Nuclear Instruments and Methods in Physics Research B 340 (2014) 5–10

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Subsurface and interface channeling of keV ions in graphene/SiC

Yudi Rosandi [a,b], Herbert M. Urbassek [a,*]

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

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

ARTICLE INFO

Article history:
Received 5 February 2014
Received in revised form 24 July 2014
Accepted 25 July 2014
Available online 10 September 2014

Keywords:
Graphene
Silicon carbide
Sputtering
Defect formation
Channeling

ABSTRACT

Using molecular-dynamics simulation, we study the impact of 3 keV Ar and Xe ions on a β-SiC (1 1 1) surface covered by a single graphene layer. At glancing ion incidence angles, we observe the ions to undergo interface channeling between the graphene and the first SiC surface layer. This behavior is particularly pronounced for Xe ions, where at incidence angles of 70–75° more than 50% of the ions are channeled. This process is accompanied by abundant damage production and sputtering in the graphene layer. Similarities and differences to subsurface channeling in elemental materials are discussed.

1. Introduction

Damage and sputtering produced by keV ions impinging at glancing incidence on substrates has recently received considerable interest. Metals [1–7], semiconductors [8,9], and ionic surfaces [10] have been studied both experimentally and by computer simulation. Such glancing impact gives rise to the phenomenon of subsurface-channeling where the projectile is channeled immediately under the surface. In this channeling mode the ion creates characteristic damage, such as vacancy islands aligned with the ion incidence direction (projected onto the surface) and even nano-grooves.

For a heterogeneous system the situation is more complex. In this respect, Standop et al. [11] studied glancing ion incidence on an Ir (1 1 1) substrate covered by a single graphene sheet. Here they found evidence for channeling of the irradiating ions in the interface between the substrate and the overlayer sheet.

Interface channeling differs in several respects from the ordinary sub-surface channeling in homogeneous materials: (i) The interface width, which defines the channel, can be larger than in a homogeneous material; thus both the fraction of channeled ions and the length of the channeled trajectory may be larger than in homogeneous materials. (ii) In the case of weak (van der Waals) bonding across the interface, the electron density and thus also the electronic stopping in the channel are even smaller for interface channeling than for sub-surface channeling. (iii) The mass difference on both sides of the channel, and the different continuum potentials, make the channeled trajectory anisotropic. Thus interface channeling provides novel features as compared to sub-surface channeling in a homogeneous substrate.

In the present paper, we report on a dedicated molecular-dynamics study of interface channeling. As substrate we choose a SiC crystal; the so-called epitaxial graphene on SiC is easily synthesized and has been much studied due to its promising electronic properties [12,13]. While fixing the ion impact energy to 3 keV, we consider a light (Ar) and a heavy (Xe) ion, and discuss systematically the effect of the incidence angle on the possibility to break through the graphene overlayer and the induced sputtering and damage production.

2. Methods

The target consists of a β-SiC substrate with a (1 1 1) Si-terminated surface; on top of it we place a single-layer graphene sheet. β-SiC is also known as 3C-SiC; it has a cubic zincblende structure. Motivated by Ref. [14], we assume a large $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ coincidence lattice, see Fig. 1. It consists of 169 graphene unit cells and of 108 SiC (1 1 1) unit meshes. This structure is considered more realistic than the so-called covalently bound stretched graphene (CSG) model with $(\sqrt{3} \times \sqrt{3})R30^\circ$ surface reconstruction [15,14].

* Corresponding author.
E-mail addresses: rosandi@physik.uni-kl.de (Y. Rosandi), urbassek@rhrk.uni-kl.de (H.M. Urbassek).
URL: http://www.physik.uni-kl.de/urbassek/ (H.M. Urbassek).

http://dx.doi.org/10.1016/j.nimb.2014.07.031
0168-583X/