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Simple model of surface roughness for binary collision sputtering simulations

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ABSTRACT

It has been shown that surface roughness can strongly influence the sputtering yield – especially at glancing incidence angles where the inclusion of surface roughness leads to an increase in sputtering yields. In this work, we propose a simple one-parameter model (the "density gradient model") which imitates surface roughness effects. In the model, the target's atomic density is assumed to vary linearly between the actual material density and zero. The layer width is the sole model parameter. The model has been implemented in the binary collision simulator IMSIL and has been evaluated against various geometric surface models for 5 keV Ga ions impinging an amorphous Si target. To aid the construction of a realistic rough surface topography, we have performed MD simulations of sequential 5 keV Ga impacts on an initially crystalline Si target. We show that our new model effectively reproduces the sputtering yield, with only minor variations in the energy and angular distributions of sputtered particles. The success of the density gradient model is attributed to a reduction of the reflection coefficient – leading to increased sputtering yields, similar in effect to surface roughness.

1. Introduction

It is well known that ion bombardment roughens the target surface [1], which in turn may influence the sputtering yield [2]. In a recent study [3] we demonstrated that the simulation of sputtering yields for grazingly incident ions requires the consideration of surface roughness. Grazing incidence conditions are typically found during transmission electron microscopy (TEM) sample preparation, one of the most important applications of focused ion beams (FIB) [4,5]. Glancing incidence angles may also occur during FIB milling of holes [6] or during irradiation of nanowires, for instance, when the nanowires bend towards the beam [7]. Recently, several groups have developed Monte Carlo binary collision (BC) codes that are capable of simulating ion bombardment of 2D and 3D micro- and nanostructures [8–14]. They all lack models of surface roughness, prohibiting meaningful simulation of glancing angle effects.

BC simulation studies of the effect of surface roughness on sputtering have mostly used geometrically modified flat surfaces, employing square waves [2], sinusoidal waves [3], or by applying fractal surface models [15,16]. All these models would be difficult to implement in 2D and 3D simulations, since the simulation needs to store a rough surface geometry interspersed with any mesoscale topographies of interest.

Yamamura et al. [2] have shown that reducing the target density in a surface layer has a similar effect as a geometrically defined rough surface. However, they used a monoatomic surface layer only, which limited the degree of roughness that could be introduced. In the present work, we generalize Yamamura's idea by using a surface layer with a density that decreases linearly towards the surface, which we henceforth call density gradient model. The sole parameter of this model is the thickness of the layer, which may be larger than monoatomic. This removes ambiguity from the model as compared to, e.g., the sinusoidal model where fits to the experimental data are available across multiple pairings of wavelengths and amplitudes [3]. Equally important, the density gradient model is easily implemented in 2D and 3D BC simulations.

To validate the model, we compare sputtering yields and energy and angular distributions of sputtered atoms with the predictions of three geometrically defined models with wave vectors parallel to the projection of the ions' incidence direction to the surface. To aid the construction of a realistic rough surface, we have also performed molecular dynamics (MD) simulations of sequential Ga impacts on a Si surface.

This study is carried out for 5 keV Ga ions impinging on Si. The simulations are compared to experimental data obtained at FEI

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Company [17]. A lower ion energy is used than in our previous study [3] mainly to facilitate the MD simulations.

2. Simulation specifics

2.1. MD modeling

MD modeling was carried out at Jagiellonian University using a modified version of LAMMPS [18]. The simulation cell was 120 Å × 120 Å × 80 Å initially filled with single-crystalline (100)-Si with a (2 × 1) reconstructed surface. The number of Si atoms in this cell was 57112. Periodic boundary conditions were used in the lateral directions. Stochastic and rigid layers, 7 Å and 3 Å thick, respectively, were used at the bottom to simulate the thermal bath that kept the sample at the required temperature and to keep the shape of the sample. The simulations were run at 0 K temperature. The target was sequentially bombarded with 5 keV Ga ions at polar angles of 89° and 85° and an azimuthal angle of 35° with respect to the cell edge which is a [010] direction. The latter was chosen as to minimize possible artifacts of the periodic boundary conditions due to the passage of the ions over regions they have previously interacted with while slowly glancing off the surface. Each impact was simulated for 2 ps. The resulting structure was used as initial condition for the subsequent impact after removal of all sputtered atoms and any excess kinetic energy from the system. The latter was achieved by an energy quenching procedure that involved application of gentle viscous damping forces to the entire sample for 0.2 ps. A Tersoff-3 potential [19] was used for Si-Si interactions, and the ZBL potential [20] splined with a Lennard-Jones (LJ) potential for Ga-Si interactions.

2.2. BC modeling

Monte Carlo simulations using the BC approximation were carried out at TU Wien using the simulator IMSIL [21,22]. As in our earlier work [3] we use the ZBL interatomic potential [20], the Oen– Robinson model for electronic stopping [23] with a cutoff energy of 10 eV, and a planar surface potential with a surface binding energy between Si and Si of 4.7 eV. Since the refraction of the incident ions at the surface potential is significant under the conditions studied, the choice of the surface binding energy between Ga and Si is also critical. We use a value of 2.82 eV [24]. All of the BC simulations were carried out using the static mode of IMSIL, wherein the target starts in an amorphous state as pure silicon, and its modification by the implanted gallium is not taken into account over the course of the simulation. 25,000 impacts were carried out for sputter yield calculations and 5 million impacts for determining the energy and angular distributions of sputtered atoms.

2D geometries are specified in IMSIL by polygons which are converted to a signed distance function defined on a Cartesian grid covering the simulation domain [13]. IMSIL was adapted for this research through the addition of a periodic geometry mode, which allowed to set the lateral size of the simulation domain equal to one wavelength. The vertical size was chosen 300 Å plus the roughness amplitude, which led to a negligible forward sputtering yield of 2×10^{-4}, thus indicating sufficient thickness to simulate an infinitely thick target. In order to exclude any significant discretization errors, we used 2000 segments for the polygons and 1 million cells for the internal grid.

Three geometric surface models were used: Cosine, triangular, and double cosine (Fig.1). The double cosine function is defined by the superposition of two cosine functions with wavelengths differing by a factor of three:

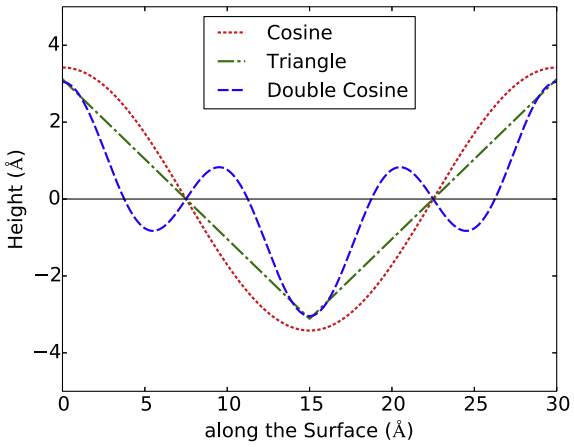

Fig. 1. Geometric roughness models used in this study, shown for a wavelength of 30 Å: Cosine, triangular, and double cosine. All surface models are shown with best-fit parameters.

$$z(x) = \frac{A}{2}\left(\cos\frac{2\pi}{\lambda}x + \cos\frac{6\pi}{\lambda}x\right), \tag{1}$$

where A is the amplitude and λ is the period. The choice of the wavelength λ is not very critical and will be estimated from the results of the MD simulations. The amplitude A will be determined by fitting to experimental sputtering yield data.

The density gradient model is implemented by creating collision partners at the end of the free flight paths with probabilities

$$p = \begin{cases} 1 & \text{for } d \geqslant w \\ d/w & \text{for } 0 < d < w \\ 0 & \text{for } d \leqslant 0, \end{cases} \tag{2}$$

where d denotes the signed distance from the surface (negative values outside the target) and w is the width of the density gradient layer. Effectively this means that the density of target atoms decreases linearly towards the surface within the layer $0 < d < w$, as illustrated in Fig. 2a. The parameter w will be determined by fitting to the experimental sputtering yield data. Note that in the limit of zero wavelengths the geometric surface models correspond to reduced-density layers. These densities are shown in Fig. 2b and are compared with the density gradient model.

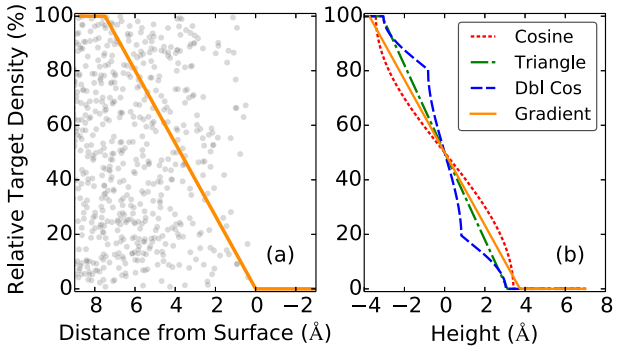

Fig. 2. (a) Schematic drawing of the target density in the density gradient model. Filled circles represent atoms. (b) Comparison of the density with equivalent density profiles of the geometric roughness models. The height axis in (b) has been shifted with respect to (a) so its origin is at the center of each roughness layer. All surface models are shown with best-fit parameters.

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