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Experimental and computer investigation of the diagnostic mirror behavior under sputtering and duct material deposition

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Abstract

Experiments on stainless steel duct material, W and Mo mirror surfaces as well as modeling of the experiment using a new computer code which takes into account scanning tunnelling microscope measured surface topography are described. Simulations of the sputtering yield as a function of the primary ion energy and the angle of incidence for ion irradiated targets demonstrated the difference in behavior for ideally smooth, non-irradiated and irradiated targets.

1. Introduction

The reflectivity of the diagnostic mirrors in fusion devices is influenced mainly by sputtering with charge exchange neutrals and by deposition on the mirror surface of impurities contained in plasma [1,2]. The mirrors located far from the plasma in deep diagnostic ducts can be covered with redeposited layers of duct material [3,4]. In quantitative computer evaluation of the surface layer behavior under impact of various atoms, one should take into account the real surface microrelief and composition change during operation. The generation of surface roughness is very important for the efficiency of diagnostic mirrors, as the dimensions of roughness should be an order of magnitude less than the wavelength used for diagnostic. The mirror surface response to irradiation with atomic particles is also important for mirror efficiency prediction.

There are widely used computer programs [5], which agree with experiments for atomically smooth surfaces (TRIM, TRIM.SP, etc.). But rough surfaces that, in fact, correspond to plasma-exposed mirrors in fusion devices exhibit strong deviations in values of sputtering yield Y, as well as in angular and energy distributions of reflected [6–9] and sputtered particles [10,11].

Different models have been applied to describe rough surfaces using small size regular structures on the surface [7,12] or fractal dimensioning of the surface [13]. The first attempt to use results of scanning tunnelling microscope (STM) measurements of the surface topography for more realistic modeling of roughness was made in [14,15] where the surface was simulated as a distribution of the local angles of ion incidence.

To make computer simulations more realistic, the modified code SCATTER-R, which included the STM measured data of the real surface microtopography, was developed. The first results on comparison of calculations with experiments on low energy deuterium ions incident on a Nb target [16] showed reasonable agreement with the experimental data.

In this paper we describe some features of the code and results of its application to simulations of ion interaction with mirrors exposed to high fluence ion irradiation. A brief description of the benchmark experiment on simulation of mirror behavior under sputtering and deposition of differing material is also given.

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2. Simulation code features

The code developed to take into account real surface topography measured with STM is based on the TRIM-like SCATTER code [17].

To incorporate an STM image into calculations, instead of a $z = 0$ condition (valid for smooth surface), a $z = f(x, y)$ condition is used, where z is the coordinate normal to the total scan surface, and x, y are planar coordinates on the target surface. The function $f(x, y)$ is defined with a linear approximation of z values for four nearby STM image points. The model surface for the 'striking' or 'emerging' point of a projectile is also determined with the help of these values. The binding energy is considered within the frame of a planar potential barrier. As the model strip of the surface is limited by STM scan dimensions, various scenarios of particle trajectory calculations (in the case of its escaping from the scan area) are considered. Namely, one can stop particle trajectory calculations and consider the particle as reflected or trapped, or continue calculations in a translated scan image.

3. Experimental

The STM SMM-2000T was used for the in air analysis of samples before and after ion beam irradiation. The surface roughness analysis is available including determination of R_q, the root-mean-square roughness of profile; R_a, the mean roughness of profile; D_a, the mean local profile slope; and other parameters. Each characteristic of the target topography was measured several times with different scanning directions.

High flux irradiation with deuterium ions was carried out on the SLEIS device [18]. Parameters of irradiation were as follows: primary energy 200 eV; incidence of the beam along the normal to the surface; beam composition: D_3^+ – 83.3%, D^+ – 14.1%, impurities (O^+, C^+) – 2.6% (this ion composition corresponds to energy distribution of incident particles: D, 67 eV – 93.7%, D, 200 eV – 5.3%, impurities, 200 eV – 2.6%); total current density 1 mA/cm^2; fluence 10^{20} cm^{-2}.

The medium-energy mass monochromator [19] was used for the sputtering and redeposition experiments with the two-target assembly (Fig. 1). A beam of Ar^+ ions with energies from 5 to 10 keV and current density of 1–10 μA/cm^2 (energy spread $\Delta E/E < 3 \times 10^{-4}$, angular divergence less than 0.4°) was used in the experiments. The position of the two targets (22 mm in diameter and 3 mm in thickness) can be changed in such a manner that the front surface of one of the targets is centred at the goniometer axis. This target can be irradiated with the ion beam. Reflected or knocked out ions were analysed with a spherical electrostatic deflector (energy resolution is 0.005, solid angle of registration is 0.0074 sr, angular resolution $\Delta\Theta = \pm 1.0°$) providing medium-energy spectroscopy of scattered ions and ionised recoils (MEIS). A laser with a wavelength $\lambda = 670$ nm was used for monitoring surface reflectivity under ion irradiation. This monitoring system is based on the comparison of the intensities of the primary laser beam with the reflected one. The relative accuracy of the reflection coefficient change measurements is equal to 0.01. Surface composition and reflectivity of the sample can be measured in situ during ion irradiation. The second target collects sputtered atoms and can be placed, in turn, for analysis (and sputtering) at the previous position of the first target. The temperatures of both targets are controlled in a range 300–700 K. Residual gas pressure in the target chamber is 10^{-8} mbar. W, Mo, and stainless steel (SS) targets were used. The in situ MEIS analysis showed that no external impurities were present on the surface of a pure W target.

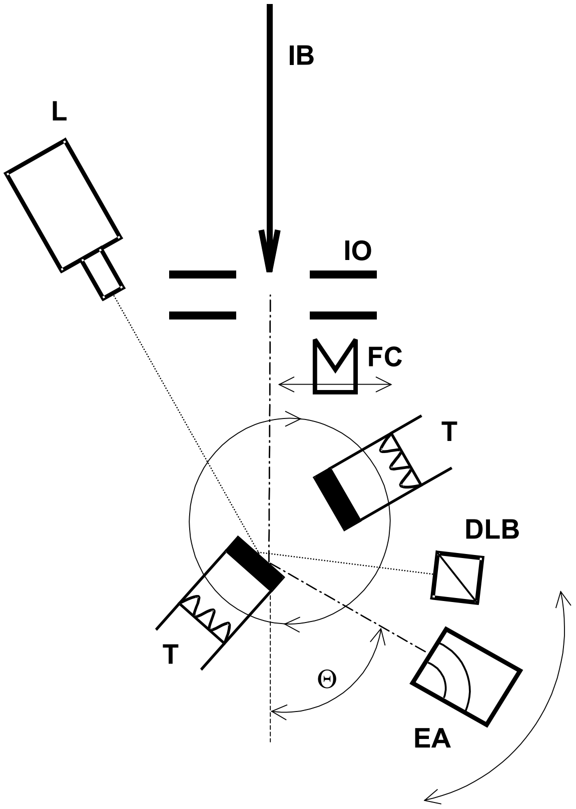

Fig. 1. Scheme of the benchmark experiment on deposition of material from SS duct sample on W mirror under ion irradiation. IB: mass separated ion beam, IO: ion optics, T: target with heating and temperature control system, EA: electrostatic energy analyzer, L: laser, DLB: detector of reflected laser beam, and FC: Faraday cup.

4. Results and discussion

The change of Mo surface reflectivity after irradiation did not exceed 5% in the wavelength range $300 < \lambda < 800$ nm. The characteristic topography parameters measured with STM were $R_q = 2.5$ nm, $R_a = 1.9$ nm, $D_a = 8.3°$.

The binding energy for the computer simulations was set equal to the energy of sublimation for Mo (6.28 eV). Calculations stopped at 1 eV for deuterium projectiles and at 6.28 eV for Mo recoils. The total number of calculated trajectories is approximately 10^7. As one can see from Fig. 2, where calculations of the sputtering coefficient Y for smooth and irradiated targets are shown, the surface roughness slightly increases Y for angles less than 70°. At grazing incidence in accordance with data of [13,14], Y is less than those for the smooth surface. Energy dependence of the sputter yield (Fig. 2(b)) reveals close coincidence of Y values for smooth and rough surfaces for high ($\sim 10^4$ eV) energies of deuterons. Computer analysis showed that at grazing incidence energetic projectiles could penetrate through the surface relief structures, in increasing Y for the rough surface. So, in spite of small decreases in mirror reflectivity due to the high fluence irradiation with low energy deuterons, the change of surface response to sputtering can be considerable.

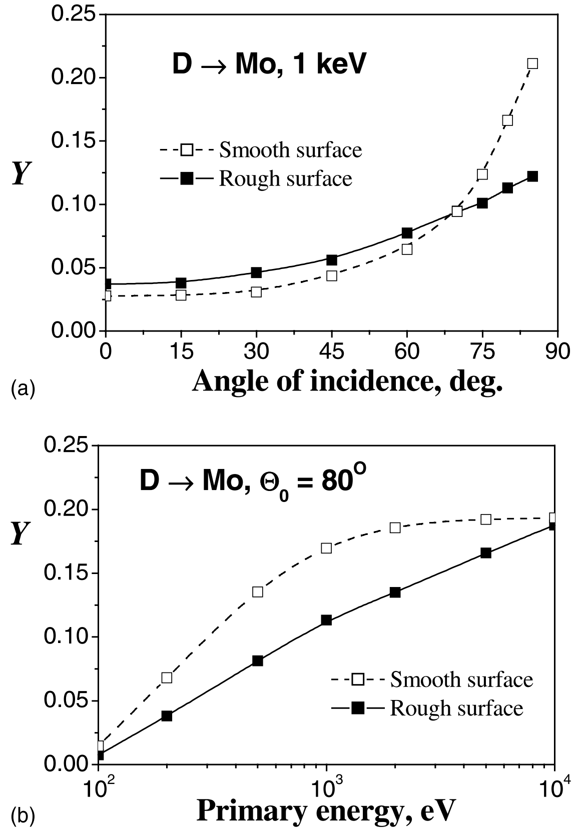

Fig. 2. Calculations of the sputtering coefficient Y for smooth and irradiated targets: (a) the angular dependence of Y and (b) the energy dependence of Y.

Samples of rolled H16N11M3T SS (Russian analogue of SS 316L) and polished pure W mirror were used for two-target sputter–redeposition experiments. The treatment of the samples before the experiment was limited by degreasing and long term heating in vacuum at ~600 K. The primary surface topography of the SS sample shown in Fig. 3(a) is typical for mechanical treatment ($R_a = 86.9$ nm, $R_q = 97.9$ nm). After irradiation with high fluence ($\sim 10^{20}$ cm^{-2}) 10 keV Ar$^+$ ions, the surface becomes more rough ($R_a = 123.6$ nm, $R_q = 151.6$ nm) with less regularity of the surface relief structure (Fig. 3(b)).

The surface relief of SS samples had a minor influence on calculated values of sputtering yield under Ar$^+$ ion bombardment. The roughness influence on the angular dependence of sputtering yield $Y(\Theta)$ becomes slightly more pronounced as the energy of Ar ions decreases down to 1 keV (Fig. 4).

The analysis of the SS deposition on the mirror surface was carried out using a Rutherford back scattering (RBS) technique (deposition of atoms sputtered from SS sample with high fluence deuterium beam at the SLEIS facility on Al substrate at room temperature) and LECO quantitative depth profiling (deposition of atoms on W mirror maintained at 600 K during Ar$^+$ bombardment of the same SS sample shown in Fig. 1). Results of the RBS analysis of the Al substrate with deposited layer using 1 MeV ^{4}He$^+$ beam show that the main components detected on the Al surface are O and Fe + Cr, while Mo and W are the minor species (O – $(6 \pm 1.5) \times 10^{16}$ cm^{-2}, Fe + Cr – $(2.2 \pm 0.5) \times 10^{16}$ cm^{-2}, Mo – $(2.4 \pm 1.5) \times 10^{14}$ cm^{-2}, W – $(8.6 \pm 2.5) \times 10^{14}$ cm^{-2}). An unexpected high percentage of W can be connected with the initial content of W in the SS sample and conditions of the SS sample rolling procedure. The possible presence of W ions in the primary ion beam of the SLEIS facility should be excluded due to the direct Auger analysis of a pure Cu target exposed to the beam. (Subsequent analysis of the SS sample with LECO quantitative depth profiling confirmed W presence at the level of ~1–2%.) The composition of deposited layer does not correspond to the primary SS sample composition due to the large amount of oxygen. But comparison of experimental and calculated data on the relative content of Fe + Cr and Mo in the deposited layer shows that these ratios are very close: 27.5 ± 1.0 and 34.2 ± 4.0, respectively.

LECO quantitative depth profiling of the W mirror with a deposited layer (formed from SS target atoms sputtered with the argon beam) showed that the layer

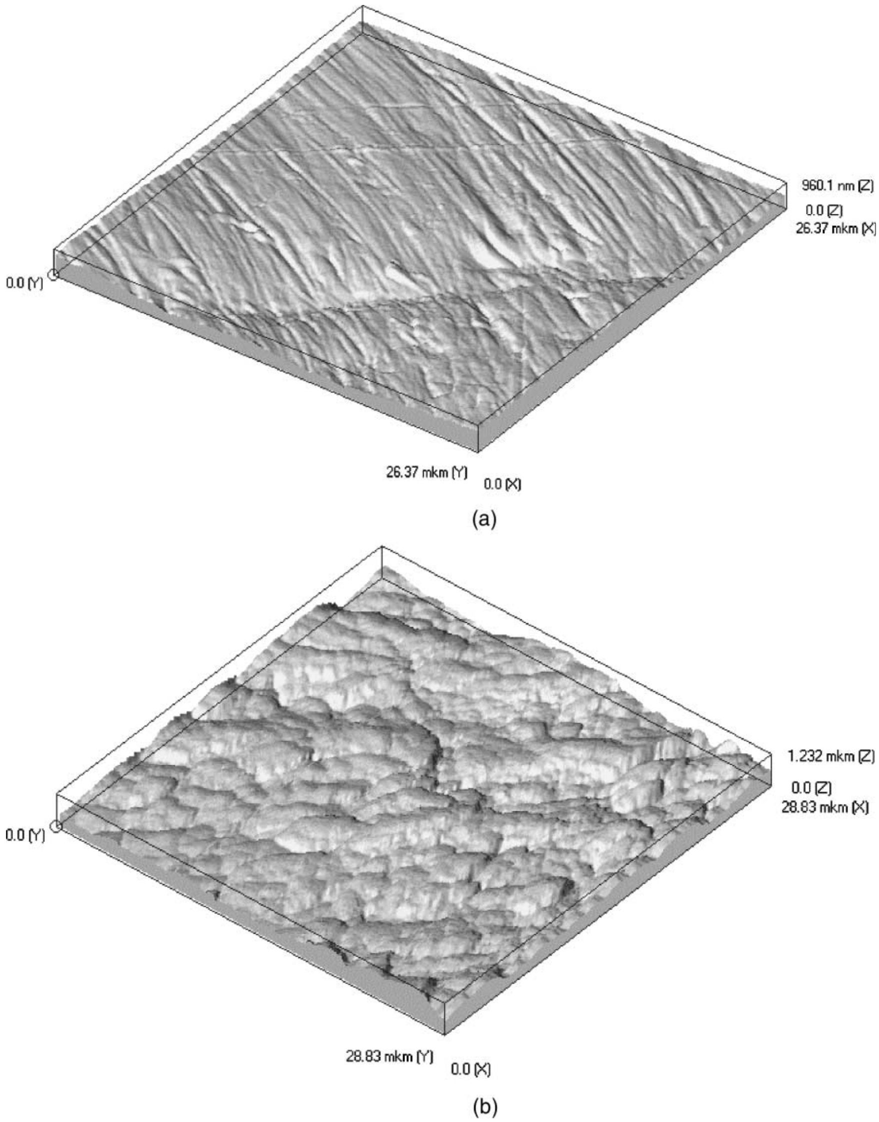

Fig. 3. STM image of SS surface: (a) surface of rolled SS sample before irradiation, scan size $26.37 \times 26.37 \times 0.96$ μm^3 and (b) the same after irradiation with Ar^+ 10 keV ions with fluence $\sim 10^{20}$ cm^{-2}, scan size $28.83 \times 28.83 \times 1.232$ μm^3.

contains all components of this steel (Cr, Fe, Ni, Mn, Ti) and is enriched with C (7.5%) and W (27%) but the ratio of $(Fe + Cr + Ni)$ to Mo is approximately the same as for the RBS analysis. The surface density of foreign atoms within the area of analysis on the W target was approximately two times less than the value calculated with the modified code. The reason for the difference between measured and calculated values can be explained an assumption of too much of a surface topography change during irradiation, as well as underestimation of impurities taking part in sputtering and deposition. The difference in the composition of the deposited layer in these two experiments can be caused by different conditions of deposition. The latter attempt to compare experiment on sputtering with calculations should be considered preliminary and mainly a demonstration of the method for code validation.

5. Conclusion

A computer code has been described for calculations of ion–solid interactions, taking into account STM measured surface topography. It is applicable for

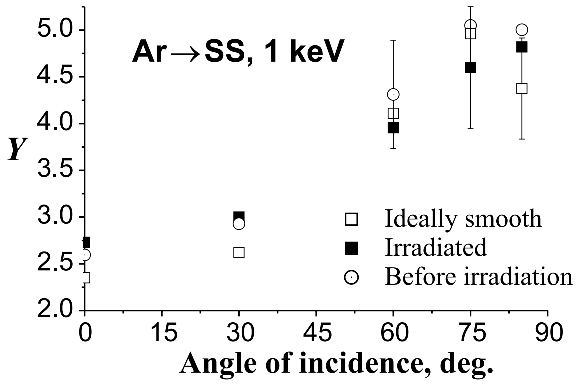

Fig. 4. Surface topography influence on calculated values of Y for sputtering of SS with Ar^+ 1 keV ions.

simulations of diagnostic mirror behavior in fusion devices, as well as for benchmark experiments on the code validation.

Simulations of the sputtering yield as a function of the primary energy and the angle of incidence for various ion irradiated targets including Mo and W mirrors and diagnostic duct SS sample demonstrated the difference in yield as a function of ion energy and incidence angle $Y(E)$ and $Y(\Theta)$ for ideally smooth, non-irradiated and irradiated targets. The small influence of the real surface roughness on the value of sputtering yield under Ar^+ bombardment was demonstrated. A non-monotonic dependence of $Y(E)$ for smooth and rough surfaces in the case of grazing incidence of deuterium ions on Mo mirror was found.

Experiments on the SS duct material deposition onto mirror surfaces with RBS and LECO quantitative depth profiling analysis of the deposited layers revealed some difference in the composition of the layer in different simulation experiments. Further experiments are necessary for the quantitative code validation using these two methods of quantitative analysis of deposited layers.

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