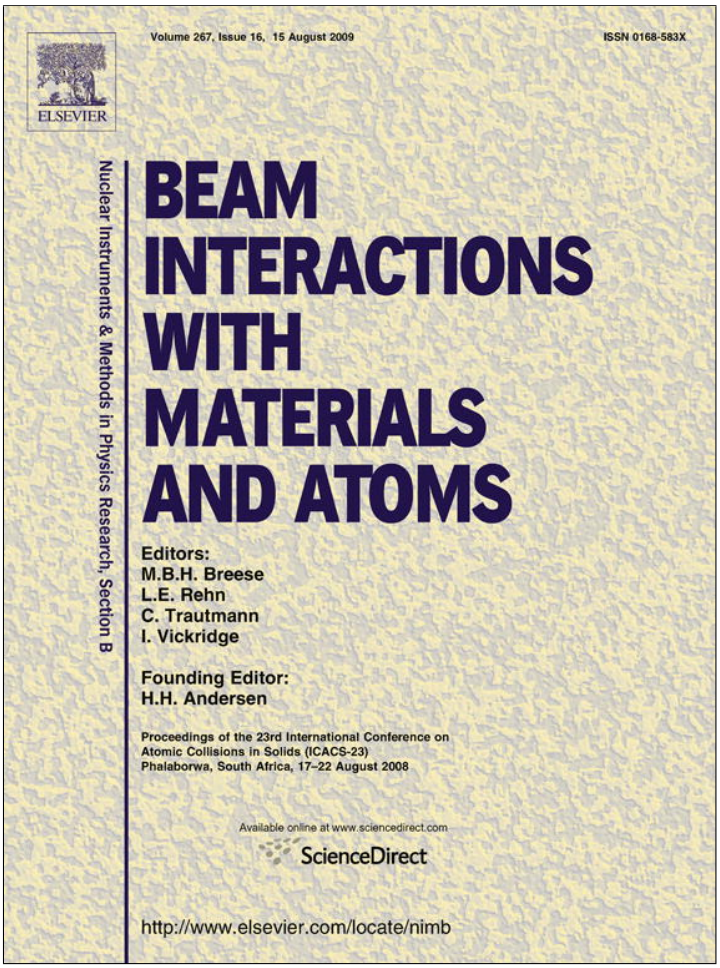

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Competition of terrace and step-edge sputtering under oblique-incidence ion impact on a stepped Pt(1 1 1) surface

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ABSTRACT

Using molecular-dynamics simulation, we study the sputtering of a Pt(1 1 1) surface under oblique and glancing incidence 5 keV Ar ions. For incidence angles larger than a critical angle ϑ_c, the projectile is reflected off the surface and the sputter yield is zero. We discuss the azimuth dependence of the critical angle ϑ_c with the help of the surface corrugation felt by the impinging ion. If a step exists on the surface, sputtering occurs also for glancing incidence $\vartheta > \vartheta_c$. We demonstrate that for realistic step densities, the total sputtering of a stepped surface may be sizable even at glancing incidence.

1. Introduction

Ion impact at glancing incidence is particularly sensitive to surface defects. If the perpendicular energy of the ion is only of the order of a few tens of eV, the ion will be reflected specularly from the surface without inducing defect formation or sputtering. If the ion scatters at a surface defect – such as an adsorbate or an adatom, or as in the present work, a surface step – a substantial amount of the ion energy may be transferred to the surface, inducing defect formation and sputtering. This mechanism has been investigated recently both by molecular-dynamics simulation and by experimental measurements based on scanning tunneling microscopy [1–7]. The phenomenon is of immediate interest to the field of the nanopatterning of thin films [8,9] with applications, e.g. as a template for the adsorption of large molecules [10], for the manipulation of magnetism [11] or for tuning the chemical reactivity of catalytically active surfaces [12].

If the ion beam is inclined further from the target surface and the perpendicular energy of the ion increases, not only defects but also the flat terrace itself will contribute to sputtering. In the present paper, we address the question how the contribution of the flat terrace to sputtering starts increasing, and finally dominating, for less glancing incidence angles. At the same time, we inquire how the contribution of step edges to sputtering evolves as a function of the ion incidence angle. These questions will be answered for the specific case of 5 keV Ar impact on the Pt(1 1 1) surface, since this system has been characterized particularly well in the past [7]. The use of molecular-dynamics simulations allows us to study the sputter process in atomistic detail and in particular to include surface defects, such as the step edge, in a realistic way.

2. Method

Our MD simulation procedure is briefly described in the following [1,2]. The simulation target is a Pt crystallite with a (1 1 1) surface. For simulations with a flat target terrace, it contains about 19,210 atoms, arranged in nine layers. Each layer extends 160 Å in the direction of the ion velocity and is 87 Å broad. For simulations with a stepped target surface, the crystallite contains 62,144 atoms, arranged in 17 layers plus one half-layer on top of it. The size of the layers is 264×87 Å^2, and the half-layer was cut at a position 107 Å from the edge of the crystal to form an ascending B-step. In all cases, the crystallite is initially at 0 K.

We employ a many-body interaction potential [13] to describe the Pt–Pt interatomic interaction, which has been splined at high energies to the ZBL [14] potential. The Ar–Pt interaction is modeled to be purely repulsive according to the ZBL potential. The potentials are cut-off at 5.1 Å. We simulated the processes occurring after ion impact for 10 ps. Sputtered atoms are identified as those atoms which have no further interaction with the target surface. The data presented are averages over 100 events per unit cell for

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