Subsurface channeling of keV ions between graphene layers: Molecular dynamics simulation

Yudi Rosandi,[1,2] Maureen L. Nietiadi,[1] 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 3 October 2014; revised manuscript received 23 February 2015; published 31 March 2015)

Using molecular dynamics simulation, we study the impact of 3 keV Xe ions at glancing incidence on a β-SiC (111) surface covered by graphene. On top of a full graphene layer covering the substrate, we add a graphene half-layer; the step forming where the half-layer terminates allows the entrance of glancing-incidence ions into a subsurface channel between graphene layers. We find a high channeling probability which leads to only little sputtering and damage formation. Typically, vacancy defects are formed at periodic intervals when the ion hits the uppermost graphene layer from below. Extended damage occurs when the ion hits the step edge itself. There we find several kinds of defects varying from adatoms over the formation of sp^1-bonded chains to hillocks.

DOI: 10.1103/PhysRevB.91.125441 PACS number(s): 79.20.Rf, 61.80.Jh, 79.20.Ap

I. INTRODUCTION

Ion irradiation of nanostructured and "two-dimensional systems" has recently gained interest. In their review [1] Krasheninnikov and Nordlund give an overview of recent research which concentrated in particular on carbon systems such as nanotubes and graphene layers. In [2] an overview of the defects induced in graphene by perpendicular ion impact is given. However, particularly interesting features appear under glancing ion incidence. Thus, recently Michely and co-workers studied ion impact on a graphene layer covering a metal—the Ir (111) surface—both by experiment and computer simulation; and highlighted interface channeling, defect formation, and ion trapping [3]. Further simulations studied ion impact on SiC covered by a graphene layer and discussed the differences between subsurface channeling in the substrate and interface channeling between the substrate and the graphene cover layer [4].

Glancing ion incidence on metals has been studied in considerably greater detail, both by experiment and by simulation [5–11]. 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 nanogrooves. This ample body of evidence for metallic targets is supplemented by more scarce studies of semiconductors [12,13] and ionic surfaces [14].

Several simulation studies have been published that analyzed the defects formed in two-dimensional carbon structures under ion impact. Electron irradiation of graphene produces isolated defects such as single vacancies or adatom-vacancy pairs [15]. Ion irradiation of carbon nanotube bundles was found to create intertube links which correspond to a change of sp^2 to sp^3 bonding [16]. The ion irradiation of two-shell (onionlike) fullerene structures was studied by DFT-based tight-binding simulations; again the creation of regions with sp^3-bonding characteristics was observed [17]. Ion irradiation of graphite also gives rise to the formation of sp^1- and sp^3-bonding defects [18,19]. Reference [1] gives an overview of radiation damage created in nanostructured carbon materials.

In the present paper we study glancing ion incidence on a SiC substrate covered by a multilayer (more precisely: one and a half layer) graphene sheet. Epitaxial graphene on SiC is easily synthesized and has been much studied due to its promising electronic properties [20,21]. The extra half layer of graphene on the substrate creates a surface step between the graphene layers which allows easy entrance for glancing ions in the subsurface graphene channel. Besides the channeling probabilities of such a system, we study the consequences of ion irradiation, viz. surface damage and sputtering.

II. METHOD

The target consists of a β-SiC substrate with a (111) Si-terminated surface; on top of it we place one full and one half-layer of graphene, see Fig. 1. β-SiC is also known as 3C-SiC; it has a cubic zincblende structure. Details of the structure are given in [4]. In short, the SiC crystallite consists of 18 SiC (111) layers and has a thickness of 42.5 Å. The area of the target surface amounts to 154×107 Å^2. A full graphene sheet is put on top of it with a lattice parameter of 2.46 Å; the nearest-neighbor distance amounts to 1.42 Å. Another half-layer of graphene is set on top of it, see Fig. 1.

The silicon atoms and substrate carbon atoms interactions are modeled by the Tersoff potential [22,23]. The high-energy region is splined to the Ziegler-Biersack-Littmark (ZBL) repulsive potential [24,25]. The interaction of carbon atoms in the graphene layers is modeled by the AIREBO potential without torsion term [26]. The interaction between graphene and the substrate is modeled by two Lennard-Jones potentials, one for the C and one for the Si atoms of SiC, with different σ and ϵ parameters. Between graphene and the substrate C atoms, the same parameters as in the van der Waals interaction in AIREBO are used: $\sigma_{\text{Gr-C}} = 3.4$ Å, and $\epsilon_{\text{Gr-C}} = 2.8$ meV. The interaction of graphene with the substrate Si atoms is fitted to the surface binding energy of 0.34 eV/(graphene unit cell) and the interlayer distance to the Si-terminated surface of $\Delta h = 2.58$ Å as calculated by DFT [27]. This gives us $\sigma_{\text{Gr-Si}} = 2.65$ Å and $\epsilon_{\text{Gr-Si}} = 0.117$ eV. The corrugation of the

*urbassek@rhrk.uni-kl.de; http://www.physik.uni-kl.de/urbassek/

