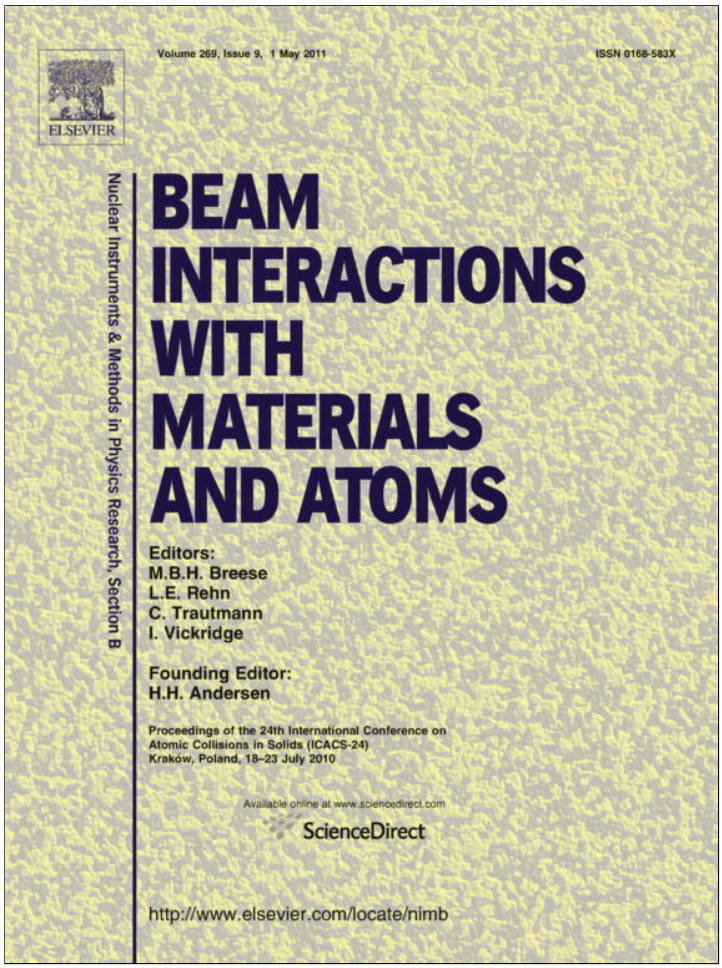

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News on sputter theory: Molecular targets, nanoparticle desorption, rough surfaces

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ABSTRACT

Sputtering theory has existed as a mature and well-understood field of physics since the theory of collision-cascade sputtering has been developed in the late 1960s. In this presentation we outline several directions, in which the basic understanding of sputter phenomena has been challenged and new insight has been obtained recently.

Sputtering of molecular solids: after ion impact on a molecular solid, not all of the impact energy is available for inducing sputtering. Part of the energy is converted into internal (rotational and vibrational) excitation of the target molecules, and part is used for molecule dissociation. Furthermore, exothermic or endothermic chemical reactions may further change the energy balance in the irradiated target.

Nanoparticle desorption: usually, the flux of sputtered particles is dominated by monatomics; in the case of a pronounced spike contribution to sputtering, the contribution of clusters in the sputtered flux may become considerable. Here, we discuss the situation that nanoparticles were present on the surface, and outline mechanisms of how these may be desorbed (more or less intact) by ion or cluster impact.

Rough surfaces: real surfaces are rough and contain surface defects (adatoms, surface steps, etc.). For grazing ion incidence, these influence the energy input into the surface dramatically. For such incidence angles sputtering vanishes for a flat terrace; however, ion impact close to a defect may lead to sputter yields comparable to those at normal incidence. In such cases sputtering also exhibits a pronounced azimuth and temperature dependence.

1. Introduction

The theory of the sputter process induced by atomic or cluster impact is rather a mature field which has been reviewed repeatedly in the recent past [1,2]. Still, due to the possibility of performing novel experiments (such as STM experiments to characterize surface damage by single ions), to the need to understand sputtering in more exotic situations (such as sputtering of condensed gases, even though this has a long history [3]), and due to the possibilities of simulating the sputter process in detail and thus extracting relevant information, our understanding of the mechanisms underlying sputtering has been extended in several areas.

In this review, we shall focus on three aspects of sputtering which can be subsumed under the above categorization: the sputtering of molecular targets, mechanisms underlying the desorption of nanoparticles, and the sputtering of rough or nanostructured surfaces. Certainly this selection is rather personal as we have been engaged in this work. We wish to mention that further important work in sputtering has been performed recently, such as the role of electronic excitations in metals during and after ion impact, sputtering of macromolecular and biomolecular targets, formation of nano-scale surface patterns by sputtering, sputtering by cluster impact, and sputtering of biomolecular targets; these results are contained elsewhere in these proceedings.

The results discussed below have been obtained using the method of classical molecular dynamics simulation [4,5]. As physics input, it needs only a knowledge of the interatomic interaction forces, and the electronic stopping. Hence this method has proven to provide atomistic insight into the mechanisms of sputtering and the properties of sputtered particles.

2. Molecular solids

The sputtering of molecular targets is of interest for novel applications in SIMS, in which depth profiling of materials containing large biomolecules is now investigated. In these cases, often clusters are used as projectiles – in particular small Au_n or Bi_n ($n = 1$–3) clusters or fullerene C_{60} molecules. Other applications reside in the astrophysical and planetary sciences, where the ice surfaces of moons, comets, dust grains, etc., are irradiated by stellar wind or dust particles.

Let us consider a diatomic homonuclear molecule like O_2. Its dissociation energy is $D_0 = 5$ eV, and the cohesive energy of the molecular solid is $U = 0.1$ eV. When a target consisting of these molecules

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