Sputtering at grazing ion incidence: Influence of adatom islands

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When energetic ions impinge at grazing incidence onto an atomically flat terrace, they will not sputter. However, when adatom islands (containing N atoms) are deposited on the surface, they induce sputtering. We investigate this effect for the specific case of 83°-incident 5 keV Ar ions on a Pt (111) surface by means of molecular-dynamics simulation and experiment. We find that—for constant coverage Θ—the sputter yield has a maximum at island sizes of $N \cong 10-20$. A detailed picture explaining the decline of the sputter yield toward larger and smaller island sizes is worked out. Our simulation results are compared with dedicated sputtering experiments, in which a coverage of $\Theta = 0.09$ of Pt adatoms are deposited onto the Pt (111) surface and form islands with a broad distribution around a most probable size of $N \cong 20$.

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I. INTRODUCTION

Energetic ion incidence on surfaces is responsible for surface erosion and damage production. However, at grazing incidence angles these effects are strongly reduced. Flat surfaces reflect ions at glancing incidence with only little energy input into the surface. However, even slight imperfections of the surface may alter the situation dramatically. The effect of surface steps has been analyzed in detail.[1–4] It was shown that if the ion impact point is in the vicinity of an ascending step edge, an ion may sputter as many atoms as for normal incidence. The sputter yield of a stepped surface is thus primarily governed by the step density. Similarly, the influence of single adatoms on a surface was analyzed and it was found that for small coverages, the sputter yield is linear in the adatom coverage.[5–7]

Real surfaces may be covered by adatom (and vacancy) islands as well, and the question arises how the sputter yield is influenced by these islands. One might think that adatom islands simply interpolate between the effects of isolated adatoms and straight step edges. However, this view is too simple, and a detailed picture of the effect of adatom islands on sputtering will be developed here.

Grazing-ion incidence on surfaces is interesting from a fundamental point of view but it also finds applications. Here, we mention, in particular, their ability to pattern surfaces, and to induce ripple structures on the surface.[8] Recently, the application of glancing-ion incidence on nanopatterning of surfaces has been investigated and the detailed atomistic aspects of glancing-ion incidence on surfaces were shown to be relevant for an understanding of the initial stages of pattern formation on metallic surfaces.[2,9,10]

The effect of surface defects on the trajectories of incident ions has already been considered in the 1970s. Interest in this question arose due to the technique of low-energy ion scattering which was used successfully to study the composition and structure of the surface.[11–14] It allowed to measure preexisting surface defects and also adsorbates.[15–18] These experiments could be interpreted using simulations based on the binary-collision approximation, in which the result of the ion impact on the target could be ignored.[11,12] These simulations did not allow to determine sputtering or ion-induced damage. Therefore, in our present analysis of the effect of surface defects on sputtering, we have to go beyond the binary-collision approximation and to employ full molecular-dynamics simulations.

In this paper we approach the question as to how adatom islands contribute to sputtering at grazing incidence by experiment and simulation. Using molecular-dynamics simulation we can address this question systematically, at least for small island sizes, and obtain a detailed atomistic view of the sputter processes in dependence of the ion impact point. These simulations are performed for 5 keV Ar impact on the Pt (111) surface at an incidence angle of 83° to the normal. At this angle, a flat terrace reflects the ion beam without being damaged or sputtered, and hence all damage can be attributed unambiguously to the adislands at the surface. We note that we investigated previously the effects of a varied incidence angle on sputtering from surface steps and found qualitatively similar results. For the 5 keV Ar impact at 83° incidence onto the Pt (111) surface, where already a considerable body of information on the sputtering behavior both from experiment and simulation is available,[1–7] we perform dedicated experiments. Here, the Pt surface is initially covered by Pt adatom islands which have been deposited on the surface prior to ion bombardment. Simulations and experiment agree satisfactorily, when the size distribution of the adatoms is taken into account.

II. METHOD

A. Simulations

We consider the impact of 5 keV Ar atoms on a Pt (111) surface at a fixed incidence angle of 83° toward the surface normal. The incidence azimuth is chosen such that its projection onto the surface is aligned in the $[\bar{1}\bar{1}2]$ direction. Our simulation crystallite contains 15 layers; each layer extends

