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Effects of faceted surface topography on high-fluence sputtering of graphite

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ABSTRACT

Effects of ion-induced faceted surface relief on high-fluence sputtering of graphite under 30-keV Ar and 15-keV N ion bombardment have been studied by means of binary-collision computer simulation. Taking into account experimental observations of surface topography, the relief was modeled by an α-dependent ridge-like periodic function (α = the ion incidence angle measured from the normal to macroscopic surface plane). It was shown that for normal incidence the sputter yield S represents a non-monotonic function of the relief aspect ratio and is saturated at $x \sim 100$–200 nm (x = the half-period of the relief). The simulations stressed the importance of the relationship between the dimensions of surface roughness and atomic collision cascades and allowed to explain the $S(\alpha)$-dependences found experimentally. It was shown that a strong (about 2 times) decrease of S at α = 60–80° is due to a shadowing mechanism which is also clearly revealed in the angular distribution of sputtered atoms.

1. Introduction

Ion bombardment of solids often leads to the appearance of surface topography, which can be observed by using, for example, scanning electron and atomic force microscopy. The variety of observed topographic structures is striking: arrays of pits, cones, facets, pyramids, ripples, etc. Such structures, chaotic or periodic, can cover large areas of the surface and greatly affect its sputtering characteristics. Nano- and micro-architectured surfaces are of interest for practical applications. The topographical evolution is energy-dependent and, in the regime of nuclear stopping of the bombarding ions, is governed by the interplay between surface erosion due to sputtering and surface diffusion. The formation and evolution of surface topographies under ion bombardment of solids is a complex phenomenon and still a stimulating task for the sputter community (e.g. [1–4]).

One of the most stable elements of surface topography are known to be the structures of a facet-type nature [5–9]. Originally such structures were observed on mono- and polycrystalline metals, but recently they were found on (0001) highly oriented pyrolytic graphite (HOPG) surfaces under high-fluence (10^{18}–10^{19} cm^{-2}) irradiation with 30 keV Ar and 15 keV N ions [10,11]. For 30-keV Ar ion irradiation, the slope angles of facet planes with respect to the nominal (macroscopic) surface plane, β_1 and β_2, were also measured [10] using the laser goniophotometry technique. The angles lie between 15° and 35° and are close to $\pi/2 - \alpha$ when the incident angle $\alpha > 50°$. It is of interest that at all α the values of β_1 and β_2 were found to be almost identical, indicating the symmetry of surface structures, by analogy with that of ripples (e.g. [7]). A pronounced faceting (crimping) of the surface was also observed on (0001) HOPG-based composite fibers [4,11] and explained in terms of the Bradley–Harper model of relief formation [12].

Many other examples of faceted surfaces are cited in [13] where the theory of terraced topographies produced by oblique-incident ions at the late stage of ion erosion is presented. In this regard, it is pertinent to recall the earlier theoretical works [7,8], which investigated the dynamics of the faceting process on rippled surfaces. For (0001) HOPG, such surfaces were clearly recognized at intermediate ion fluences of about 10^{17} cm^{-2} [14].

The aim of the present study is to reproduce by means of classical trajectory simulations the experimental $S(\alpha)$-dependences reported in [10,11]. For 30 keV Ar ions, such dependence is compared in Fig. 1 with the results of simulations performed for a flat amorphous graphite (carbon) surface by use of the TRIM.SP and OKSANA programs (e.g. [15]). The comparison is justified taking into account the mosaic structure of HOPG, which may largely suppress crystallographic effects, especially at high fluences when HOPG structure is approaching that of isotropic polycrystalline graphites [4]. Fig. 1 demonstrates a striking difference between the measured and calculated sputter yields at α = 60–80°. The question arises whether the model of faceted surface is able to minimize the difference. This issue will be discussed below.

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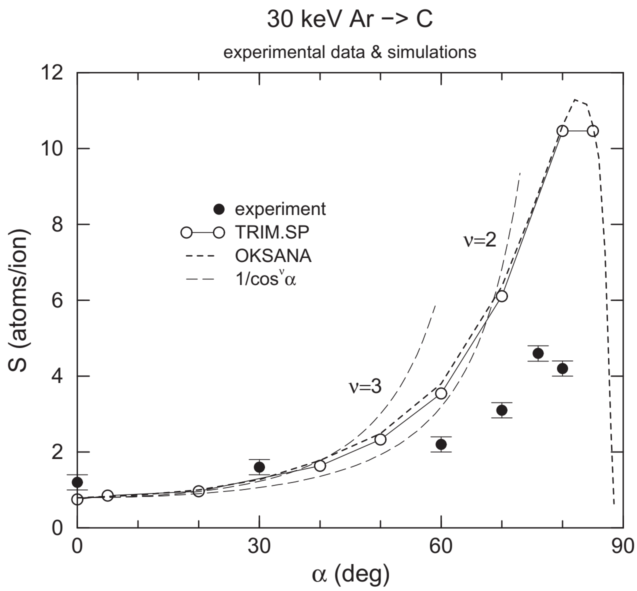

Fig. 1. Survey of measured [10] and calculated sputter yields for a graphite target bombarded with 30 keV Ar ions. Simulations were carried out for a flat surface using the computer codes TRIM.SP and OKSANA. The results of TRIM.SP simulations were taken from [10]. Also shown are the inverse cosine dependences approximating the simulated data.

Another issue that will be briefly considered is the angular distributions of sputtered atoms which may, but have not yet been studied experimentally.

2. The simulation program

The simulations were performed using the computer code OKSANA described in detail earlier [16]. Briefly, trajectories of bombarding ions and recoiling atoms generated in collision cascades are calculated in the binary collision approximation taking into account weak simultaneous collisions at large distances. For the reasons mentioned above, only disordered (amorphous) targets are considered. The target is simulated by rotation of a crystalline atomic block, the procedure of rotation being repeated from collision to collision. The screened Coulomb potential of Ziegler–Biersack–Littmark (ZBL) [17] was used as the interatomic potential. Inelastic energy losses were calculated according to the Firsov formula [18]. The direction of the incident ion beam was 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; the fall of the bombarding ions in the X–Z plane is always assumed (Fig. 2). The relief was modeled by a two-dimensional ridge-like function with a period $2x$ and a height z. The slope angles of ridge planes relative to the basal X–Y plane were identical (Fig. 2), as found experimentally [10].

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, was used for ejected atoms – candidates for sputtering. In accordance with common practice, the surface binding energy was assumed to be equal to the energy of sublimation. It should be noted that the OKSANA program allows to follow the trajectories of sputtered atoms until they are much above the surface but before the final escape such atoms (like scattered ions) can be recaptured by the side walls of the relief and contribute to sputtering. Since the steady-state regime of sputtering was simulated, no changes in the surface relief, originally specified, were considered.

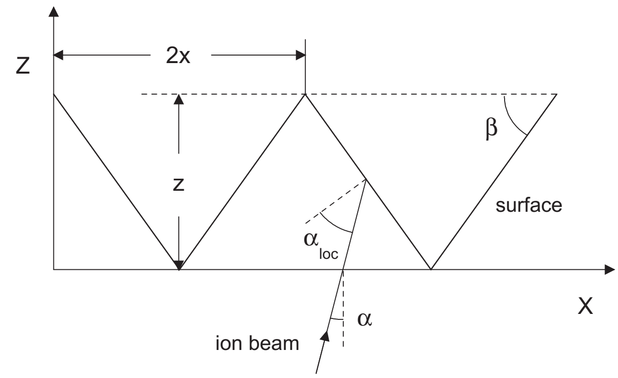

Fig. 2. Ridge-like model of surface relief used in the present simulations. x is the half-period of the relief along the X-axis, z the depth of the relief, α the angle of incidence measured from the normal to the basal plane X–Y, α_{loc} the local incidence angle, and $\beta = \text{atan}(z/x)$ the slope angle of a ridge plane.

The ejection direction of a sputtered atom was characterized by the azimuthal, φ, and polar, θ, angles. The angle φ is counted from the X–Z plane, the angle θ from the surface normal. The number of incident ions was chosen high enough to ensure that the values of Y were calculated with an accuracy of about ±1%. A typical run consisted of 100,000–200,000 sputtered atoms.

3. Results and discussion

Consider first the results for graphite sputtered with normally-incident Ar ions. Some idea of the collision process leading to sputtering of a relief surface is given in Fig. 3, which shows the trajectories of bombarding particles and the initial positions of sputtered atoms in the projection on the X–Z plane at $x = z = 50$ nm taken as an example. The figure predicts the penetration depth of the ions in the range 30–50 nm. It is seen that for heavy (compared to carbon) argon atoms the probability of ion backscattering is close to zero.

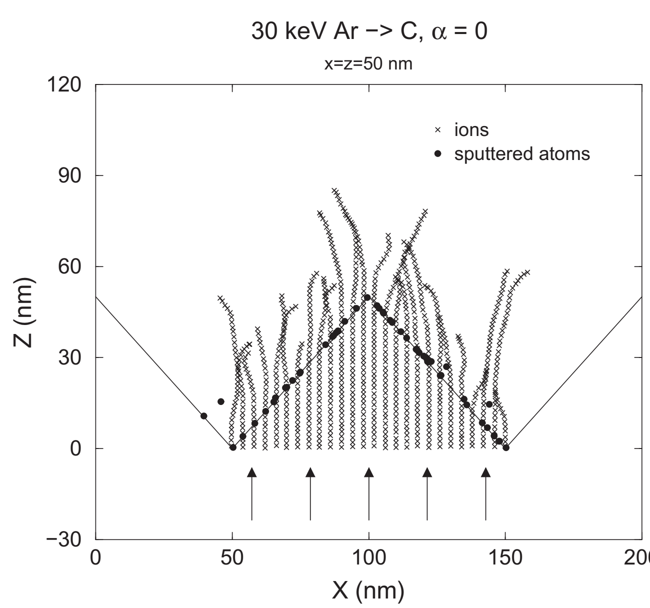

Fig. 3. Trajectories of 30 keV Ar ions incident on a ridged graphite surface at $\alpha = 0$ and $x = z = 50$ nm. The filled circles indicate the initial positions of sputtered atoms, i.e. at the moment of their birth in collision cascades. The broken line shows the solid surface.