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Modeling of substrate impacts on formation of bilayer silicene

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ABSTRACT

Energy bandgap opening has been found in buckle-free bilayer silicene (BLSi) under uniform tensile in-plane strain. Practically such in-plane strain can be provided from the substrate lattice mismatch. In this work, we performed a theoretical study using density functional theory (DFT) to investigate the substrate-induced impacts on bilayer silicene. Several common semiconductor substrates have been examined for simulating epitaxial grown bilayer silicene with excessive in-plane strain. The existence of three characteristic equilibrium distances between the BLSi and the substrate was observed. The value of the optimal distance depends on the substrate materials and the surface terminated atoms. Highest electron transfer occurrence was observed when a BLSi directly deposited on a substrate, associated with strong chemical bonding at the smallest equilibrium separating distance. At the intermediate or large metastable distances, the interactions between BLSi and substrate surface atoms transformed into weak partial coupling or almost complete decoupling. For the BLSi on Ga-terminated GaSb substrate (GaSb_Ga) strong bonding strength results a fixed interface distance at 0.8173 **Å** and increased bandgap than free-standing BLSi**.** As the separation in the range of **2.6 to 2.9 Å**, the system can be established at a metastable state via partially coupling with a reduced bandgap less than 40 meV. Above 2.9 **Å** , electron transfer is insignificant and BLSi acts as a free-standing one. By contrast, the GaSb_Sb system sustains a large-range and continuous energy bandgap opening (up to 57 meV) across a wide Δd_0 range of **3.0 to 4.3 Å**. This founding suggests that direct epitaxial growth will result in strong bonding which is impractical to well-control bandgap opening and to physically separate the as-grown BLSi from the substrate. Remote epitaxial is more promising by inserting an inert passive material or even an airgap with an appropriate separating distance between the BLSi and substrate.

1. Introduction

Integrated Circuits (ICs) have been integrated into every modern electronics in our daily lives. However, innovation and breakthrough of electronics have been predicted to encounter a performance bottleneck as the mainstream silicon-based IC chips approach the physical limits. The state-of-the-art ICs technology will be soon below 3 nm. At such a scale, the short channel effect and power consumption become the dominant factors impeding further development [1]. To tackle the challenge, a thinner channel layer, projected by the ITRS (International Technology Roadmap for Semiconductors), seems to be the most viable solution.

2D materials have received a lot of attention associated with their atomic-thin thickness, distinct optical, electrical, magnetic, thermal, and mechanical properties [2]. A variety of 2D materials have been found followed by the discovery of graphene, like silicene, germanene, phosphorene, MoS_2, WS_2, $MoSe_2$, HfS_2, $HfSe_2$, GaS, and InS etc. The major challenge of applying graphene in large-scale digital circuits is its lack of energy bandgap. Among all other 2D materials, silicene appears to be one of the most favored candidates for its excellent compatibility with standard silicon technology [3–6]. Up to date, monolayer, bilayer, and a few layer silicenes have been experimentally fabricated on metallic, semiconducting, and insulating substrates via various approaches [7–17], accelerating their implementation.

Monolayer silicence (MLSi) has been extensively studied both computationally and experimentally in the aspects of structure, stability, and electronic properties [3–6]. It is well-accepted that stable free-standing MLSi has a lattice constant of 3.866 Å with buckling height

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of 0.5 ± 0.05 Å depending on experimental or computational accuracy. Pristine free-standing buckled MLSi, similar to flat graphene, shows the Dirac cone-shaped energy band diagram but zero bandgap. MLSi is attractive for its high intrinsic mobility and linear dispersive Dirac cone, and has been experimentally demonstrated in laboratories for field-effect transistors (FET), Neuromophic, Photodetectors etc [18]. Its bandgap can be opened up to 200 meV via applying high electric field or alternating its chemistry through oxidation etc. [18–22] These strategies are either undesirable or impractical in practical device processing. Self-structuring or straining via substrate mismatch is more favorable [23–25]. This strategy has been widely used to improve electron and hole mobilities in silicon technology. However, in-plane strain will not induce any band gap opening in MLSi. Further, intrinsic MLSi is unstable in air and readily interacts with most common substrates [3–6]. These intrinsic limitations of MLSi have prevented it immediate implementation in the mainstream semiconductor industry.

Bilayer silicene (BLSi) offers numerous notable advantages over MLSi. Benefiting from the interlayer coupling, BLSi is much more stable than MLSi and hence, much less reactive towards environment and substrates. The buckling in silicene brings about rich variations in BLSi structure, rendering wealthy and unique electronic and optical properties. Over the past decade, new discoveries related with BLSi continue to emerge [26–34]. To date, five up to ten dynamically stable structures and many metastable phases with distinct atomic configurations, symmetries, and periodicities are reported in BLSi. The various BLSi metastable phases have similar cohesive energies. The distinct electronic and optical properties in each phase can be realized via facile phase transformation. Therefore, BLSi can be finely tuned in a wide range, transition from metallic to semiconducting states. Compared to monolayer silicene, bilayer silicene is more robust with tunable and wider bandgap, allowing for better transistor behavior. In addition, light–matter interactions in BLSi are stronger than in MLSi. The unique and rich relationship between structure and electronic and/or optical properties in BLSi has more profound applications to nanoelectronics, optoelectronics, photonics, spintronics, and electromechanical devices etc.

Our previous computation studies show that the most common five free-standing BLSis are all buckled, presenting Dirac-cone shaped energy band diagram with zero energy band gap. Under uniform tensile in-plane straining, these free-standing BLSis exhibited gradual reduction in buckling height and several local minima in total energy. At an excessive tensile biaxial strain in the range of 10.7 – 15.4 %, BLSi transformed into atomically flat AA-stacked structures with zero buckling height. Different from MLSi, the strain-flattened BLSi showed energy band gap opening up to 0.17 eV [35]. However, up to date, the maximum in-plane strain experimentally achieved is around 7% in the epitaxial silicene grown on Au (111) [36]. For practical applications of BLSi, the challenge lies in selecting appropriate substrates and identifying criteria for BLSi on substrate with desired bandgap opening and also weak bonding to facilitate easy release from the substrate. The primary objective of this study is, by employing the density functional theory (DFT), to investigate the substrate-induced impacts on structural and electronic properties of bilayer silicene films. Specifically, the lattice mismatch induced strain on BLSi has been taken into account in the modeling. Further, the feasibility to add an airgap interlayer between BLSi and the substrate has been studied to facilitate physically separating the BLSi from its substrate.

2. Modeling details

Modeling of atomic structure was carried out using Synopsis Atomistic Tool-Kit (ATK) software package (Quantum ATK) based on first-principle density functional theory. Details of the computational optimization can be found in our previous works [37–40]. In this study, Generalized Gradient Approximation (GGA) and Quasi-Newton method were employed to optimize the atomic structures with Hellmann-Feynman forces smaller than 0.0001 eV/Å. The density mesh cutoff energy, electron temperatures, and Monkhorst-Pack K-points mesh were selected to be 75 Hartree, 300 K, and 15*15*1, respectively. Energy band diagrams were calculated using Perdew, Burke, and Enzerhof (PBE) approximations [41,42]. Non-Equilibrium Green's Function (NEGF) was utilized to compute the electronic transport properties including current and charge densities under finite bias in nanoscale electronic devices [43–45]. The in-plane lattices were denoted as “A” and “B” axes. A large constant in C-axis, i.e. c = 60Å, was selected to ensure no interaction among layers within the vacuum spacing.

We have conducted a verification process using free-standing monolayer silicene. Both structure and energy band diagram are consistent with others under the above computational conditions. As benchmarks, stable states of free-standing BLSi w/o tensile strain were computed. The atomic model of free-standing BLSi consists of four silicon atoms in two atomic layers in AA-stacking or AB-stacking. Periodic boundary conditions have been employed for unit cells 1 x 1, 2 x 2, and 3 x 3 to optimize the atomic structure. The unstrained BLSi is buckled in each layer and has lattice constant of 3.866 Å, same as MLSi. Afterwards, the lattice constant is gradually increased to mimic the silicene under uniform tensile in-plane strain. In this case, all the four silicon atoms are allowed to relax in the c-axis.

Considering the desired lattice mismatch and technology's scaling up potential and compatibility with the mainstream semiconductor industry, groups of II-VI, III-V and IV semiconductor substrates, e.g. CdSe, InAs, GaSb, AlSb, were selected in this research [35,37–40,46]. Substrate's terminating atoms are known to play a crucial role and have determinant impacts on the BLSi structures. In this study, calculations were also carried out on both GaSb_Ga (with Ga as the atop atom) and GaSb_Sb (with Sb as the atop atom) substrates.

The atomic model of BLSi on substrate consists of four silicon atoms in two atomic layers on top of the selected substrate with six atoms (see Fig. 1). In the stabilized substrate structure, the six atoms in three pairs are labeled as S1, S2, and S3. These pairs stacked in the ABC pattern along the C-axis reflecting the (111) orientation of the cubic-structured substrate. To mimic semi-infinite substrate, the base pair (S1) was fixed but the top two pairs were allowed to adjust their positions during optimization. Before optimization, the buckled stable BLSi with lattice constant of 3.866 Å was set on top of the substrate. All the four silicon atoms were allowed to relax during the structural optimization process. The interface spacing or thickness is defined by the separation between the top terminated atom of the substrate and the lowest silicon atom of BLSi. The initial separation between BLSi and substrate Δd_i was varied in the range 1 to 10 Å. The separation of the optimized system is Δd_o. To study the relationship between Δd_o and Δd_i, the in-plane lattice constants (A and B axes) of the strained BLSi and the substrate were kept identical to those at the optimized stable case. The systems with BLSi on all the selected substrates converged with a minimum energy, suggesting they can reach metastable state. After the BLSi/substrate system optimization, the interfacial electron density was analyzed. The band structure and energy bandgap of BLSi was computed using the optimized BLSi structure with the substrate removed.

3. Results and discussions

Results have shown that BLSi on the four metal-terminated substrates, whether the starting BLSi is in AA-stacking or AB-stacking with small perturbation, is stabilized at hexagonal honeycomb structure with AA-like stacking configuration. The lattice constants are aligned with the four selected substrates. Relative to the lattice constant of free-standing stable BLSi (a_o = 3.866 Å), the BLSi on the selected substrate, e.g. CdSe, InAs, GaSb, AlSb, has experienced significant biaxial tensile strain ($\epsilon = \frac{a-a_o}{a}$) which is induced by the substrate. However, the highly strained BLSi is still slightly buckled although the buckling height reduced significantly. This observation shows that BLSi on substrate is