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Sputtering of a silicon surface: Preferential sputtering of surface impurities

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ABSTRACT

We present molecular-dynamics simulations of the sputtering of an impurity atom off a Si 2×1 (100) surface by 2 keV Ar ions. The impurity is characterized by its mass and its binding energy to the Si substrate. We find that sputtering strongly decreases with the mass and even more strongly with the binding energy of the impurity atom to the matrix. The velocity of the impurity perpendicular to the surface is reduced with increasing impurity mass and binding energy. In terms of available ionization theories we can conclude that heavier impurities will have a smaller ionization probability.

1. Introduction

Silicon is arguably the most important material used in surface characterization techniques. For ion-irradiation based surface-analysis 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].

Often surface analysis techniques are needed to inquire about the near-surface composition of impurities in silicon. Then besides the sputter properties of the Si matrix, also an understanding of the preferential sputtering of impurity elements is required. The calculation of the sputter yield of an impurity atom from a Si matrix is nontrivial. In general it depends on the impurity mass, its binding to the matrix, but also to the local relaxation of the matrix around the impurity atom.

Additionally, besides monatomic species, as a rule also dimers and larger clusters are found in the sputtered flux. Again, an understanding of the properties of sputtered molecules is necessary for a reliable interpretation of sputtered-particle mass spectra and surface analysis. The understanding of preferential sputtering effects has a long and successful history [5–9], and computer simulation could contribute substantially [10–15]. However, most simulation studies have been performed for metallic targets, and a dedicated analysis of preferential sputtering from a Si surface is still missing.

Here we use molecular dynamics to examine the sputtering behavior. Since the sputtering yield of Si is low ($Y < 1$), and the impurity is diluted, this is a computer-time consuming task. For the calculation of preferential sputtering effects, we use here a novel strategy. We run a simulation in pure Si. If an atom (let us call it 'atom *i*') has been sputtered, we rerun this simulation, but with exchanging before the start of the simulation atom *i* by the impurity atom X. We can thus determine the probability that the impurity X is sputtered relative to the probability that the Si atom was sputtered.

Since here we are not interested in the exact chemical nature of the impurity and of its interaction with Si, we model it by its two most important characteristics: its mass M_x and its binding energy ϵ_x. All other parameters of the interaction are kept fixed, and identical to Si. This also guarantees that the Si lattice is not distorted around the impurity atom.

2. Method

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 5 boundaries were kept fixed, surrounded by an energy-damping zone [16]. 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

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