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Measurements and modeling of the angular-resolved sputtering yield of D-soaked Be by 100, 300, 500 and 700 eV D^+

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Abstract

The angular-resolved sputtering yield of Be by D^+ was predicted and then measured. An ion beam at 100, 300, 500 and 700 eV from a Colutron ion source was focused onto S-65 C grade Be samples. The sample was exposed in situ to a 350 V dc D plasma to remove oxide, load the surface with D and more-nearly simulate the surface which would be found during steady-state fusion device operating conditions. The angular distribution of the sputtered atoms was measured by collection on a highly ordered pyrolytic graphite witness plate. The areal density of Be (and BeO, after exposure to air) was then measured using a scanning Auger spectrometer. Total deposition was measured by deposition onto a quartz crystal oscillator placed alongside the witness plate. A three-dimensional version of vectorized fractal TRIM (VFTRIM3D), a Monte-Carlo computer code which includes surface roughness characterized by fractal geometry, was used to predict the angular distribution of the sputtered particles and a global sputtering coefficient. One-quarter million trajectories were simulated to determine the azimuthal and polar angle distributions of the sputtered atoms. A fractal dimension of 2.05, and a surface binding energy of 3.38 eV, both standard values for Be, were used. Results show reasonable agreement between the code and experimental values for total yield with the experimental yields somewhat lower. The measured angular distribution is broader (less forward peaked) than predicted by the computer simulation.

Keywords: Plasma–wall interaction; Sputtering measurements; Monte-Carlo model; Be

1. Introduction

The experimental determination of sputtering yields at the relative low-energy found in the edge region of tokamaks has always been problematic. At low energies the surface roughness and the gas adsorbed on and absorbed in the surface will affect the yield. Ion beam driven experiments which determine the sputtering through weight loss measurements [1] do not mimic the surface in a tokamak, nor do they measure the angular distribution of the sputtered material needed for sheath-impurity transport calculations [2]. Plasma simulator results [3] only produce measurements of the yield integrated through an assumed transport model that is dependent on the plasma sheath, magnetic field and other conditions unique to the specific simulation device.

We introduce an apparatus and method which allows Be samples to be cleaned and 'filled' by the bombardment of D^+ in situ, and then measured. Both the absolute yield and the angular-resolved yield of the sputtered flux can be determined as a function of ion energy and angle of incidence. In this paper the experimental apparatus, independent computer modeling, and the results are described.

2. Experiment

A modified Colutron ion gun [4] produces a D^+ current of approximately 100 nA from a D plasma. The beam passes through a $E \times B$ filter to select a charge to mass ratio for D^+. The beam is decelerated through a custom-designed series of cylindrical lenses to the desired energy and bent to eliminate neutrals [5]. The doses on the Be sample ranged from 1.1×10^{15} to 2.2×10^{15} cm^{-2}.

The beam strikes the sample at a predetermined incident angle (45° for the work presented here.) This angle

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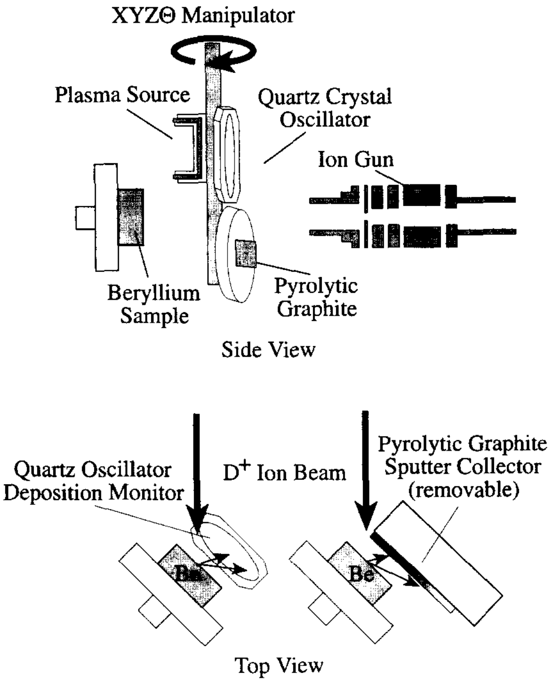

Fig. 1. Schematic of the target and diagnostic apparatus. A $X-Y-Z-\Theta$ manipulator can position either a dc-plasma source, a quartz crystal oscillator, or a highly-ordered pyrolytic-graphite-crystal witness plate in front of the Be sample.

was chosen to closely resemble the average incident angle for ions at the wall of a fusion device. The S-65 C grade beryllium sample is a candidate material for ITER and was supplied by Brush Wellman. It came from lot 4763 and was machined to 32 μinch RMS or better without EDM and then etched in a 2–2–2 solution.

On a $X-Y-Z-\Theta$ manipulator arm three different devices are mounted. See Fig. 1. The first is a 2 cm diameter, 1 cm deep cylindrical cup, insulated by Pyrex from a slightly larger and deeper cup kept at ground potential. When the cup is placed 1 cm over the grounded sample, and the pressure in the chamber is raised to 700 mTorr of D_2, +350 V is placed on the inner cup. This creates a locally intense dc plasma. The measured ion current density to the sample was 0.4 mA/cm^2, enough to remove one monolayer every 7.7 s. This plasma cleaning and D-filling of the sample was carried out for 20 min before each measurement.

To measure the sputtering yields the ion current to the sample is summed over the length of the exposure. Previous work measured the ion-induced electron emission [6] from Be. To eliminate the need for a correction to the total measured current, the surrounding structures were biased several volts negative with respect to the sample to repel the emitted electrons and drive them back.

After the cleaning/filling one of two diagnostics can be placed over the sample: an Inficon quartz-crystal oscillator (QCO) or a crystal of highly ordered pyrolytic graphite (HOPG). The signal from the QCO is used to determine the total weight gain from the collection of sputtered material. This allows an absolute determination of sputtering yield into the azimuthal and polar angles subtended by the QCO.

The HOPG is mounted on a vacuum transfer cassette and serves as a 'witness plate'. A fresh surface is cleaved prior to each experiment. After the Be sample is bombarded by the ion beam, the HOPG witness plate is transferred to a Physical Electronics model 660 scanning Auger spectrometer. En route it is briefly exposed to air intentionally in order to oxidize the deposited Be. The

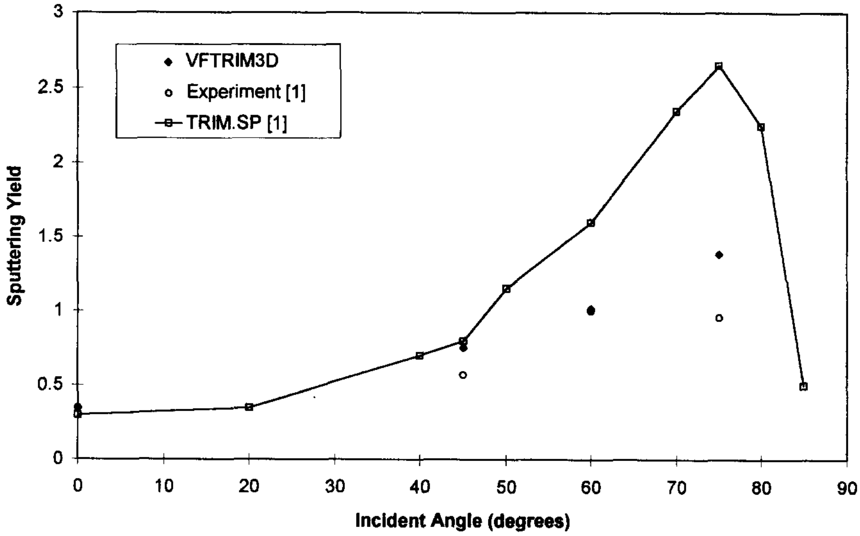

Fig. 2. VFTRIM3D data for the self-sputtering of 1000 eV Be as a function of incident angle overlaid on previously published TRIM.SP and experimental data [1].

Auger spectrometer determines the absolute surface density of the BeO from the differentiated peak-to-peak heights of the 510 eV O, 275 eV C, and 108 eV Be lines. Merely exposing a freshly cleaved HOPG sample to air which has not collected Be does not show any evidence of the O line.

3. Simulation

In parallel with the development of the experimental apparatus, the TRIM.SP [7] computer code has been modified to include the effect of the surface topography using a fractal surface model [8]. Recently, this fractal surface model has been extended to three dimensions [9,10] in order to properly predict the azimuthal yields of sputtered and reflected material. Fig. 2 shows the effect of the surface model. VFTRIM3D results are overlaid on previously published data [1]. The effect of the surface roughness decreases the reflection and sputtering at higher angles of incident and more nearly represents the experimental data of Roth.

For the VFTRIM3D data in all the figures and Table 1 and for comparisons to our own experiments a fractal dimension of 2.05, a surface binding energy of 3.38 eV and a bond energy equal to 10% of the surface binding energy were used. This fractal dimension is in agreement with the published atomic level roughness of many metals ([11], for example.) A D$^+$ beam incident at 45° struck a surface composed of 1 D atom for every 3 Be atoms. This 0.33 D to Be ratio was taken from recent room temperature saturation experiments [12]. The resulting sputtered flux from 250,000 incident flights was binned into the proper geometrical swaths for direct comparison to the experimentally determined areal densities.

4. Results

Fig. 3 shows the absolute sputtering yield as a function of energy for D$^+$ incident on D-exposed Be from the QCO data. This data has been corrected by the VFTRIM3D factors shown in Table 1 which account for the sticking coefficient of the Be onto the Be-covered gold-plated crystal, the resputtering of the stuck Be by the reflected D atoms, and the weight of the D deposited on the QCO. These corrections add between 2.6% and 6.6% to the measured experimental flux, and are taken into account in the data shown in Fig. 3. Overlaid on Fig. 3 are the calculated sputtering yields from VFTRIM3D. The computer code predicts a slightly higher sputtering yield than is observed at some energies.

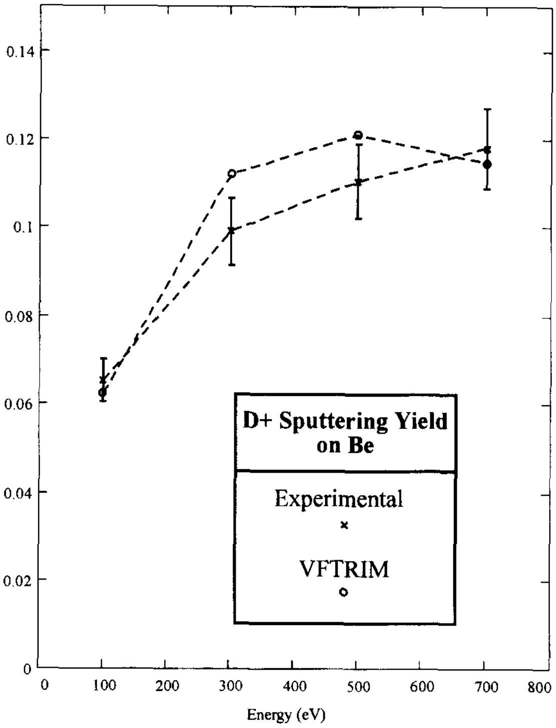

Fig. 3. Total sputtering yield as a function of energy for D$^+$ on D-bombarded Be at 45°. Modeling results are from VFTRIM3D. Experimental points are from deposition onto a quartz crystal oscillator and are corrected (by about 10%) for the sticking coefficient for Be and the resputtering by the reflected neutrals.

The statistical uncertainties on the computer-simulated data come from the square root of the number of flights and are very small in Figs. 2 and 3. The experimental errors are due to the limits of the detected frequency shift in the oscillator and the error in reading the total current to the sample, and, for Fig. 4, the uncertainty from the Auger analysis.

Table 1
Modeling results to determine the correction to the experimental data for sticking of Be and re-sputtering by the reflected D from the quartz crystal oscillator

D$^+$ energy on Be surface	Energy peak of sputtered Be	Sticking coefficient for sputtered Be	Reflection coefficient of incident D$^+$	Average energy of reflected D	Sputtering yield of reflected D onto 5 nm of Be over Au	Scaling factor for experimental data
100 eV	4 eV	0.93	0.236	35 eV	0.1029	1.102
300 eV	4 eV	0.93	0.197	105 eV	0.2771	1.137
500 eV	4 eV	0.93	0.178	173 eV	0.3409	1.145
700 eV	4 eV	0.93	0.160	235 eV	0.3245	1.134

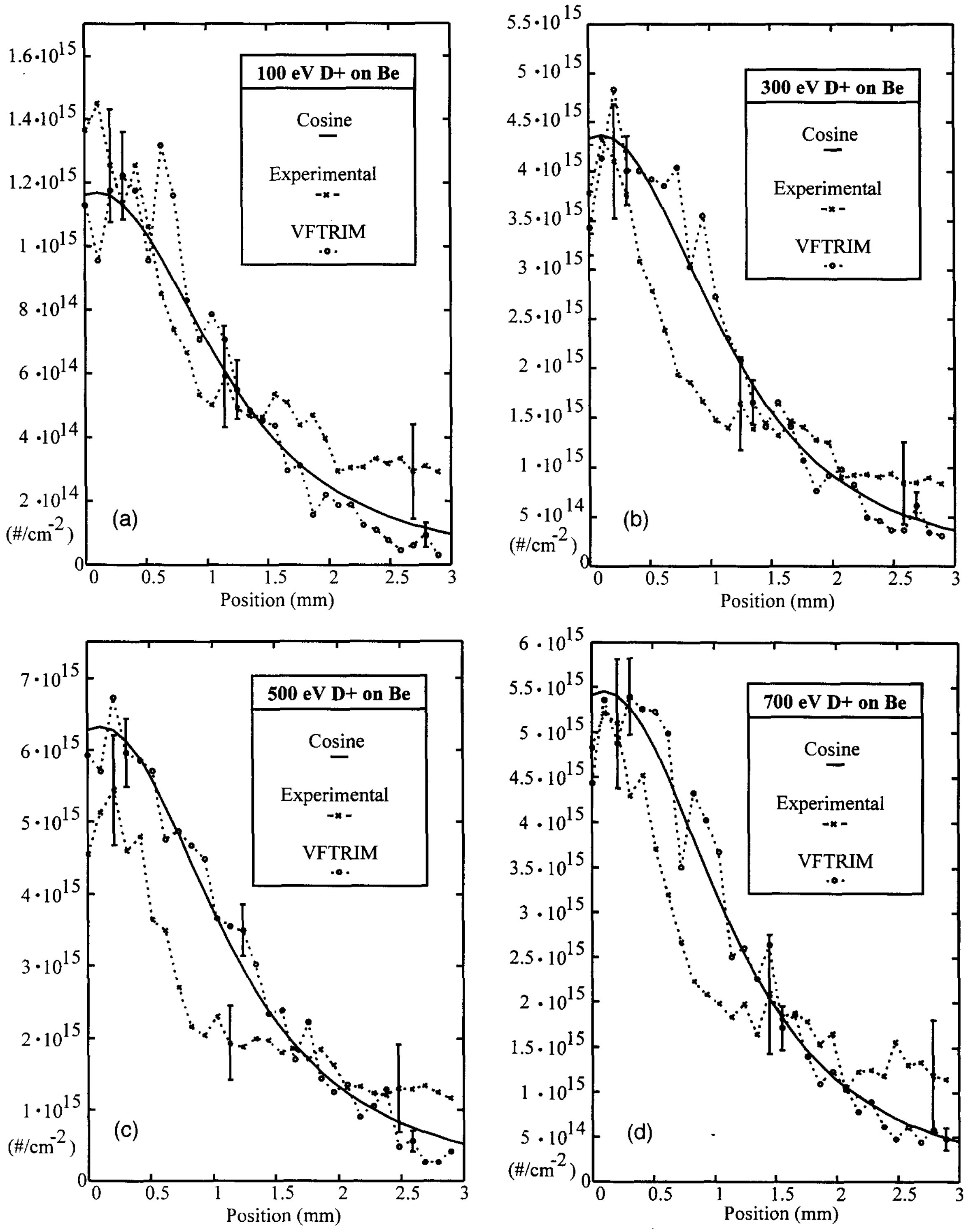

Fig. 4. Angular distributions of the sputtered Be flux. The solid line represents a cosine distribution and is sealed to the computational VFTRIM3D results. The experimental points are from Auger scanning spectrometer areal densities of BeO_2 on highly-oriented pyrolytic graphite witness plates. The incident angle for the D^+ was 45° at (a) 100 eV, (b) 300 eV, (c) 500 eV, and (d) 700 eV.

Data reduction from a scan of peak-to-peak differentiated Auger line intensities, to the number of atoms per cm^2 at a position along the witness plates was accomplished with the aid of MathCAD. Fig. 4a–d show the experimental areal densities as a function of position along the witness plate. The data extends for 3 mm along the witness plate and collects the sputtered flux with polar angles from 0 to 65°. In the figures the signal peaks at the point which is perpendicular to the ion beam spot. The data 3 mm away represents sputtered particle trajectories at 65° from normal.

The experimental data from the auger spectrometer is scaled by the absolute yield obtained form the QCO. This adjustment of a factor of approximately 11 is needed to calibrate peak-to-peak Auger line intensities to areal densities. This accounts for the potential non-oxidation of all the surface atoms and the burial of Be beneath the graphite surface.

Overlaid on the experimental data are the VFTRIM3D results for the same geometry. The magnitudes of these two plots are not scaled. A cosine distribution (scaled to the VFTRIM3D data) is also shown on the graphs as a dashed line. Note that the simulation results fall very close to a cosine distribution while the experimental results show more evidence of having a higher angular flux at larger angles. The small peak at 2.8 mm is in the correct position to account for material preferentially sputtered in a specular direction. This presumably arises from the knock-on collisions of ions specularly reflected off of interior Be atoms.

As the energy is increased the computational results become more and more cosine-like. The experimental results develop a less-peaked angular distribution. More particles are emitted at higher angles of incidence and fewer at intermediate angles. The number emitted normal to the surface compares favorably at all energies.

5. Conclusions

Angularly resolved and total sputtering yields at low (less than 1000 eV) energies can now be determined in a routine fashion under conditions relevant to fusion research devices. This apparatus and analysis technique should help determine the suitability of differing materials as well as manufacturing and finishing techniques for a given material. The computational development of VFTRIM3D compliments the experimental effort and allows a benchmarking of the code. Though no attempt was made to do so here, adjustable parameters in the code such as fractal dimension and the ratio of SBE to bondbreaking energies could be adjusted to more closely match the experimental data and then used in a predictive mode for cases outside the capabilities of the present experimental apparatus. The data shows evidence for a small degree of specular sputtering and a non-cosine distribution of sputtered material.

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