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Molecular dynamics simulation of graphene bombardment with Si ion

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HIGHLIGHTS

- We provides a model to prepare graphene-based SiC material using ion bombardment.
- The parameters required to develop graphene devices by controlling defect formation.
- It study the Si ion impact the graphene sheet based on molecular dynamics simulation.
- The presents of Si–C tetrahedron can be provides a thought to develop quantum dot.

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ABSTRACT

Molecular dynamics simulations with Tersoff–Ziegler–Biersack–Littmark (Tersoff–ZBL) potential and adaptive intermolecular reactive empirical bond order (AIREBO) potential are performed to study the effect of irradiated graphene with silicon ion at several positions and energy levels of 0.1–1000 eV. The simulations reveal four processes: absorption, replacement, transmission and damage. At energies below 110 eV, the dominant process is absorption. For atom in group (a), the process that takes place is replacement, in which the silicon ion removes one carbon atom and occupies the place of the eliminated atom at the incident energy of 72–370 eV. Transmission is present at energies above 100 eV for atom in group (d). Damage is a very important process in current bombardment, and there are four types of defects: single vacancy, replacement-single vacancy, double vacancy and nanopore. The simulations provide a fundamental understanding of the silicon bombardment of graphene, and the parameters required to develop graphene-based devices by controlling defect formation.

1. Introduction

Graphene is a material of single layer of carbon atoms densely packed into a benzene-ring structure. It has received considerable attention since it was first discovered in 2004 by Geim et al. [1]. Graphene is extensively used in transistors [2,3], transparent electronic materials [4], and sensors [5,6] because of its excellent electronic properties [7,8], as well as its predominant thermal [9,10], mechanical [11], and optical properties [12]. Recently, simple graphene-based devices have become feasible, but most applications require control over band structure and electrical properties. Improving the electrical and structural properties of materials can be effectively achieved through functionalization [13], but this approach is not easily achieved. Another method of modifying the electronic structure of graphene is defect formation and defects can be created intentionally by ion bombardment [14]. And energetic ions have been used widespread to modify the structure and properties of nanostructured carbon materials with high precision, and it has been successfully used to tune the structure of carbon nanotube as well as graphene [14,15]. Both experiments and simulations on the electron or ion bombardment of various nanostructures demonstrate that this approach presents beneficial effects [16–19]. Based on the experiment of Ar^+ ion impact graphene, Dobrik et al. [20] investigated the effect of atomic scale defects and disorder on the low-energy electronic structure of graphene, and this study showed that defect results in the substantial reduction in the Fermi velocity. Performing molecular dynamics simulation, Bellido and Seminario [21] studied the effect of irradiating graphene with carbon ion at different positions and energies. The simulation discussed the interaction between same kinds of atom (C–C interaction) in the bombardment, it is essential to study the interaction of different kinds of atom, such as silicon–carbon interaction, due to the Si–C semiconductor devices has a wide range of applications on electronic field. Using density functional theory (DFT), for example, Zhou et al. [22] studied the structural and electronic properties of Si-substituted graphene and found that the band gap of graphene can be continuously tuned with differently substitutional concentration. To utilize such processes-induced band structure and electrical properties changes, a special design

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is proposed to fabricate graphene-based quantum well device such as graphene-based SiC device. Zhao et al. [23] used two types of clusters to determine the influence of such clusters on graphene after bombardment, and demonstrated that by choosing a suitable cluster species and controlling its energies, nanopores of desired sizes and qualities can be fabricated in a graphene sheet. Therefore, by carefully choosing the parameters of the incident ion such as the type of ion and initial kinetic energy, it is possible to intentionally fabricate the electrical and structural properties of graphene sheet.

In the current study, we investigate the Si ion bombardment of graphene in a variety of sites and at several shooting energies by molecular dynamics simulations based on hybrid Tersoff–ZBL potential and adaptive intermolecular reactive empirical bond order (AIREBO) potential. Four processes—absorption, replacement, damage, and transmission—are analyzed, and the relationship between these processes and incident energy is discussed. This research provide a potential for the development of electronic devices with exceptional properties, such as low density, wide-band gap. And the physics behind the substitutional process of ion bombardment of graphene with silicon ion will provide a possible model with their parameters to prepare graphene-based SiC (SiCNR [22]) material.

2. Simulation conditions and methods

2.1. Potential between atoms

In this study, the surface reconstructions of irradiated graphene with silicon ion at different energies are simulated by MD simulation techniques. The interaction between silicon and carbon atoms were described with a hybrid Tersoff–ZBL potential [24–27]. The Tersoff–ZBl potential giving the energy E of system atoms as:

$$E = \frac{1}{2}\sum_i\sum_{j\neq i} V_{ij} \tag{1}$$

$$V_{ij} = (1 - f_F(r_{ij}))V_{ij}^{ZBL} + f_F(r_{ij})V_{ij}^{Tersoff} \tag{2}$$

f_F is a fermi-like function used to smoothly connect the ZBL repulsive potential with the Tersoff potential. A_F are control parameter of the function shape, and r_C is essentially the cutoff for the ZBL potential.

$$f_F(r_{ij}) = \frac{1}{1 + e^{-A_F(r_{ij} - r_C)}} \tag{3}$$

The ZBL potential has two factors:

$$V_{ij}^{ZBL} = \frac{1}{4\pi\varepsilon_0}\frac{Z_i Z_j e^2}{r_{ij}}\phi(r_{ij}/a) \tag{4}$$

The first factor is the Coulomb repulsive term, with Z_i, Z_j as the atomic number of the two atoms, e as the electron charge, ε_0 as the permittivity of vacuum. The second term, ϕ is the ZBL universal screening function, with a_0 being the Bohr radius and a function is only accurate for small separation (<1 Å).

$$a = \frac{0.8854a_0}{Z_i^{0.23} + Z_j^{0.23}} \tag{5}$$

$$\phi(x) = 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x} \tag{6}$$

The Tersoff potential has four terms:

$$V_{ij}^{Tersoff} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})] \tag{7}$$

where f_C is a smooth cutoff function to limit the range of the potential and goes from 0 to 1 in a small range D around R.

$$f_C(r) = \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin(\frac{\pi}{2}\frac{r-R}{D}) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \tag{8}$$

The functions

$$f_R(r) = A\exp(-\lambda_1 r) \tag{9}$$

and

$$f_A(r) = -B\exp(-\lambda_2 r) \tag{10}$$

are repulsive and attractive Morse-like potentials, respectively. The b_{ij} functions are measures of bond order:

$$b_{ij} = (1 + \beta^n\zeta_{ij}^n)^{-\frac{1}{2n}} \tag{11}$$

and depends on the ζ_{ij} function:

$$\zeta_{ij} = \sum_{k\neq i,j} f_C(r_{ik})g(\theta_{ijk})\exp\left(-[\lambda_3^3(r_{ij} - r_{ik})^m]\right) \tag{12}$$

where the $g(\theta)$ function is defined as:

$$g(\theta) = \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos\theta - \cos\theta_0)^2]}\right) \tag{13}$$

where θ represents the angle between bonds ij and ik and γ_{ijk} is a parameter used to strengthen or weaken bonds between different types of atoms [20]. Parameters used in the simulation are shown in Table 1 [24].

The C–C interatomic interactions in graphene were calculated with the adaptive intermolecular reactive empirical bond order (AIREBO) potential [23,28]. This potential enables the breaking and creation of covalent bonds, and has been successfully applied in studying the properties of carbon-based nanomaterials [29,30]. The AIREBO potential consists of three terms:

$$E = \frac{1}{2}\sum_i\sum_{j\neq i}[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{TORSION}] \tag{14}$$

the E_{ij}^{REBO} gives the model its reactive capabilities and only describes short-ranged C–C interactions ($r < 2$ Å), the E_{ij}^{LJ} term adds longer-ranged interactions ($2 < r <$ cutoff), and the $E_{kijl}^{TORSION}$ term is an explicit 4-body potential that describes various dihedral angle preferences in hydrocarbon configurations.

2.2. Initial conditions

The graphene target used in the simulations has dimensions of 10×10 nm^2 and consists of 3807 atoms. The graphene sheet was centered at the origin of coordinates, lying on the x–y plane; a silicon ion was positioned 4 nm from the graphene in the z-axis (Fig. 1). Two opposite ends of the graphene are fixed to simulate a suspended system.

Table 1
Parameters of the ion bombardment simulation.

Parameter	Value	Parameter	Value
m	1.0	B	432.15 eV
γ	1.0	R	2.36 Å
λ_3	0.0 Å^{-1}	D	0.15 Å
c	19981	λ_1	2.9726 Å^{-1}
d	7.034	A	1681.7 eV
h	−0.33953	Z_i	6
n	0.99054	Z_j	14
β	4.1612×10^{-6}	r_C	0.95 Å
λ_2	2.0913 Å^{-1}	A_F	14