Glancing ion incidence on Si(100): Influence of surface reconstruction on ion subsurface channeling

Yudi Rosandi[1,2] and Herbert M. Urbassek[1,*]

[1]*Fachbereich Physik und Forschungszentrum OPTIMAS, Universität Kaiserslautern, Erwin-Schrödinger-Straße, D- 67663 Kaiserslautern, Germany*

[2]*Department of Physics, Universitas Padjadjaran, Jatinangor, Sumedang 45363, Indonesia*

(Received 7 November 2011; revised manuscript received 29 February 2012; published 13 April 2012)

We demonstrate that a Si target may exhibit the phenomenon of subsurface channeling for glancing incidence ions. To this end, we perform molecular-dynamics simulations of 3 keV Ar^+ ion impact at grazing incidence (83° toward the surface normal) on a Si (100) surface. Both an unreconstructed and a (2×1) dimer-reconstructed surface are investigated. In both cases, the ion is reflected from the flat terrace and creates neither damage nor sputtering. The situation changes when a surface step is introduced on the surface; ion incidence in the vicinity of the step induces both damage and sputtering. We find that the phenomenon of subsurface channeling plays a dominant role in damage creation at the step edge. Subsurface channels aligned in the $\langle 110 \rangle$ direction are created under the reconstructed surface; they run parallel to the dimer rows. If the ion incidence geometry is favorable—incidence azimuth aligned along $\langle 110 \rangle$ and the ion approaching an unbonded B step—the ion can enter these channels. Without surface reconstruction no subsurface channeling can occur. Subsurface-channeled ions generate peculiar surface damage patterns which may allow their identification in experiment.

DOI: 10.1103/PhysRevB.85.155430 PACS number(s): 79.20.Rf, 61.80.Jh, 79.20.Ap

I. INTRODUCTION

Surface patterning of silicon by ion bombardment has been studied in the recent past.[1–3] Particular attention has been paid to the ripple patterns induced by ion impact at normal and off-normal incidence angles.[4] However, the effect of single-ion impacts at glancing incidence on the flat silicon surface has, up to now, not been sufficiently evaluated.

It is known that, at glancing incidence, ion impact creates distinctive damage on the bombarded surface. The underlying mechanisms have been studied in detail for a metal surface, Pt (111).[5–8] Under this condition, pre-existent surface defects play an essential role in transferring the ion energy to the target crystallite. In particular, the existence of surface steps enables a very special type of ion trajectory, which features the so-called subsurface-channeling phenomenon. Its characteristic is the creation of an aligned row of periodic damage islands. Using a suitably massive ion, it is also possible to generate a vacancy groove decorated with adatom islands on its sides.[9,10]

In this paper, we study glancing-ion incidence on the Si (100) surface at incidence angles where the flat terrace reflects the ion, and only surface steps allow them to perform sufficiently violent collisions to induce damage at the surface and sputtering. We focus on the possibility that the ion enters the target in a subsurface-channeled trajectory and elucidate the role of this phenomenon for target modification and sputtering.

Our prediction of subsurface channeling in a Si crystal was not anticipated. Compared with the well-studied case of Pt, Si crystals differ strongly in their crystal structure and in their possibility of surface reconstruction. In addition, Si atoms are lighter than typical projectile ions (Ar in our case), while Pt is much heavier; thus the response of the target (damage—in particular destruction of the channels while the projectile passes through it) is expected to be larger than in Pt. We believe that our results will also be interesting in the field of surface patterning and ripple formation of Si surfaces under glancing-ion impact, since we describe the damage processes occurring under individual-ion impact. The generation of surface damage aligned in the ion-incidence direction, such as we describe it here, may influence the damage patterns evolving under higher fluences.[5] While continuum theories of surface topography evolution are quite developed,[11,12] their need for atomistic input has recently been acknowledged.[13,14] Our work demonstrates the anisotropic damage developing under grazing-incidence ion impact on Si, such as is relevant for ion-induced surface topography modification.

The Si (100) surface usually exhibits the (2×1) reconstruction during which dimer rows, aligned in [110] direction, are created.[15] These dimer rows form subsurface channels, which are able to trap the incoming ions. We shall show that, when an incoming ion impinges at glancing incidence in front of a monolayer surface step, it can enter the channel and propagate in it for a relatively long distance below the dimer rows. During channeling the reconstruction pattern is destroyed and surface defects, vacancy islands, and other extended defect structures are left behind. The defects are aligned in the ion-propagation direction. An unreconstructed surface does not exhibit surface channeling, since the channels formed by the dimer rows do not exist. As a consequence the damage patterns on this surface differ considerably from those on the reconstructed surface. For the unreconstructed surface, channeling is only possible in deeper layers or inside the bulk, when ions penetrate the surface layers. Besides the surface damage produced by glancing-ion impact, we shall also discuss the consequences on sputtering. We shall demonstrate that a monolayer step leads to strong sputtering; again the features found for reconstructed and unreconstructed surfaces differ in a characteristic way.

II. SIMULATION METHOD

We consider a Si (100) target consisting of 100 926 atoms; it extends 310 Å in the direction of the ion beam, has a width of 160 Å, and is 40 Å thick. A monolayer step is created on the surface by removing the topmost atomic layer up to the position $x = 103$ Å; the remaining

