Step-edge sputtering through grazing incidence ions investigated by scanning tunneling microscopy and molecular dynamics simulations

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Scanning tunneling microscopy is used to quantify step-edge sputtering of Pt(111) at 550 K by grazing incidence ion bombardment with 5 keV Ar^{+} ions. For bombardment conditions causing negligible erosion on terraces, damage features associated with step bombardment allow us to visualize step retraction and thus to quantify the step-edge sputtering yield. An alternative method for step-edge yield determination, which is applicable under more general conditions, is the analysis of the concentration of ascending steps together with the removed amount as a function of ion fluence. Interestingly, the azimuthal direction of the impinging ions with respect to the surface significantly changes the sputtering yield at step edges. This change is attributed to the orientation dependence of subsurface channeling. Atomistic insight into step-edge sputtering and its azimuthal dependence is given by molecular dynamics simulations of ion impacts at 0 and 550 K. The simulations also demonstrate a strong dependence of the step-edge sputtering yield on temperature.

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I. INTRODUCTION

Patterning of metallic and semiconductor surfaces through grazing incidence ion bombardment has gained increasing interest in the last decade. The ability to create nanogrooves and ripple patterns[1–6] with tunable lateral periodicity and amplitude has several potential applications. The resulting morphology can be used as a template for the adsorption of large molecules,[7] for the manipulation of magnetism[8] or for tuning the chemical reactivity of catalytically active surfaces.[9] Grazing incidence ion beams are also of interest in ion beam assisted deposition[10] and were shown to effectively change texture and roughness of thin films.[11]

A practical prerequisite for future applications of grazing incidence ion beams is knowledge of how fast the surface erodes for a given ion flux of a specific energy. For normal incidence ion bombardment, the erosion rate is largely temperature and morphology independent. The sputtering yield $\bar{Y}$—the average number of sputtered particles per incident ion—may be readily calculated with fair accuracy by analytical formulas[12,13] or Monte Carlo simulations based on the binary collision approximation [e.g., TRIM (Ref. 14)]. Knowledge of this is thus sufficient for the prediction of erosion rate.

For grazing incidence ions, the situation is considerably more difficult. The erosion rate or the average sputtering yield $\bar{Y}$ is a sensitive function of the surface morphology and, thus, also of temperature and ion fluence, as we have shown in our previous work.[15] Whereas the ion is reflected from flat terraces without sputtering—this process is termed *surface channeling* in the ion-surface scattering community—large angle scattering and significant sputtering take place if ions interact with step atoms or point defects.

In this paper, we describe two methods of measuring the sputtering yield Y^{step} characterizing the interaction of grazing incidence ions with surface steps. The first, which is a very direct method, visualizes Y^{step} by measuring step retraction through scanning tunneling microscopy (STM) topographs. While this method is only applicable under extremely grazing incidence conditions, the second method is generally more applicable. It relies on the determination of the step concentration and on measuring the removed material. We show that with knowledge of the step-edge concentration and of the normal incidence amorphous yield Y^{amorph}, the fluence dependent global erosion rate or $\bar{Y}$ may be predicted with an accuracy of a factor of 2. Finally, with the help of molecular-dynamics (MD) simulations, we are able to understand the significant dependence of Y^{step} on the azimuthal direction and find a strong dependence of the yield on temperature.

II. GEOMETRICAL MODEL

Above, we already referred to the step-edge yield Y^{step}. To clarify terminology and as a prerequisite for the presentation of the experimental results, we briefly summarize some of our previous work related to sputtering and damage at grazing incidence ion bombardment.[15,16] As sketched in Fig. 1(a), for the grazing incidence geometry, we distinguish two classes of ion trajectories. The first class consists of ions hitting an ascending (illuminated) step edge either indirectly, after reflection from the lower terrace [trajectory labeled 1 in Fig. 1(a)], or directly [trajectory labeled 2 in Fig. 1(a)]. The second class consists of all other ions from which the majority consists of ions hitting the terrace [trajectory labeled 3 in Fig. 1(a)]. Also, ions approaching the surface at or close to descending steps belong to this class. We label the distance of the ion penetration point through the plane of the upper terrace layer nuclei [dashed line in Fig. 1(a)] to the step-edge atom nucleus by ξ. All ions with $\xi \in [-x_c, 0]$ belong to the first class. Here, x_c characterizes the width of the zone of influence with Δh being the step height; it is $x_c = 2\Delta h \tan \vartheta$ from geometry.

The ions of the first class enter the zone of influence in front of an illuminated step edge [compare Fig. 1(b)]. Thus, they hit the step edge and cause step-edge sputtering with a yield Y^{step}. For all other ions, a terrace impact takes place

