increases with $E_t$, Fig. 5. As $\theta$ increases, $E_r$ drops sharply and $E_e$ increases, lowering $E_t$. On the other hand, $E_t$ increases from 9.7 to 11.5 by the increase of $R$ from 6000 to 9000 Å. The largest $E_t$, 12.3, was obtained for $h = 6.4$ μ.

Field and equipotential lines and trajectories of He ions field-ionized above the tip surface at $V_t = 10$ kV are shown in Figs. 6–9. Although the high field regions are well confined in a narrow space around the tip apex and the field lines are smoothly curved, the ion trajectories spread fairly straightly into the radial directions of the tip apex, indicating the projection of an enlarged image of the tip apex on a screen like an ordinary FIM.

5. Discussion and conclusion

The tip voltage, $V_t$, required to generate $E_t = 4.5$ V/Å, the ionization field of He, is above 20 kV for a conventional FIM with a tip of $r = 1000$ Å.
Å. However, the present tip–electrode configuration yields $E_\tau > 4.5 \text{ V/Å}$ at $V_t = 10 \text{ kV}$ because the high field is confined in a small space. This implies that even the apex of an obtuse tip with $\theta = 90^\circ$ can be observed and mass-analyzed by the SAP. Table 1 also indicates that $E_e$ is high and few tip–electrode configurations give $E_\tau > 10$. If we visualize the tip as a core cable and the electrode as an outer cylinder, the field distribution between the tip and the electrode is somewhat similar to the distribution expected in a cylindrically symmetric space. The analogy becomes obvious as $d$ reduced to 0 and becomes negative when the tip is inserted into the open hole of the electrode. Then, $E_\tau$ should be proportional to the ratio $\phi/2r$ which is 2.0 for $\phi = 2.4 \mu$ and $r = 6000 \text{ Å}$, and is about 1/5 of $E_\tau$. The proportional constant varies gently with $h$, $\theta$, $d$, $\phi$ and $R$, as shown in Table 1.

Present discussions indicate that the SAP allows the observation of atomic arrangements and the mass-analysis of individual atoms of gentle peak apexes with $\theta > 90^\circ$ on a grooved specimen surface. Present results also suggest that it is desirable to set $\phi > 5r$, $h > 2\phi$ and $R > 5r$. Then the SAP can inspect each peak apex about 10 μ apart on a grooved surface.

Realization of the proposed SAP requires the fabrication of the grooved specimen surface and the micro-extraction electrode. Trial fabrication was conducted by drilling through a gold-plated Si tip of an atomic force microscope by irradiating a 30 keV Ga ion beam for about 1 min. The beam diameter was 0.2 μm and the ion current was $\sim 30 \text{ pA}$. A funnel-shaped electrode with an open hole of less than 2 μm in diameter was fabricated. The success in the trial fabrication is a promising step for the development of a SAP.

Fig. 8. Equipotential and field lines around the tip with a large cone angle and the electrode. $r = 1000 \text{ Å}$, $h = 3.2 \mu$, $\theta = 90^\circ$, $d = 0$, $\phi = 3.4 \mu$, $\alpha_1 = 30^\circ$, $\alpha_2 = 35^\circ$ and $R = 6000 \text{ Å}$. $E_t$ and $E_e$ for $V = 10 \text{ kV}$ are 4.5 and 1.04 V/Å, respectively, and $E_\tau = 4.3; \Delta V$ is 200 V.
with unique features in the micro-analysis of various flat specimens which cannot be investigated by the existing AP.

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7. References