Nuclear Instruments and Methods in Physics Research B 343 (2015) 48–51

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

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

Formation of nanopore in a suspended graphene sheet with argon cluster bombardment: A molecular dynamics simulation study

Zabiholah Zabihi, Houshang Araghi *

Department of Physics, Amirkabir University of Technology, Tehran, Iran

ARTICLE INFO

Article history:
Received 14 July 2014
Received in revised form 18 September 2014
Accepted 7 November 2014
Available online 26 November 2014

Keywords:
Nanopore
Suspended graphene sheet
Argon cluster
Molecular dynamics simulation

ABSTRACT

Formation of a nanopore in a suspended graphene sheet using an argon gas beam was simulated using molecular dynamics (MD) method. The Lennard-Jones (LJ) two-body potential and Tersoff–Brenner empirical potential energy function are applied in the MD simulations for different interactions between particles. The simulation results demonstrated that the incident energy and cluster size played a crucial role in the collisions. Simulation results for the Ar_{55}–graphene collisions show that the Ar_{55} cluster bounces back when the incident energy is less than 11 eV/atom, the argon cluster penetrates when the incident energy is greater than 14 eV/atom. The two threshold incident energies, i.e., threshold incident energy of defect formation in graphene and threshold energy of penetration argon cluster were observed in the simulation. The threshold energies were found to have relatively weak negative power law dependence on the cluster size. The number of sputtered carbon atoms is obtained as a function of the kinetic energy of the cluster.

1. Introduction

The carbon atoms in graphene condense in a honeycomb lattice due to sp^2-hybridized carbon bond in two dimensions [1]. It has unique mechanical [2], thermal [3,4], electronic [5], optical [6], and transport properties [7], which leads to its huge potential applications in nanoelectronic and energy science [8]. One of the key obstacles in the development of graphene based nanoelectronics is the absence of a band gap in pristine graphene [9,10]. One of the solutions of such problem is modify the electronic band structure of graphene. Experimental and theoretical studies have shown that chemical doping of graphene with foreign atoms and some vacancies of carbon atoms within the graphene sheet can lead to Fermi level shifting and also a band-gap opening [11–14]. For example, Pedersen et al. [15] obtained,

$$E_g = K\left(\frac{\sqrt{N_r}}{N_T}\right) \quad (1)$$

where E_g is the energy band gaps, N_r is the number of removed carbon atoms, N_T is the number of atoms before the pore is made and $K = 25$ eV.

Graphene nanopores can have potential applications in various technologies, such as DNA sequencing, gas separation, and single-molecule analysis [16,17]. Generating pores with precisely controlled subnanometer sizes is the key challenge in the design of a graphene nanopore device. Various techniques have been employed to punch nanopores in graphene sheets, including electron beam from a transmission electron microscope (TEM) and heavy ion irradiation [18].

Using electron beam technique, Fischbein and Drndic [19] drilled nanopores with the width of several nanometers and stable; but, this high cost method is not fully controllable at nanoscale. Russo and Golovchenko [20] used energetic ion exposure technique to create nanopores with radius as small as 3 Å. Zhao et al. [21] indicated that energetic cluster irradiation was more effective in generating of nanometer-scale pores in graphene, because their much larger kinetic energy could be transferred to the target atoms. Recent experimental works have further confirmed that cluster irradiation is a feasible and promising way in the generation of nanopores [22]. Numerical simulations have demonstrated that a nanopores of controlled sizes and qualities can be fabricated in a graphene sheet by choosing a suitable conditions of collision between nanocluster and graphene such as impacting cluster energy, cluster size, temperature and cluster species [21].

One robust method for studying the influence of different conditions of collision between cluster and graphene on the formation

* Corresponding author. Tel.: +98 64545243.
E-mail address: araghi@aut.ac.ir (H. Araghi).

http://dx.doi.org/10.1016/j.nimb.2014.11.022
0168-583X/

Table 1
Lennard-Jones potential parameters.

	σ (A)	ε (eV)
Ar–Ar	3.4	0.0104
Ar–C	3.385	0.005

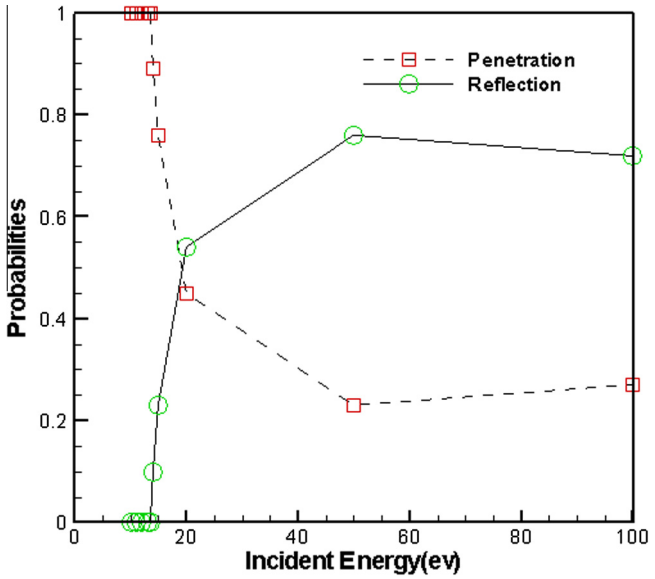

Fig. 1. Incident energy dependence of the reflection and penetration probabilities.

of nanopore is molecular dynamics (MD) simulation [23]. The numerical simulations results may be useful in explaining experimental results and predicting suitable conditions for generating graphene nanopores.

In this paper, MD simulations were performed for the collisions between an argon cluster and graphene. The phenomena of argon cluster–graphene collisions and mechanism of the atomic nanopore formation in graphene were investigated. Effects of cluster size on the threshold incident energy of defect formation in graphene were also discussed.

2. Molecular dynamics method

MD simulations were performed for the collisions between an argon cluster and graphene. For present simulations we used an effective code LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator, written by Sandia National Laboratories [24]. Length (along the X axis) of the graphene sheet was 11 nm, its width (along the Y axis) was 10 nm. Graphene sheet located in the center of the cubical simulation cell .periodic boundary conditions was imposed on both lateral directions. In the simulation, the Tersoff–Brenner empirical potential energy function (PEF) was utilized to simulate the energy of covalent bonding between carbon atoms in the structure of graphene layer [25,26]. The initial configuration of graphene was fully relaxed at room temperature before the collision simulations. The Ar nanocluster was arranged by cutting a sphere from bulk crystals, which were set to be maintained at 0 K. The Ar cluster was placed above the graphene sheet within simulation cell so that there would be no interaction between the Ar cluster and graphene sheet.

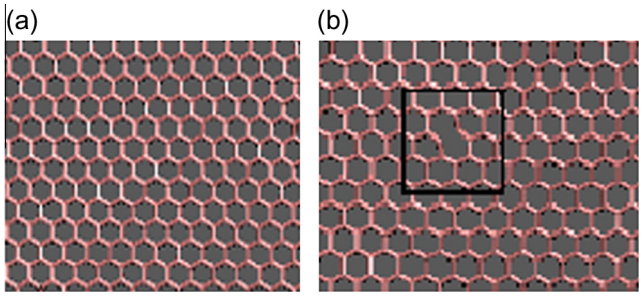

Fig. 3. Atomic configurations to X–Y plane when the collision energy is: (a) 10 eV, and (b) 11 eV.

Then, a initial translational velocity component of the cluster atoms was assumed .Incident angle of the argon cluster to the graphene was 0°. During the collision phase, the borders of graphene were attached to the thermostat which were set to be maintained at 300 K by rescaling the velocities of atoms at every time of step. Lennard-Jones (LJ) two-body potential was employed to simulate the interactions of Ar–Ar and Ar–C atoms. The form of LJ potentials was:

$$V = 4\sum_{i}\sum_{j>i}\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad (2)$$

In the LJ potential, σ is the distance at which the potential is zero and ε is the depth of the potential well. Note that the constants were obtained from the mixing rules given by $\sigma_{ij} = (\sigma_i + \sigma_j)/2$ and $\varepsilon_{ij} = (\varepsilon_i\varepsilon_j)^{1/2}$. The parameters for ε and σ used in the present simulation are shown in Table 1 [27]. Position of the atom was updated by integrating the classical equation of motion using the velocity Verlet algorithm with a time step of 0.5 fs. To reduce the calculation time, the potential cutoff radius was introduced. The Van der Waals interaction of Ar–Ar and Ar–C atoms with the distance of 11A or above was neglected.

3. Result

Studying the effect of incident energy in ranging 1–120 eV/atom was chosen to demonstrate two distinctive phenomena: (i) Argon atoms were just reflected, and (ii) some argon atoms penetrated through graphene. Fig. 1 demonstrates the probabilities of reflection and penetration of the Ar_{55} cluster.

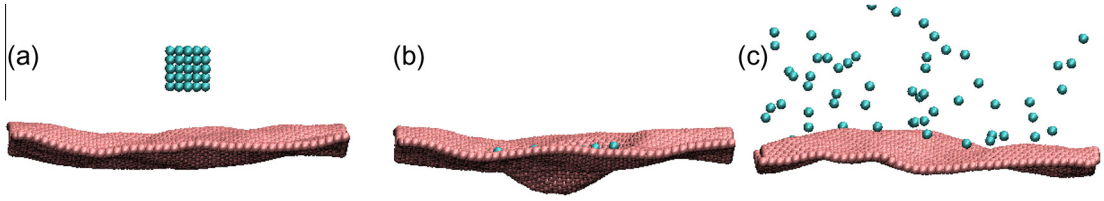

Fig. 2. Snapshots of Ar_{55} clusters collision on graphene sheet: (a) t = 0 ps, (b) t = 1 ps, (c) t = 6 ps.