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Sputter yield of rippled surfaces: A simulation study



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ABSTRACT

Atomistic (binary-collision) simulation is used to study the sputter yield from rippled surfaces in a wide range of ion incidence angles. Most simulations refer to amorphous carbon bombarded with 7 keV Ga ions, and sinusoidal ripple morphology is assumed. Results are compared with the analytical predictions and Monte Carlo simulations based on continuum models of sputtering from sine- and ridge-shaped surfaces. Both atomistic and Monte Carlo simulations do not confirm a sharp increase in the sputter yield with increasing the ripple amplitude predicted theoretically (Makeev and Barabási, 2004). Significant differences between the results are also observed in the yield dependence on the angle of incidence.

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1. Introduction

Sputtering is the release of atoms from a solid surface subjected to bombardment by energetic atomic particles, for example ions. Ion-beam sputtering has been studied for a long time, but it is still one of the top areas of research, owing to many applications in research and technology. For applied purposes, one of the most requested characteristics of sputtering is the sputter yield, defined as the average number of ejected atoms per incident ion. The sputter yield depends on a number of beam and material parameters such as the type, energy, and direction of incidence of the beam, as well as the composition and ion-induced surface topography. Many of these dependences are well studied, but the impact of surface roughness on the yield is still a stimulated task for the sputter community (e.g. [1–4]). In this regard, of great interest is the sputtering of surfaces with different shape, including wave- and ridge-contoured surfaces observed experimentally for different materials in a wide range of ion energies and incidence angles [5–8]. Such data are of vital importance in the study of dose effects in sputtering of sinusoidally rippled and faceted (step/terrace) surfaces [9].

For sinusoidal surfaces, a comprehensive theoretical study of the sputter yield Y was carried out by Makeev and Barabási (MB) [10,11] in the framework of Sigmund's theory [12,13]. It was shown that the wave surface structures (ripples) may cause significant variations in the yield, depending on a complex interplay between the wavelength and amplitude of ripples and the energy

deposition depth. For the angles of incidence $\alpha = 35\text{--}65^\circ$ characteristic of the formation of ripples (α is measured from the surface normal), the MB theory predicts a sharp (by 1.5–2.5 times) increase in the yield with increasing the ripple amplitude. This prediction, however, contradicts the experimental data of Adams et al. [9] on sputtering of diamond targets with 20 keV Ga ions, showing rather the opposite behaviour of Y . This contradiction inevitably raises some doubts about the adequacy of the model used. This model really has some limitations [14,15], however, it is difficult to expect that they are so significant to cause a qualitative disagreement with experiment.

To clarify the above, this paper presents the results of computer simulations performed using the author's program OKSANA [16] developed to calculate sputtering from smooth and periodically modulated surfaces. Most simulations refer to 7 keV Ga ion bombardment of amorphous carbon for reasons of comparison with the MB theory. The calculated sputter yields are compared with the results of Monte Carlo simulations that implement the MB model of ion sputtering, and with the analytic estimates of Y in terms of the Wittmaack model of sputtering from faceted surfaces [5].

2. Simulation methods

2.1. BC simulation

The version of the program OKSANA used in the present work is described in [16]. Briefly, the program is based on the

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binary-collision approximation (BCA) and takes into account weak simultaneous collisions at larger distances. The program provides simulation of sputtering from crystalline and disordered (amorphous) targets, but in this study we deal only with the latter. As in MARLOWE [17], an amorphous target is modeled by rotation of a corresponding crystalline atomic block, the procedure of rotation being repeated for each new collision. The classical scattering in atomic collisions is described by the screened Coulomb potentials of Ziegler, Biersack and Littmark (ZBL) [18]. Inelastic energy losses in atomic collisions are described as default by the Firsov formula [19] that defines the losses through the impact parameter of the collision. All other parameters are identical to those in the standard model [20].

The direction of ion bombardment is given in a Cartesian coordinate system, in which the X' and Y' axes lie in the surface plane of the target, and axis Z' is directed inside the target. It is assumed that in all cases the axis of the ion beam is parallel to the X' - Z' plane (Fig. 1). The surface profile is modeled by a sine-wave function with a period $2x$ and a height z (Fig. 1). Collision cascade atoms of all generations are traced, and those atoms which overcome the surface potential barrier are considered as sputtered. Locally planar potential barrier, which takes into account particle stopping upon leaving the surface and trajectory refraction, is used for ejected atoms – candidates for sputtering. In accordance with common practice [21], the surface binding energy is assumed to be equal to the energy of sublimation (7.41 eV for carbon), and the bulk binding energy is taken equal to zero. The trajectories of ejected atoms are traced until they are much above the surface but before the final escape such atoms (like scattered ions) can reach the closest flanks of ripples and cause their sputtering. For a correct comparison with the MB theory, no changes in the surface topography, originally specified, are made (the static mode).

When bombarding rough surfaces, some part of the surface may be in shadow. For sinusoidal surfaces, this happens at $\alpha > \alpha_s$, where $\alpha_s = \arctan(2x/\pi z)$ is the shadowing angle [22]. Strictly speaking, the model of sinusoidal surface is more or less realistic only at $\alpha < \alpha_s$, since at higher angles of incidence the surface has a tendency to be faceted [22]. However, for a more complete comparison with the MB results, the sputtering in the regime of shadowing ($\alpha > \alpha_s$) will be considered as well.

OKSANA makes it possible to record the spatial distribution of the deposited energy and to determine the energy deposition depth d , which is necessary for comparison with the MB theory (see below). For control, such calculations were performed for 5–50 keV Ar and Xe ions on carbon and gave good agreement with the TRIM data [23]. For 1–20 keV Ga ions on C, the calculated

values of d lie in the range of 1.5–10.5 nm. Some idea of the collision process near a curved surface is given in Fig. 2, where the density of dots is proportional to the deposited energy. More examples of such distributions can be found, for example, in [15].

2.2. MC simulation

As already mentioned, the sputter yield of rippled surfaces was calculated by Makeev and Barabási [10,11] on the basis of the Sigmund theory of continuum sputtering [12,13]. In Sigmund's theory, it is assumed that sputtering of a target by energetic ions is the result of atomic collision cascades and that the sputter yield is determined by the energy deposited near the surface. In a simplified form, the deposited energy distribution is given by the Gaussian [12,13]:

$$E_D(\delta, \xi, \eta) = \frac{\varepsilon}{(2\pi)^{3/2} \sigma \mu^2} \exp\left\{-\frac{(\delta-d)^2}{2\sigma^2} - \frac{\xi^2 + \eta^2}{2\mu^2}\right\}, \quad (1)$$

where ε is the initial energy of an incident ion, σ and μ denote the standard deviations of the distribution along the longitudinal and two lateral directions respectively, and d is the energy deposition depth, mentioned above. This distribution is centered at a point located at a distance d from the surface, and the contours of equal energy deposition are ellipsoids of rotation of the type that follows from Fig. 2.

Integrating the distribution (1) over a sinusoidal surface, Makeev and Barabási succeeded in calculating the relevant sputter yield. This approach is also realized in the present work, but instead of analytical evaluation of the yield the problem is solved by Monte Carlo (MC) technique for a large number of ion impact points lying on the surface within one period of the sine wave. The impact points are distributed in such a manner to match the ion beam, uniform in cross section. The sputter yield corresponding to a single impact point is determined by summing up the deposited energy, Eq. (1), over the entire surface. Such (partial) sputter yields are then summed for all impact points to find the total yield Y , more precisely, the quantity proportional to it. The proportionality factor is irrelevant, since only normalized values of Y are considered. Following [10,11], it is assumed that $\sigma = d/2$ and $\mu = d/4$, which corresponds to an asymmetric deposited-energy profile elongated in the direction of ion bombardment. Fig. 2 suggests that for the Ga-C pair the distribution (1) with the above relations for σ

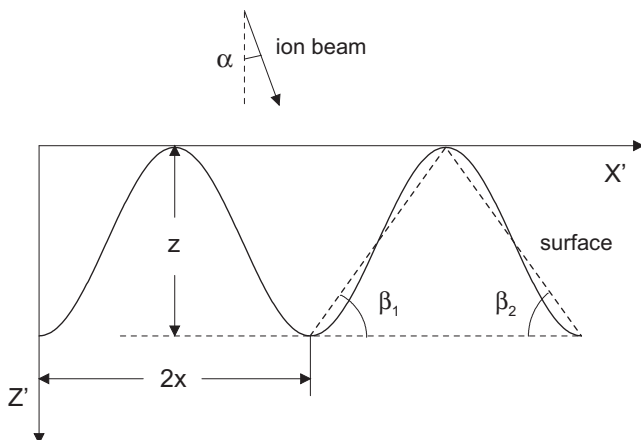


Fig. 1. Scheme of ion beam incidence on a sine-shaped surface of the target.

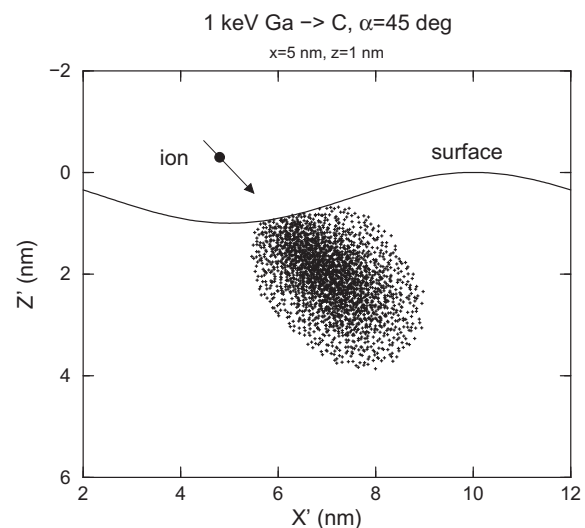


Fig. 2. Distribution of deposited energy for a single impact point of 1 keV Ga ions incident on a sinusoidal carbon surface at $\alpha = 45^\circ$.

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