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Biased sample holder for complete correction of SIMS transmission losses with tilted samples

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ABSTRACT

For investigation of fundamental aspects of secondary ion mass spectrometry (SIMS) such as secondary ion distributions, roughness formation or simply for optimisation of a particular analysis, the ability to tilt a sample is vital. However many instruments suffer transmission losses when the sample is tilted. This phenomenon has been investigated for the Cation Mass Spectrometer (CMS) instrument using Monte Carlo simulations and the cause determined to be modification of the extraction field arising from the sample tilt. A new sample holder incorporating biasing electrodes has been developed to eliminate transmission losses during SIMS analysis when using tilted samples. Simulations and experimental result confirm complete elimination of transmission losses for sample tilts of up to 20°.

1. Introduction

Secondary ion mass spectrometry (SIMS) is a well known and widely used analysis technique [1–3] . During the SIMS processes, a sample is sputtered by a primary beam and the resultant secondary ions are extracted and analysed according to their mass. In this way elemental image, depth profiles or full 3D chemical maps of a sample may be produced.

For the studies of fundamental processes in SIMS and for optimising individual analyses the ability to tilt the sample with respect to the primary beam is important as secondary ion angular distributions, concentration of implanted species, sputter yield, primary beam–sample interactions, depth resolution and roughness formation are all affected by the angle of incidence of primary ions. The cation mass spectrometer has been developed to study both fundamental processes and improve quantitative analysis using MCs^+ ions. The instrument, described in detail elsewhere [4], is based on a Cameca 3f and has dual gallium/caesium primary ion columns and a patented system for in-situ neutral caesium deposition. At normal incidence between the sample and extraction system the instrument benefits from an absolute transmission of up to 50%. However, the transmission of the instrument decreases dramatically as samples are tilted (see Fig. 1).

To determine the cause of this transmission loss and investigate the potential for correction, the instrument was simulated using SIMION versions 7 and 8 [5].

2. Simulation

A potential array containing the extraction system was created and loaded into SIMION's ion optics bench. As the tilted sample means the system no longer has rotational symmetry, planar (3D) models were used. To determine where the transmission losses occurred, a large number of particles were flown through the system and the positions where ions collided with electrodes were recorded. To ensure the accuracy of the results, Monte Carlo methods were used to generate secondary ions on the sample with the correct initial distributions. The most important factors are secondary ion energy and angular distribution. The energy distribution of secondary ions may be modelled by the Sigmund–Thompson distribution given in Eq. (1) [6,7] where U is the surface binding energy

$$N(E) \sim \frac{E}{(E+U)^3} \quad (1)$$

The angular distribution may be approximated by a cosine raised to a power n, where n is sample dependant and normally between 1 and 2 [7]. In this study a value of 1 was used for the exponent. The effect of raster size is ignored in this study as previous investigations of the extraction system by the author showed that for raster sizes up to $250 \times 250\ \mu m^2$ the raster size had no effect on the transmission. For this study only positive secondary ions were considered; however the results would be applicable to negative ions simply by reversing the polarity of the appropriate voltages.

SIMION produces random numbers uniformly distributed between zero and one. To generate probability distributions, these numbers must undergo a mathematical transform. To generate

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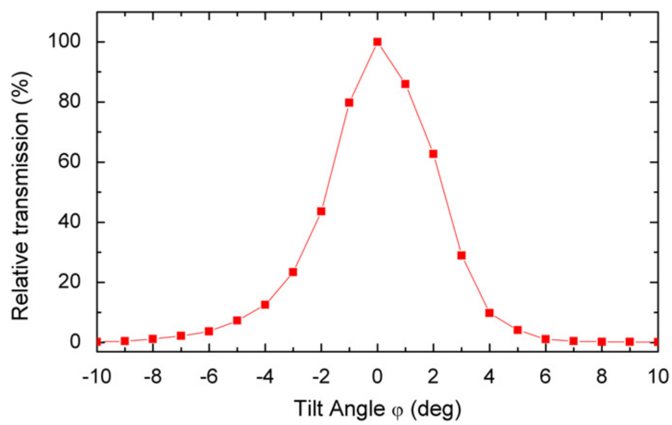

Fig. 1. Variation in relative transmission with sample tilt angle for the CMS instrument (measured experimentally).

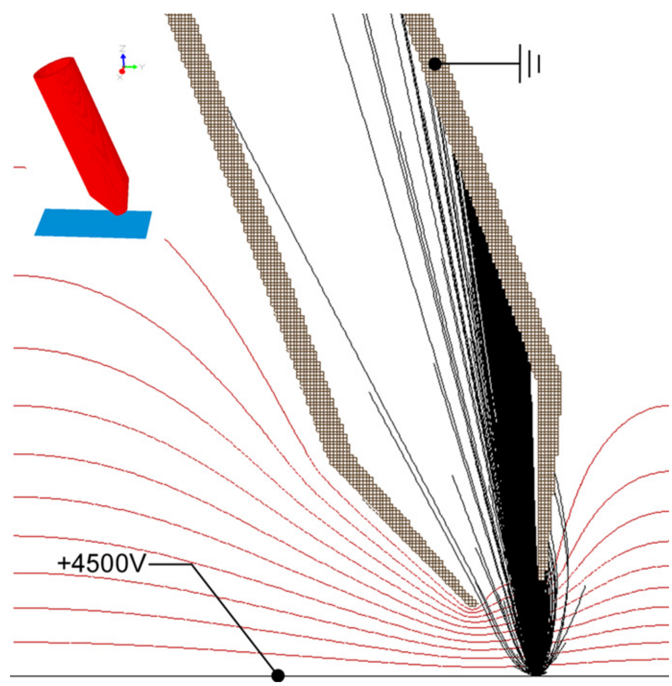

Fig. 2. Cross-section through CMS extraction system for sample tilt of 20° with equipotentials. The sample is biased to +4500 V and the extraction electrode is grounded. Trajectories are for 10,000 ions with realistic angular and energy distributions. Inset 3D model of electrode geometry.

secondary ions with the appropriate distributions, the initial angle and energy are assigned random numbers and these are then converted into energy and angle by the transforms. A detailed description of the transforms required for each distribution may be found in Ref. [8]. Once the initial angle and energy are determined for each ion, these are translated into SIMION's co-ordinate system after an arbitrary rotation to allow centring of the initial angular distribution on any vector. This allows ions to be launched with the angular distribution centred on the normal (or at some other angle) to a tilted sample. Code for generating ions with appropriate distributions was written first in the sl language and later updated to lua.

Fig. 2 shows cross-section through the extraction system potential array with a sample tilted at 20°. The extraction field is produced by biasing the sample to +4500 V while grounding the extraction electrode. The sample is modelled by a flat plane. To avoid artefacts introduced by flying ions from positions close to a jagged surface, the sample plane was maintained parallel to SIMION's virtual grid and the extraction electrode rotated about the eucentric point. A total of 10,000 ions were flown through the system with the initial angular distribution centred on the sample normal. As the figure shows, most of the ions collide with the extraction electrode after a very short distance. This is because the extraction field above the sample is no longer axially symmetric when the sample is tilted. This causes the angular distribution of secondary ions to be centred on an axis at an angle to that of the extraction system. If the field asymmetry can be corrected for a tilted sample, then the original transmission should be recovered.

A first attempt at correction involved using an un-tilted plane to determine the macroscopic field, while the sample was mounted on a small tilted region just below the extraction electrode. Several designs (hill, valley and hill+valley), shown in Fig. 3(a), were simulated based on this approach and their efficacy compared with a flat tilted sample plane for angles up to 20°. For ease of comparison of simulation and experimental data the relative transmission, defined as the number of ions passing successfully through the system for a tilted sample compared with that of an un-tilted system, was used. For the simulations the relative transmission is that of just the extraction system, while for experimental results the relative transmission is of the whole instrument. This will result in some discrepancy between the results; however, the general trends remain comparable.

Fig. 3(b) shows the results for bundles of 10,000 ions. It is clear that the only configuration that offers an improvement over a tilted sample is the valley configuration and here the improvement is still not particularly significant. For this reason a more complex modification involving correction electrodes was investigated.

As the field from a tilted sample introduces an angular deflection in the secondary beam, it should be possible to correct for the angular shift using a simple dipole field. To produce a dipole field, electrodes were added on either side of the sample post and biased symmetrically with respect to the sample voltage (see Fig. 4(a)). For a 20° sample tilt, 10,000 ions were flown through the system and the variation in relative transmission was recorded as the magnitude of the corrector bias was increased. Fig. 4(b) shows that with this configuration it is possible to recover 100% relative transmission. However, further simulations showed that the width of the distribution and the voltage required for complete correction is significantly affected by the precise geometry of the correction electrodes and sample post.

A simple prototype, shown in Fig. 5, based on this idea was developed. It consists of a line of sample posts each machined to a precise length and angle with correction electrodes mounted on either side. In this way the tilt angle of the sample could be modified simply by translating the sample stage, without affecting the working distance (as this affects the transmission). Five sample posts with angles 0°, 5°, 10°, 15° and 20° were tested with three mountable in the sample holder at the same time. The prototype was simulated for tilt angles up to 20° and, as expected from the dipole geometry, for each angle it was possible to recover 100% relative transmission. The voltage required for complete correction varied linearly with tilt angle as one might expect.

3. Experimental

The prototype was mounted on the sample holder of the CMS instrument and the relative transmission of the instrument measured for comparison with the simulations. High work function metal foils (100 μm W and Au) were glued to each sample post using silver glue. To determine the relative transmission, a 5.5 keV Cs primary beam of ~5 nA was used to sputter the samples and the