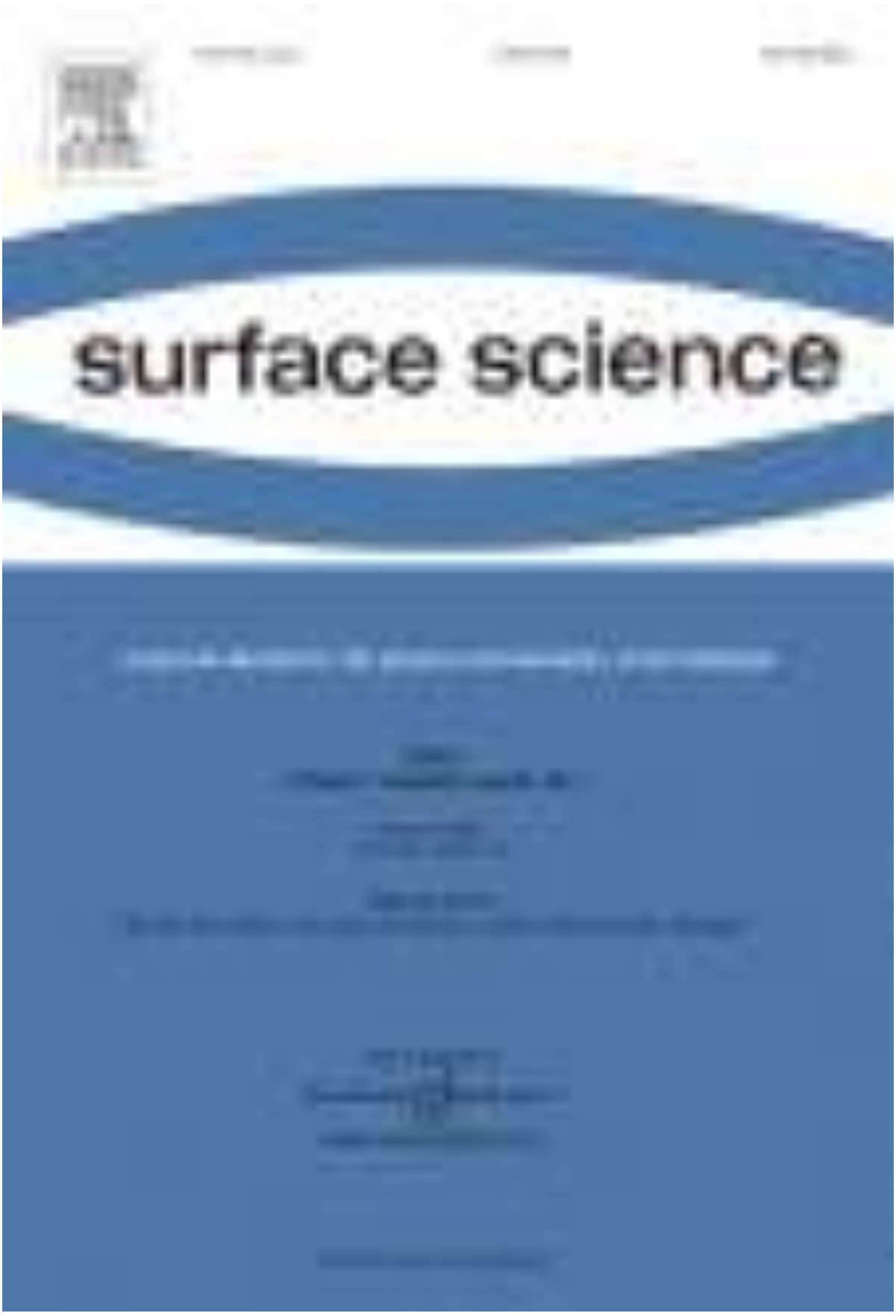
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Grazing incidence impact of ions on an adatom-covered surface: Molecular-dynamics study of sputtering, surface-damage formation and ion-induced adatom mobility

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Received 19 September 2005; accepted for publication 16 December 2005
Available online 14 February 2006

Abstract

Using molecular-dynamics simulation, we study the exemplary case of 5 keV Ar impact onto a Pt(1 1 1) surface at 83° incidence angle towards the surface normal. Under these conditions, on a flat terrace, the ions are specularly reflected, inducing neither damage nor sputtering of the surface. This situation changes drastically, if the surface is covered randomly with a coverage Θ of adatoms. For $0.1 < \Theta < 0.5$, average sputter yields and damage of up to a value of 5 and 9, respectively, are achieved. For coverages around $\Theta = 0.3$–0.4, 50 adatoms are relocated on the average on the surface, affecting an area of around 1000 Å^2. This ion-induced mobility promotes adatom clustering, which typically leads to a rim-like structure around the ion impact point.

Keywords: Molecular dynamics; Ion–solid interactions; Radiation damage; Surface structure, morphology, roughness, and topography; Platinum

1. Introduction

Interest in glancing-ion incidence on surfaces has been increasingly high in recent years both from an applied and a fundamental point of view [1]. In fundamental studies, glancing-ion reflection or channeling along the surface has been used as a means for surface analysis and has brought interesting insight into many aspects of surface science, including electron emission [2], surface magnetism [3], and surface topography [4]. Furthermore, at slightly less glancing incidence angles, ion beams are used to pattern surfaces, inducing pronounced ripple structures on the surfaces. This phenomenon has been found for a variety of materials and may find applications in nanopatterning of surfaces [5]. Recently, 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 [6].

While in the studies of glancing-ion surface interaction, it is usually stated that the interaction is strongly affected by any defects existing on the surface [7], the theoretical analysis or simulation of the interaction is often performed using binary interaction codes and concentrates on the fate of the projectile ion [8,9]. However, in the cases of structure formation under glancing-ion incidence, also the fate of the target—i.e., damage formation and sputtering—is of importance. Here, the interaction of glancing-incidence ions with surface steps has already been investigated recently, and a strong influence of steps on both damage and sputtering has been found [10,6].

In the present paper, we wish to investigate the effect of adatoms present on the surface. To this end, we study ion impact on an atomistically rough surface, which is constructed as a surface covered randomly with atoms. We chose to study the specific case of 5 keV Ar impact on the Pt(1 1 1) surface under 83° incidence angle since this system is being used in actual experiments [6].

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doi:10.1016/j.susc.2005.12.063