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The sputter cross section of a surface-vacancy island

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ABSTRACT

Using molecular-dynamics simulation we investigate the effect of surface-vacancy islands on ion-induced sputtering. As an exemplary case, the sputtering of a Pt(1 1 1) surface by 5 keV Ar^+ ions incident at 83° towards the surface normal is investigated. We find that only the ascending step of the island induces sputtering. Wide vacancy islands exhibit the direct-hit, indirect-hit and channeling zones previously identified for surface steps and adatom islands. A special role is played by the descending step edge. Even though it is not sputtered itself, it deflects ion trajectories and may direct them to the ascending step edge thus enhancing sputtering. We derive a simple criterion based on the shadow cone of the descending step to decide whether a vacancy island contributes to sputtering or not.

1. Introduction

Surface defects influence ion bombardment at glancing incidence angles significantly. At normal incidence the sputter yield is dominated by impacts onto the flat terrace and the effect of defects is minor. When the ion beam is gradually inclined towards the surface, the yield does not decrease smoothly with increasing incidence angle. Rather, at a characteristic angle, the sputter yield decreases abruptly to zero. The motion of the approaching ions is steered by the collective repulsive ion-surface potential away from the surface; thus the ions are reflected specularly off the surface. For 5 keV Ar^+ ions, the effect appears at an angle of around 75° towards the surface normal, until at angles steeper than 83°, the flat terrace has zero sputter yield. At such incidence angles, the contribution of the defects to sputtering is decisive. The role of such defects – ascending surface steps, adatom islands, or a distribution of isolated adatoms – has been investigated experimentally and by molecular-dynamics simulation thoroughly in the past [1–12]. For adatom islands, the front of the defect (the ascending step edge) plays the decisive role such that the island size is of minor influence. However, atoms at the descending step edge of an adatom island are not sputtered.

Surface defects can be created in a controlled manner. After deposition of atoms of the same species on the surface, at low temperature the deposited atoms will be distributed almost randomly on the surface. When the surface is annealed, the atoms agglomerate forming compact adatom islands. However, for coverages >0.5, the surface can be viewed to be covered by vacancy islands rather than by adatom islands.

Glancing-incidence ion bombardment at keV energy has been used as a method to create nano-patterns on surfaces [1–3,13]. The method is used, for instance, in the fabrication of templates for large-molecule adsorption [14], surface magnetism [15–17], and for tuning the chemical reactivity of catalytically active surfaces [18].

In this paper we use molecular-dynamics (MD) simulation to investigate the question how surface vacancy islands influence sputtering at grazing incidence. The role of the (beam-facing) descending step will be analyzed. We focus on vacancy islands which are one monolayer deep, and do not consider deeper (crater-type) islands.

2. Method

2.1. Simulation

We consider a Pt crystallite with a (1 1 1) surface. Its lattice constant is 3.924 Å; in the following the nearest-neighbor distance $r_{NN} = 2.775$ Å, and the interlayer spacing of (1 1 1) planes, $h = 2.26$ Å, will be important. Ar^+ ions with an energy of 5 keV and an impact angle of $\vartheta = 83^\circ$, measured with respect to the surface normal, impinge on it. The azimuth of the incident ions is aligned with the $[\bar{1}\,\bar{1}\,2]$ crystallographic direction. At this angle, terrace sputtering is zero [5,6], and hence sputtering is induced only by the surface defect.

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