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Influence of the ion impact azimuth on glancing-incidence keV ion impact on the Si(100) surface

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ABSTRACT

Using molecular-dynamics simulation, we study the impact of 3 keV Ar^+ and Xe^+ ions at glancing incidence onto the Si(100) surface. The (2×1) reconstructed surface forms subsurface channels, which are able to trap the incoming ions. We choose two azimuth angles of the impinging ions, parallel and perpendicular to the dimer rows on the target surface. Surface steps allow glancing ions to enter these subsurface channels. The probability of subsurface channeling is pronouncedly larger for ion impact along the dimer rows, since for this azimuth the subsurface channels have a larger cross section. Finally, our simulation results demonstrate that surface-channeling events can be identified by their characteristic damage features.

1. Introduction

The study of Si surfaces is of great importance in view of their potential for technological applications. As electronic devices are continuously decreasing in size, a profound understanding of nanoscale material processes is mandatory. Theoretical as well as simulational studies may provide important microscopic input to understand and also to propose novel methods for advanced atomic-scale fabrication techniques.

Theoretical and experimental research on the Si surface has started decades ago, providing a huge amount of information which assisted the rapid growth of silicon-based technologies [1]. As a prominent example, the reconstruction characteristics of Si surfaces and their potential for self-organized nano-patterning have been reported [2–6]. However, the interaction of the Si surface with single-ion impact under glancing incidence has not yet been sufficiently explored [7].

Ion interaction with Si has attracted considerable attention, since, under certain conditions, sputtering by ion beams induces surface patterning of the Si surface. Surface structures such as ripples and nano-dots are created and can be controlled by tuning the energy and/or the incidence angle of the ion beam [8]. However, in the low-energy range (at a few keV), the spontaneous process of pattern formation may also turn out to be disadvantageous for controlled surface modification techniques [6]. Theoretical studies on the origin of pattern formation are still under way. Both continuum models [9] and Monte Carlo computer simulations [10] have been employed to understand the underlying mechanism of nano-patterning, and have obtained satisfactory agreement with experiments in several cases.

The length scale of the self-organized surface patterns is in the range of 10 to 1000 nm. This is quite large for atomistic simulation techniques such as the molecular-dynamics method. However, atomistic simulation is able to give insight to the detailed mechanism of single-ion impact events. This knowledge may be used as input data for further modeling, such as by continuum or Monte Carlo schemes [11]. Previous work on glancing-angle ion incidence on metallic surfaces has shown how the existence of surface steps leads to clearly discernible features in the damage pattern on the surface [12–18].

The (100) surface of Si is one of the most important surface orientations [19] and its behavior has been carefully examined. The surface may undergo many types of reconstruction, which have been studied both experimentally and theoretically [3,20,21]. Also the steps on the surface have been thoroughly investigated [22].

In this work we focus on the interaction of 3 keV ions with the (2×1) dimer reconstructed Si(100) surface, both with and without a surface step. We investigate two ion beam directions: the direction parallel and the direction perpendicular to the dimer-reconstruction rows. These directions constitute two extreme cases with respect to the possibility of ion channeling. The (2×1) reconstruction is characterized by the decoration of the surface by dimer rows, which may strongly influence the nature of propagation of the impinging ions [7]. The reconstruction-induced displacement of surface atoms builds reconstructed channels below the surface that are able to trap the ion. Surface steps naturally allow the impinging ions to enter these subsurface channels, which subsequently create characteristic damage either at the step edge or behind on the upper terrace.

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