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## Determination of the variation in sputter yield in the SIMS transient region using MEIS

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### Abstract

The near-surface erosion rate in SIMS depth profiling is significantly different from that in the bulk, and varies with primary ion dose across the transient region in a currently unknown manner. Here, we describe a new method using medium energy ion scattering to measure the transient matrix sputter yield, and hence determine the erosion rate. We demonstrate its use in converting the raw dose and yield scales in a shallow depth profile to depth and concentration. We show that the surface erosion rate may be more than 10 times that in the bulk, and that the ion yield for boron in silicon apparently stabilizes before the sputter yield.

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### 1. Introduction

The near-surface sputter yield of silicon is significantly higher than in the bulk, and this difference is expected to increase as the primary beam energy is reduced [1]. The resulting change in erosion rate is one factor which causes systematic shifts in the SIMS depth scale if a uniform erosion rate is used for depth calibration. The resulting errors are serious in a modern ultra-shallow SIMS profile, and can amount to significantly more than 10% error in the top 10 nm. A novel method to accurately determine the sputter yield of the matrix in both the SIMS

transient and steady-state regions has therefore been developed, based on medium energy ion scattering (MEIS).

We exploit the ability of MEIS to measure damage levels using the blocking of channels in a single crystal with an amorphized surface, and examine the rate of change of the residual damage in a pre-amorphized sample as a result of subsequent sputtering at sub-keV SIMS primary energies [2]. The thickness of the amorphous layer is chosen to be significantly greater than that of the altered layer created by the sputtering beam. Sputtering therefore reduces the net disorder in the surface by thinning the amorphous layer, and measurement of the damage remaining in the surface as a function of sputter beam dose can be used to calculate the transient erosion rate and sputter yield.

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## 2. Experimental

The sample investigated was a 1 keV boron implant into a silicon (0 0 1) surface, pre-amorphized using 5 keV Ge<sup>+</sup> at 10<sup>15</sup> ions cm<sup>-2</sup>. Several individual craters were formed by sputtering the sample using a 500 eV O<sub>2</sub><sup>+</sup> primary beam at normal incidence with a crater size of 3 mm<sup>2</sup> with ion doses in the range 4 × 10<sup>15</sup> to 2 × 10<sup>17</sup> O<sub>2</sub><sup>+</sup> cm<sup>-2</sup>, using the EVA 2000FL SIMS tool at Warwick. MEIS saturated damage profiles were measured on the CLRC facility at Daresbury using 100 keV He<sup>+</sup> incident ions, with a total beam dose of 0.5 × 10<sup>16</sup> ions cm<sup>-2</sup>. Experiments were performed using the double alignment geometry of [1̄ 1 0] incidence and [1 1 0] blocking, corresponding to incident and scattering angles of 45° and 90°, respectively. Each sample was studied in both channelled and random directions. Part of the same wafer was capped with ~15 nm amorphous silicon layer by UHV deposition at room temperature in a VG V90S MBE system. Hence, the same boron distribution could be measured using 500 eV O<sub>2</sub><sup>+</sup> SIMS both with and without the surface transient. The uncapped profile was depth-calibrated using surface profilometry (crater depth  $z_{\text{meas}} = 86.5$  nm) and a further correction based on the MEIS data, and compared with the capped.

## 3. Results and discussion

Fig. 1 shows the MEIS spectra obtained with O<sub>2</sub><sup>+</sup> dose as a parameter, together with a schema showing how the area was calculated. (The de-channeling background in the crystalline material does not affect the intensity in the amorphized layer and so the areas are calculated without background subtraction, as shown.) There are clear signs of oxidation in the spectra, but there is also some irreproducibility in the Si edge position from one spectrum to the next. This seems to be a feature of the imaging detector in the instrument. However, as we are interested in the difference in area under the silicon surface peak, we ignore this for now. For the zero-dose spectrum the FWHM width of the amorphized layer is 16.5 nm (using a stopping power of 200 eV nm<sup>-1</sup> obtained from TRIM calculations). This agrees reasonably well with the SIMS measurement of 15.3 nm. Detailed

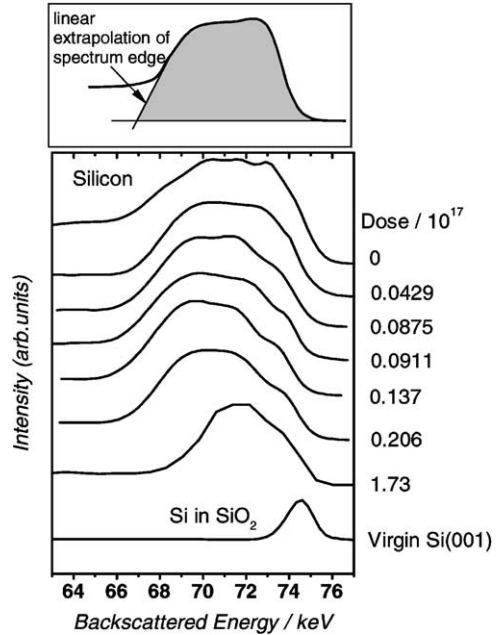


Fig. 1. MEIS channeling spectra of the Si peak with virgin Si (0 0 1) included for comparison. Shading on the insert indicates how the individual areas  $A(\phi)$  were calculated.

investigation shows an average de-channeling  $\chi_{\text{min}}$  of 0.95, indicative of complete amorphization.

Our hypothesis is that the difference in area  $\Delta A(\phi)$  between each MEIS spectrum and the zero-dose area  $A_0$  is proportional to the number of Si atoms sputtered by a dose  $\phi$  of O<sub>2</sub><sup>+</sup> ions, so that

$$\Delta A(\phi) = A_0 - A(\phi) \propto \int_0^\phi Y_{\text{Si}}(\phi) d\phi \quad (1)$$

where  $Y_{\text{Si}}$  is the silicon sputtered yield.

Fig. 2 shows the measured data for  $\Delta A(\phi)$  as a function of  $\phi$  (black circles). In principle, similar results could also be obtained for a wholly crystalline sample containing a buried heavy marker, by monitoring the marker's energy shift with respect to the Si edge as the superficial Si atoms were removed, and accounting for the effects of retained (SIMS) probe atoms. It is clear from Fig. 2 that the Si eroded as a function of  $\phi$  initially increases non-linearly as expected in the transient region. The data are well fitted by the function

$$\Delta A(\phi) = a\phi + b(1 - e^{-c\phi}) \quad (2)$$

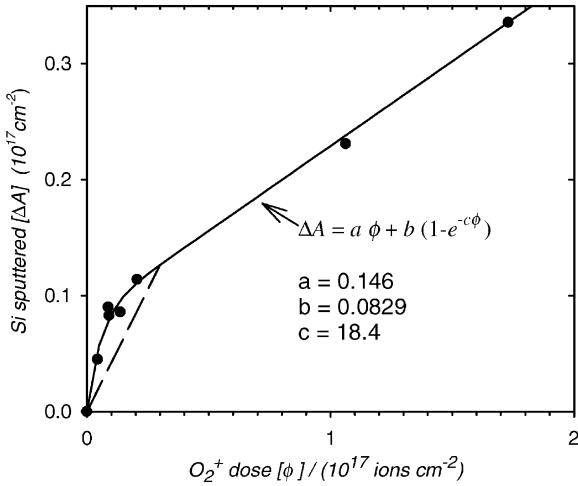


Fig. 2. Difference between area under the as-implanted damage profile and the oxygen dosed profiles from the MEIS spectra as a function of oxygen dose. The fit shown was used in the SIMS depth profile correction.

whose slope is proportional to the sputter yield of the matrix. Since eroded depth  $z \propto \Delta A(\phi)$  and  $\lim_{\phi \rightarrow \infty} z = \phi Y_{\infty} \Omega_{\text{Si}}$ , where  $Y_{\infty}$  is the bulk sputter yield, and  $\Omega_{\text{Si}} = 2 \times 10^{-23} \text{ cm}^3$  is the atomic volume of the matrix, the constant of proportionality must be  $Y_{\infty} \Omega_{\text{Si}}/a$ , so that in general

$$z = 10^{17} \frac{Y_{\infty}}{a} \Omega_{\text{Si}} \Delta A(\phi) = \frac{z_{\text{meas}}}{\Delta A(\phi_{\text{tot}})} \Delta A(\phi) \quad (3)$$

Setting  $a = Y_{\infty}$  and fitting using the 86.5 nm crater and its corresponding ion dose ( $\phi_{\text{tot}} = 2.90 \times 10^{18} \text{ O}_2^+ \text{ cm}^{-2}$ ) gives  $a = 0.146$  (in good agreement with Ref. [3]),  $b = 0.0829$ , and  $c = 18.35$ , if  $\phi$  is measured in units of  $10^{17} \text{ O}_2^+ \text{ cm}^{-2}$ . This gives the ordinate scaling in Fig. 2.

Previous measurements [4] using the dose to steady-state of the  $\text{Si}^+$  yield to obtain the transient dose  $\phi_{\text{tr}}$ , found  $\phi_{\text{tr}} \sim 1.5 \times 10^{16} \text{ O}_2^+ \text{ cm}^{-2}$  for silicon with  $\sim 1 \text{ nm}$  native oxide and  $\sim 1.7 \times 10^{16} \text{ O}_2^+ \text{ cm}^{-2}$  for clean silicon. However, the sputter yield should also be in steady-state by the end of the transient and the slope of Eq. (2) falls to within 5% of  $a$  at a dose of  $3 \times 10^{16} \text{ O}_2^+ \text{ cm}^{-2}$ , almost double that in the previous measurements.

Fig. 3 shows raw (depth proportional to SIMS beam dose) and depth-calibrated boron profiles (using Eq. (3) to obtain the depth scale) from the uncapped sample. The asterisk in the inset shows the

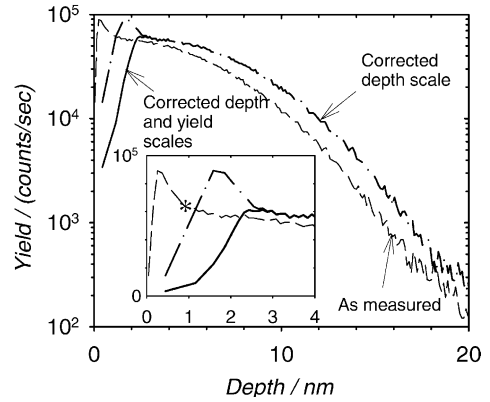


Fig. 3. As measured, depth corrected, and depth and yield corrected boron profiles. The inset shows a linear plot of the top 4 nm.

$3 \times 10^{16} \text{ O}_2^+ \text{ cm}^{-2}$  point on the raw data—at the end of the ubiquitous boron spike observed on sub-keV SIMS profiles of as-implanted material under conditions of full oxidation.

Eq. (3) has been used to correct the depth scale in Fig. 3 (dash-dot line). The inset shows the near-surface behavior on a linear scale. The corrected profile is shifted by 1.4 nm, which is more than expected ( $0.9 \text{ nm keV}^{-1}$  per  $\text{O}_2^+$  [5]). It is also apparent that the width of the transient region (the thickness of silicon sputtered to achieve steady-state) is 2.4 nm, again higher than the figure of 0.7 nm estimated for crystalline Si [4].

Elsewhere [6], we suggest that that boron ion emission, takes place at constant ionization probability  $\alpha_{\text{B}}^+$ , and therefore, after the initial steep rise (to the peak of the spike) its ion yield is proportional to the matrix sputter rate. Now, the main effect of the depth scale correction has been to stretch the surface spike laterally. Elsewhere [5], we show that the surface spike must be included in the dose integral, so the stretching has not conserved dose. To correct the boron yield  $Y_{\text{B}}^+$  we need

$$Y_{\text{corrB}}^+(\phi) = Y_{\text{B}}^+(\phi) \frac{Y_{\infty}}{Y_{\text{Si}}(\phi)} \quad (4)$$

The results of this procedure are shown by the solid curve in Fig. 3. The boron surface spike is now completely removed as one would expect for an ideal profile without transient effects. The capped sample, which is free from these, provides a reference for the

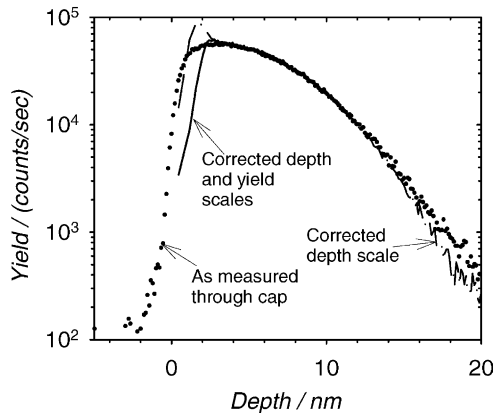


Fig. 4. Comparison between corrected and capped profiles. The depth scale of the capped profile has been offset by  $-15.3$  nm (the thickness of the cap).

yield correction. The comparison in Fig. 4 between the dotted line (as measured through the cap) and the fully corrected profile shows that the yield correction works well in the decaying part of the spike, again supporting the hypothesis that boron is sputtered at constant yield in this region.

#### 4. Summary and conclusions

We outline a method for obtaining the transient erosion rate in SIMS using MEIS, and demonstrate its

use in obtaining a corrected depth scale. The data suggest that transient widths estimated using ion yields are narrower than those based on sputter yield, and that the transient sputter yield is higher than expected. More data are required before this is certain.

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