Nuclear Instruments and Methods in Physics Research B 365 (2015) 235–239

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

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

Molecular dynamics modeling of defect formation in many-layer hexagonal boron nitride

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ARTICLE INFO

Article history:
Received 9 November 2014
Received in revised form 27 August 2015
Accepted 9 October 2015
Available online 22 October 2015

Keywords:
Ion irradiation
Ceramics
Point defects
Molecular dynamics

ABSTRACT

Molecular dynamics simulations are conducted to examine lattice defect formation in a hexagonal boron nitride lattice by high-energy xenon ion impact. This work seeks to characterize the production of defects which occur under ion irradiation. Lattice defect formation is first examined in single-layer hexagonal boron nitride. Energetic xenon ions over a range of 10 eV–10 keV are used to randomly impact the central lattice at an angle of 90° (orthogonal to the lattice basal plane). The resulting defects are analyzed for 5000 ion impacts, and results are reported for average single and double vacancy formation per impact. A similar study is conducted for a many-layer hexagonal boron nitride lattice, to assess the influence of additional layers in the formation of point defects as a function of incident ion energy. Ion impacts at both 90° and 45° are examined. The defects formed in the top layer of the many-layer lattice are qualitatively similar to the single layer results, but the presence of the bulk lattice is found to reduce the single vacancy probability in the top-most layer. Point defects are prominent in the lattice sub-layers with increasing ion energy. Orthogonal ion impacts are found to cause the most damage, as measured by the number of vacancy defects produced; the number of vacancies increases linearly with energy, while the number of defects in the oblique impact configuration reaches an asymptotic limit with increasing energy.

1. Introduction

As a wide gap semiconductor, hexagonal boron nitride (*h*-BN) is a desirable candidate material for a broad range of applications, from *h*-BN-based nano-devices to wall materials for Hall thrusters. The effectiveness of *h*-BN as an electrical insulator, and its overall thermal and electrical properties, is achieved in part by the strong, in-plane ionic bonding of the planar lattice structure. The presence of defects, either in the form of impurities or vacancies, modify the intrinsic properties of the lattice [1–8]. Lattice defects in general may be introduced in a controlled way to tailor the material properties, or they may be an undesirable consequence of exposure to environmental factors such as radiation, surface reactions or gas/plasma-surface interactions.

This work employs molecular dynamics simulations to characterize the formation of defects in many-layer *h*-BN due to impact of Xe^+ over a range of incident ion energies. Previous studies examined defect formation in *h*-BN due to electron irradiation [9,10] as well as ion impact [11,12] leading to material sputtering. The molecular dynamics study by Lehtinen et al. [11] in particular establishes a general trend of ion impact energy and angle of incidence with the type of defect introduced in a *h*-BN monolayer. This work aims to extend such studies to many-layer *h*-BN, in efforts to establish a connection between irradiation processing parameters and characteristic lattice defects in bulk *h*-BN materials. These details are best captured with molecular dynamics, while approximate BCA methods such as TRIM, may be better suited for surface phenomena.

2. Computational model

The lattice system under consideration is a 10-layer *h*-BN material comprised of an in-plane hexagonal structure with alternating boron (B, green) and nitrogen (N, blue) (Fig. 1). The basal plane is oriented in the *x*–*y* direction, with an equilibrium interlayer spacing of 3.245 Å (Fig. 1(a)). The impacting ion is introduced above the material surface (in the $+z$-direction) and strikes the top-most layer with an orthogonal (90°) or oblique (45°) angle of incidence (Fig. 1(b)). The edge of each layer is treated with a Berendsen thermostat boundary condition (Fig. 1(c)) with a target temperature of 0 K. The xenon ion is positioned above the lattice plane so

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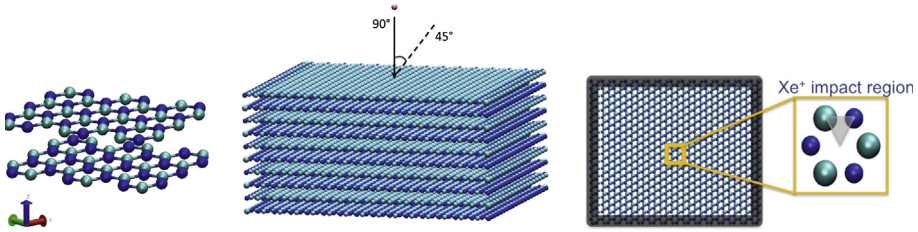
http://dx.doi.org/10.1016/j.nimb.2015.10.020
0168-583X/



(a) Lattice structure of *h*-BN

(b) Ion impact incidence (90°/45°) relative to basal plane of 10-layer lattice

(c) Edge thermostat boundary condition and ion impact region (shaded triangle)

Fig. 1. Simulation setup of *h*-BN lattice under Xe^+ ion irradiation. (a) Lattice structure of *h*-BN. Boron (green) and nitrogen (blue) form intralayer ionic bonds, with relatively weak van der Waals interlayer forces. (b) Ions are introduced above the lattice (single- or 10-layer) and impact at 90° or 45° relative to the basal plane surface normal. (c) Layers treated with edge thermostat boundary condition, and ions impact in center of lattice. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

as to impact the top-most layer within the minimum irreducible area of the central hexagonal structure [11]. The exact impact location is selected randomly for each ion impact within the shaded gray triangle shown in Fig. 1(c).

The molecular dynamics simulations are performed using the HOOMD-blue solver [13,14]. The Albe-Möller many-body analytical potential [15] is used to model the interactions between the boron and nitrogen atoms in the lattice (B–B, N–N, B–N). The Albe-Möller potential is a Tersoff-like bond-order potential fitted from *ab initio* data that accounts for bond influences by neighboring atoms, including bond lengths and angles. Interactions involving the incident ion (Xe–B, Xe–N) are modeled using the purely repulsive Ziegler–Biersack–Littmark interaction potential [16]. It is assumed that the xenon ion is neutralized by a surface electron prior to impact, which has a negligible influence on the impact dynamics for low-charge ions and is not modeled here.

An adaptive simulation time step ranging from $\Delta t = (0.1\ \text{fs}–1\ \text{as})$ is used to capture the collision dynamics involving the shortest timescales in the system. The second-order velocity-Verlet scheme is used for time-integration, and simulations are run for approximately 1 ps after the impact. This ensures that any defect configurations have reached an energy minimum, and any material sputtered out-of-plane has time to leave the system. Each ion impact is simulated with a pristine *h*-BN lattice shown in Fig. 1 (b), and the post-impact systems are then analyzed for defects in a post-processing routine. The defect statistics reported at each ion energy correspond to 5000 independent ion impacts as outlined above.

3. Results

Defects produced by a single ion impact are characterized according to the number of atoms displaced from their position in the lattice. Although a variety of complex defects can be classified, the results presented here focus on single (B/N) and double (B–N) vacancy defects and the subsequent interstitial defects introduced as a result of these vacancies. A single vacancy is defined as a point defect in which one atom is removed completely from its lattice position. A double vacancy is a defect in which two neighboring atoms are removed completely from their lattice position. The results outlined in the next sections present a validation study against single-layer irradiation results by Lehtinen et al. [11], and results from the many-layer studies are analyzed and discussed.

3.1. Defect formation in h-BN monolayer

Simulation results from the monolayer study are presented first and compared against vacancy probability per ion impact reported by Lehtinen et al. [11]. Fig. 2(a) presents the probability of single vacancy formation as a function of ion energy involving orthogonal (90°) impacts, and double vacancy probabilities are presented in Fig. 2(b). The results from the present study are represented by the open circles. The first peak in single point defects corresponds to ion energies of approximately 300 eV, when the incident ion has sufficient energy to displace the target atom. As energy increases, the incident ion has sufficient energy to displace a pair of atoms from the lattice, resulting in a peak in the probability of a double vacancy defect. Increasing the incident ion energy further reduces the effective cross section of the ion/target atom interaction, and a second peak appears in the single vacancy probability for energies above 1 keV at the expense of double defect formation. This variation in defect probability with ion energy is in very good agreement with the results by Lehtinen et al. (filled circles) [11].

3.2. Defect characteristics in many-layer h-BN

A similar analysis is conducted for single-ion impacts in a 10-layer *h*-BN slab. In order to analyze the complex defects formed by the collision cascade, the post-collision lattice is effectively deconstructed and analyzed as individual layers. The top-most layer (which interacts first with the incident ion) is referred to as layer 10, and the sublayers are numbered sequentially with layer 1 at the bottom. The single and double vacancy probability values from the top-most layer (red symbols) are compared to the monolayer results in Fig. 2(a) and (b). The general trend of the single vacancy formation (double-peak in probability as a function of energy) is very similar to the monolayer results. However, the additional sublayers are found to reduce the peak probability of single vacancy formation, at ion energies of 100–150 eV and above 1 keV (Fig. 2(a)). The double vacancy probability as a function of ion energy (Fig. 2(b)) is largely unaffected by the presence of the sublayers.

Fig. 3(a) and (b) show the many-layer *h*-BN lattice in the region near the impact site for a representative orthogonal ion impact at 500 eV, before and after impact. The intact lattice atoms are shown in light blue, and the colored atoms (with target atom shown in pink in the top layer) correspond to point vacancy sites formed after the collision cascade, which produce corresponding interstitial defects in the post-impact lattice (3(b)). The most prominent defect in layer 10 is a double (B–N) vacancy, and these atoms subsequently collide with atoms in the underlying sublayers. The effective collision energies of the subsequent secondary and tertiary interactions are reduced, owing to nuclear stopping and phonon excitation, and the maximum damage in this sample case is found in the eighth layer (indicated by four vacancy defects in purple) below which the xenon atom imparts minimal damage.