



Stable configurations of graphene on silicon

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ABSTRACT

Integration of graphene on silicon-based nanostructures is crucial in advancing graphene based nanoelectronic device technologies. The present paper provides a new insight on the combined effect of graphene structure and silicon (001) substrate on their two-dimensional anisotropic interface. Molecular dynamics simulations involving the sub-nanoscale interface reveal a most favourable set of temperature independent orientations of the monolayer graphene sheet with an angle of $\sim 15^\circ$ between its armchair direction and [010] axis of the silicon substrate. While computing the favorable stable orientations, both the translation and the rotational vibrations of graphene are included. The possible interactions between the graphene atoms and the silicon atoms are identified from their coordination. Graphene sheet shows maximum bonding density with bond length 0.195 nm and minimum bond energy when interfaced with silicon substrate at 15° orientation. Local deformation analysis reveals probability distribution with maximum strain levels of 0.134, 0.047 and 0.029 for 900 K, 300 K and 100 K, respectively in silicon surface for 15° oriented graphene whereas the maximum probable strain in graphene is about 0.041 irrespective of temperature. Silicon–silicon dimer formation is changed due to silicon–carbon bonding. These results may help further in band structure engineering of silicon–graphene lattice.

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1. Introduction

Graphene is a two-dimensional allotrope of carbon [1,2] with hexagonal lattice structure, which has several interesting electronic, magnetic, optical and thermo-mechanical properties. Several of these properties have been studied extensively since the first report on graphene [3,4]. Free-standing graphene has an electronic band structure which shows zero gap between valence and conduction bands at K point of the first Brillouin zone forming the shape of Dirac cones [5]. The lack of bandgap makes graphene a semi-metal with several interesting properties such as ballistic transport [6], long mean free path at room temperature [7], high carrier mobility with mass-less relativistic carriers called Dirac Fermions [8] and integer as well as fractional quantum Hall effect [9–11]. These distinctive properties of graphene and its composites have various potential applications such as gas sensors [12,13],

novel spintronic devices [14] and transparent electrodes for photovoltaics [15,16]. However, the absence of bandgap in graphene limits its incorporation in field effect transistors and other optoelectronic devices [17]. Therefore to facilitate various graphene based applications, techniques for engineering certain bandgap in graphene-based system are as follows: patterning holes or defects in graphene [18,19], adsorbing different molecules on the graphene surface [20–22], and/or placing graphene on various different substrates [23,24]. Our present study is concerned with the problem of graphene placement on silicon substrate for bandgap engineering.

Graphene placed on wide variety of substrates including metals [25,26], semiconductors [27,28] and insulators [29–31], have potential advantages in various field of applications. Here, we focus on the advantages of graphene on a silicon substrate. Silicon is the widely used single-crystal substrate in current micro-fabrication technology [32]. When graphene is placed on silicon substrate, one would expect the electronic energy structure of graphene to change. This is due to the removal of atomic orbital symmetry for carbon atoms that are interacting with the underlying silicon substrate [33]. Graphene layer on silicon enhances the thermal conductivity by one order of magnitude when compared to that of pristine silicon [34]. Non-local elasticity theory based ultrasonic

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wave dispersion calculations proved that flexural modes are significantly affected by the silicon substrate [35]. Graphene placed on silicon acts as a tunneling barrier for injection or detection of electronic spin into silicon when the system is placed with a ferromagnetic electric contact [36]. Recently, researchers interfaced graphene with silicon to form Schottky junctions that are useful in photo diodes [37], light harvesters [38] and solar cells [39].

Earlier studies showed formation of graphene on silicon by annealing epitaxial SiC film grown on silicon substrate at 1500 K [40]. However, direct growth of graphene on silicon surface is very attractive towards forming Schottky type junction. Other reports [37–39] used a clean silicon surface obtained from wet etching and then transferred the mechanically exfoliated graphene. Transfer of graphene on silicon (111) surface under ultra-high vacuum conditions by fusion bonding or wafer direct bonding has been discussed by Ochedowski et al. [41]. Such transfer processes result in contamination, defects and wrinkles in graphene layer [42] and the effectiveness depends largely on the uniformity of the crystal surface and surface cleanliness. Orientation dependent mechanical deformation and fracture behavior of graphene [43–45] are important input to develop the process successfully. Laser beam induced growth of graphene on silicon is a new technique [46]. Another method using the direct growth of graphene on insulating surface [31] may be extended for silicon surface as well. In such growth mechanism, a graphene layer is formed after cooling by minimizing the energetics. While minimizing energy, both translation and rotational motion is possible which may result in rotation of the graphene on silicon surface. Molecular dynamics (MD) simulations show ripples having amplitude of 0.12 nm in graphene placed on silicon terminated SiC surface at different temperatures [47]. Recent reports have shown that graphene exhibits distinct growth mechanism that depends on its in-plane orientation relative to the substrate surface orientation [48,49]. The structural symmetry of graphene breaks down when it is placed on a pure silicon (001) substrate. In such system, the natures of lattice strain and temperature effects are two important factors that have not been studied till date.

In the present study, we have comprehensively looked at the stability of graphene on silicon (001) system (Si-G system). We consider an example of nano-fabrication process that imitates the epitaxial growth of graphene on silicon involving the following temperature states. (i) Chemical vapor deposition (CVD) at a temperature of 900 K, (ii) cooling to room temperature of 300 K and (iii) further cooling to cryo condition at 100 K. At these temperatures, we search for a stable orientation of graphene on silicon surface with the help of bond density and bond energy analysis. We also evaluate the lattice strain in order to confirm the stable orientation of graphene on (001) silicon substrate.

2. Simulation scheme

MD simulations are performed to study the stability of the Si-G system where the single layer graphene is allowed to translate and rotate over the silicon substrate. Initial angular orientation is prescribed. Fig. 1(a) shows the schematic of Si-G system. A 15 nm square shaped single layer graphene sheet is placed on a silicon (001) substrate of dimensions $25 \times 25 \times 4 \text{ nm}^3$ with its center on the (001) plane of its surface aligning on the vertical axis passing through the center of the graphene layer. Initially graphene is placed at a height h from the silicon (100) surface atomic layer and with an initial orientation angle θ . We used different graphene for different orientations with the rectangular boundaries kept fixed which cut the edge atom bonds differently in each case of orientation. Fig. 1(b) show the scheme of orientation of graphene with respect to the silicon surface unit cell. Orientation of the

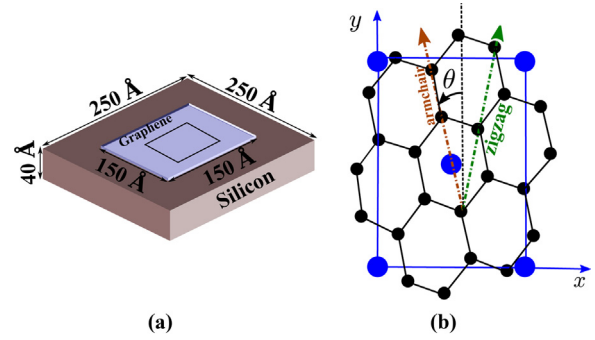


Fig. 1. (a) Si-G system used in our MD simulations. Slab represents the silicon substrate and the central region represents the graphene layer. Square box inside the graphene region indicate the effective region used for calculations. (b) Representation of graphene rotation on silicon substrate with an angle θ subtended between armchair direction and y-axis. The angle subtended between zigzag direction and y-axis is $30^\circ - \theta$. Carbon atoms in graphene are colored with black. Silicon atoms are colored as blue. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

graphene is defined as the angle θ between armchair vector and [010] axis (y-axis). Different graphene orientations are characterized by the chiral vector $\mathbf{C}_h = (i - j)\frac{a}{2}\hat{x} + (i + j)\frac{\sqrt{3}a}{2}\hat{y}$, where a is the lattice constant of graphene. i and j are the chiral indices. The armchair and zigzag directions in Fig. 1(b) correspond to $\mathbf{C}_h = \sqrt{3}a\hat{y}$ and $\mathbf{C}_h = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$, respectively. Periodic boundary conditions are assumed along in-plane directions in order to replicate the repeating unit of Si-G system considered. Atoms in the bottom two layers of lattices are fully restrained (with zero velocities) to make the substrate stationary and induce deformation at the upper layers due to the Si-G interface mis-match.

The inter-atomic interactions involved in Si-G system are modelled using a combination of Tersoff and adaptive inter-molecular reactive empirical bond order (AIREBO) potential functions. Tersoff inter-atomic potential [50] is used to study the stability and deformation of silicon crystal and SiC. AIREBO potential [51] captures various physical characteristics of graphene accurately. Combination of these potentials will help us to account for the possible interactions like silicon-silicon, silicon-carbon and carbon-carbon more accurately. The total atomic interaction energy U of the Si-G system as a function of atomic coordinates is a sum of bonded, non-bonded (Lennard-Jones + Torsional) interactions and it can be written as

$$U = \frac{1}{2} \sum_{n=1}^N \sum_{m \neq n}^N \left[U^{\text{BOND}}(r^{nm}) + U^{\text{LJ}}(r^{nm}) + \sum_{k \neq n, ml \neq n, m, k} U^{\text{TORSION}}(\omega^{nmkl}) \right], \quad (1)$$

where r^{nm} is the distance of separation between atom index n and atom index m . Atomic indices run from 1 to N , where N is the total number of atoms in the Si-G system. U^{BOND} is the inter-atomic potential energy which accounts for the bonded interactions between a pair of atoms. U^{LJ} is the non-bonded inter-atomic potential energy constructed with a series of switching functions such that U^{BOND} term is not effected. The other non-bonded interaction (U^{TORSION}) is a four-body potential that optimizes the angular configuration. The values for the parameters involved in U^{BOND} are taken from Tersoff potential for silicon-silicon and silicon-carbon interactions [50]. The carbon-carbon interaction potential parameters are considered using AIREBO potential [51]. The non-bonded interaction potential is determined for graphene

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