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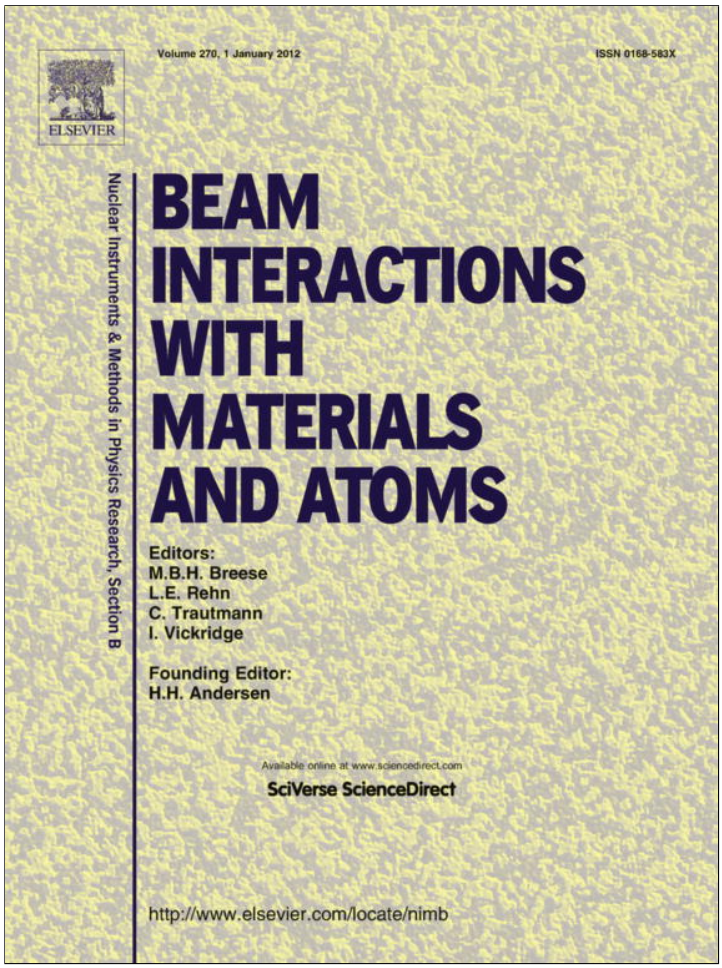

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Short Communication

Sputtering of dimers off a silicon surface

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ABSTRACT

We present experimental and molecular-dynamics simulation results of the sputtering of a Si surface by 2 keV Ar ions. Results on both the monomer and dimer distributions are presented. In simulation, these distributions follow a generalized Thompson law with power exponent $n = 2$ and $n = 3$, respectively. The experimental data, obtained via plasma post-ionization in an SNMS (secondary neutral mass spectrometry) apparatus, show good agreement with respect to the dimer fraction, and the relative energy distributions of dimers and monomers. The consequences for the dimer sputtering mechanism are discussed.

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1. Introduction

Silicon is arguably the most important material used in surface characterization techniques. For ion-irradiation based methods, such as secondary-ion mass spectrometry (SIMS) or secondary-neutral mass spectrometry (SNMS), hence a considerable amount of information about the basic sputtering process has been produced over the years, and sputter yields and sputtered particle energy distributions have become reliably known [1–4].

Besides monatomic species, as a rule also dimers and larger clusters are found in the sputtered flux. An understanding of the properties of sputtered molecules is necessary for a reliable interpretation of sputtered-particle mass spectra and surface analysis. In sputter theory, various mechanisms for the sputtering of dimers have been analyzed and discussed [5–7]; these include the so-called direct-emission mechanism [8,9], in which close neighbors are emitted, and the so-called recombination mechanism [10], in which previously unbound atoms are associated during the emission process to form a dimer. These two different mechanisms give rise to distinctly different energy distributions of emitted dimers.

Sputtering of a Si surface by keV ions has been studied repeatedly by molecular-dynamics simulation. We mention in particular the early work by Stansfield et al. [11] and by Smith et al. [12], in which the sputtering of both a reconstructed and a non-reconstructed Si (100) surface by $\leqslant 1.5$ keV Ar ions was examined. These studies used a Stillinger–Weber [13] and a Tersoff [14] interatomic interaction potential, respectively. Their results on the energy distribution and the depth of origin of sputtered monomers are comparable, while small differences in the angular emission distributions show up. No results on sputtered dimers were reported.

In the present paper, we study dimer emission from a Si surface induced by 2 keV Ar impact. We compare energy distributions obtained from an SNMS apparatus with those obtained by molecular-dynamics simulation. Our results will allow to draw conclusions on the dimer sputtering mechanism.

2. Method

2.1. Simulation

We employ a standard molecular-dynamics code for the sputtering simulation. Our target crystallite consists of 5407 Si atoms arranged in 30 monolayers. The surface is a (100) surface in 2×1 reconstruction. Apart from the free surface, the outermost atoms at the other five boundaries were kept fixed, surrounded by an energy-damping zone [15]. We checked with the help of a larger simulation target (270,504 atoms with a depth of 100 layers) that our simulation results reproduce sputtering reliably.

Ar atoms impinge with an energy of 2 keV on the Si surface, with perpendicular incidence direction. In total, we simulate 50,000 individual Ar impacts. For each impact, the exact impact point has been varied randomly within the irreducible surface impact cell [16,17]; this gives us a statistically reliable overview over all possible impact conditions. Note that each impact occurs on a

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