Silicene on substrates: interaction mechanism and growth behavior

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Abstract. Silicene, a monolayer of silicon atom assembling in a honeycomb lattice, has attracted more and more attention due to its outstanding electronic properties. The recently successful synthesis of silicene on several metal surfaces takes a big step towards the utilization of silicene in the future microelectronic devices. On the roadmap for the applications of silicene, two critical issues have to be addressed: (1) how to improve the quality of silicene; (2) how to preserve the extraordinary electronic properties of silicene. These two problems can be solved by deeply understanding the substrate effect on silicene. In this review, we systematically discuss the substrate effect on the atomic structure and electronic properties of a silicene sheet as well as the growth behavior of silicene on Ag surface, which are important for both fabrication and application of silicene.

1. Introduction

As early as in 1994, the theoretical possibility of stage corrugation in Si analogs of graphite had already been explored.[1] But until 2009, two-dimensional (2D) silicon monolayer possessing a hexagonal honeycomb lattice with a buckled height of about 0.44 Å was confirmed to be stable by phonon dispersion and ab initio finite temperature molecular dynamics calculations.[2,3] Such single atom thickness of 2D sheet silicon was thereafter named by silicene[4-34], which attracts more and more attentions recently. Most of all, silicene possesses outstanding electronic properties similar to that of graphene.[2-6,35-37] The band structure of silicene exhibit linear dispersion around Fermi level, forming the famous "Dirac cone" at the symmetric point K in the reciprocal space. This band characteristic indicates that the charge carriers in silicene sheet behave like massless Dirac fermions in a small energy range around the Fermi level $E_F$. Interestingly, the velocity of charge carriers near Fermi level in silicene was estimated to be $10^5\text{~}10^6 \text{~m/s}$,[2] comparable to that in graphene.[37-39] Both first-principle and tight-binding calculations show that silicene has a much larger band gap (about 1.55 meV) at the Dirac points opened by the effective spin-orbit coupling than graphene.[7,8] Therefore the quantum spin Hall effect can be observed in silicene in an experimentally accessible temperature regime, which may lead to some novel silicene-based spintronic devices. Moreover, first-principles calculations predicted that a tunable gap can be opened up in silicene at the Fermi level via hydrogenation,[9-11] fluorination,[12] or applying electric field.[13,14] Most attractively, easy
integration into the current Si based technology makes silicene a potential candidate for microelectronic devices.

To realize the utilization of silicene, the challenge for fabrication of silicene must be overcome. Since there is no silicon allotrope with layered structure analogous to the graphite in nature, the mechanical stripping method for fabricating graphene[35] and many other 2D materials[40] does not work for silicene. Meanwhile, the silicon oxide (SiO$_2$) is a kind of hard insulator. Thus, the method of reduction of graphene oxide[41] can’t be applied to silicene either. Up to now, the major method for synthesizing silicene is epitaxial growth on metal substrates. Before the synthesis of large-scale silicene sheet, silicene nanoribbon was successfully fabricated on Ag(001)[42] and Ag(110)[43-45] surfaces. Afterwards, Lalmi et al. reported epitaxial growth of silicene on Ag(111) substrate in 2010.[15] The lateral Si-Si distance in the $(2\sqrt{3} \times 2\sqrt{3}) R30^\circ$ superstructure observed by them was 0.19 ± 0.01 nm, shorter than the Si-Si bond lengths (0.22 ~ 0.24 nm) from previous theoretical prediction[3] and experimental observation in silicon nanoribbons[39,40]. The difference between the lateral Si-Si distance and the Si-Si bond lengths was attributed to the large buckling of silicene on Ag(111) surface.[32] More recently, several experiments were conducted to repeat the epitaxial growth of silicene on Ag(111) surface and a variety of superstructures were observed, including $(4 \times 4)$, $(\sqrt{13} \times \sqrt{13}) R13.9^\circ$, $(\sqrt{7} \times \sqrt{7}) R19.1^\circ$, $(2\sqrt{3} \times 2\sqrt{3}) R30^\circ$ with respect to Ag(111)[17-20,33,46]. The average Si-Si distances in these superstructures are 0.22±0.01 nm, in agreement with that in nanoribbon. Our first-principles simulations explained the superiority of Ag as substrate for the growth of silicene.[21] Firstly, Ag(111) surface can stabilize sp$^2$ hybridized silicene via moderate interaction between silicene and surface metal atoms. Secondly, Ag(111) surface interacts with silicene almost homogeneously and thus the local tension in silicene during the growth process can be rather small.

In addition to Ag, efforts also have been made to synthesize silicene on other substrates. For example, silicene was also successfully synthesized on zirconium diboride (ZrB$_2$) thin films grown on Si wafers through epitaxial growth[22] and Ir(111) surface by directly depositing silicon atoms and annealing the sample at 670 K[23]. The successful synthesis of silicene ribbons and sheets supplies the precondition for utilizing silicene in nanoscale materials and devices. The atomic structures, electronic properties and synthesis of silicene have been summarized in previous reviews.[47-49] Though free-standing silicene exhibits excellent electronic properties, during the growth process of silicene or in the practical utilization of silicene in microelectronic devices, it always occurs along with substrates. Thus, the substrate effects are significant and have attracted some recent efforts.[14,16,24-30,34] In this review, we will briefly summarize our current understanding on the substrate effects for silicene and the growth behavior of silicene on Ag(111) surface.

2. Interaction mechanism between silicene and substrates

2.1 silicene on insulating substrates

In the future microelectronic devices made of silicene, silicene has to be supported on some insulating substrates, similar to the cases of graphene[50-58] and MoS$_2$ sheets[59-61]. Thus, the effect of inert substrates on the electronic and transport properties of silicene is an important issue for the practical applications of silicene. Houssa et al. proposed that a silicene flake could preserve the semimetallic behavior when it is embedded between ultrathin AlN layers.[24] The ultrathin AlN was shown to be insulating with an energy gap of about 4.6 eV. Silicene flake weakly interacts with AlN layers via vdW forces. Recent ab initio calculations suggested that the excellent electronic properties of silicene can be preserved on hexagonal boron nitride (h-BN) monolayer and hydrogenated SiC(0001) surface[14,25,26] It was found that silicene retain its geometry structure with a distance of about 3 Å from the substrates (Figure 1). The cohesive energies between silicene and these substrates are about 0.07~0.09 eV per silicon atom, which can also be viewed as van der Waals (vdW) type.
As shown in Figure 2b, c, the Dirac cone of silicene was nearly preserved on the h-BN monolayer and hydrogenated Si-terminated SiC(0001) surface (Si-SiC). Therefore, h-BN and Si-SiC can provide effective mechanical support for silicene without disturbing its geometry and electronic properties. On the contrary, silicene on the hydrogenated C-terminated SiC(0001) surface (C-SiC) becomes metallic (Figure 2d). For silicene/BN (Figure 2f) and silicene/Si-SiC (Figure 2g), the partial charge densities in the energy range of $E_F - 0.2$ eV concentrate on silicene, similar to that in free-standing silicene (Figure 2e). While for silicene/C-SiC, the partial charge densities distribute widely in silicene and the substrate (Figure 2h), implying that the Fermi level has already entered the vicinity of valence band maximum (VBM) of C−SiC.

Different substrate effects on the electronic property of silicene can be explained by the work functions of substrates.[25] By setting the vacuum energy as zero, the VBM is the negative value of
work function. As shown in Figure 3a, the VBM of silicene is slightly lower than the VBM of C-SiC. The approaching of the two energy levels results in certain interaction between silicene and substrate. As a consequence, some new electronic states arise between the two VBMs due to the strong electron coupling after silicene contacting with C-SiC. Thus, the Fermi level of the silicene/C-SiC hybrid system lies between the VBM of original silicene and the VBM of original C-SiC (Figure 3b). Eventually, the Dirac cone of silicene is submerged under the Fermi level (Figure 3b) and slightly disturbed due to the electron coupling. On the contrary, for the other two substrates, the VBM of silicene locates in the gap of the substrates that is far from the VBMs of the substrates. The electron coupling between silicene and the substrates is too weak to create any new electronic states. Consequently, the Fermi levels for silicene/BN and silicene/Si-SiC still cross the Dirac points of silicene.

Figure 3. (a) Conduction band minima (CBM) and valence band maximum (VBM) of BN monolayer, Si-SiC substrate, silicene, and C-SiC substrate with respect to the vacuum level (set as zero energy). The values of CBM and VBM of silicene are exactly identical. (b) Schematic for the origin of metallic behavior in silicene/C–SiC hybrid system. Blue areas present the occupied electronic states.[25]

2.2 Silicene on metal substrates

Different from the insulating substrates, silicene sheets forms various superstructures on metal surfaces due to stronger silicene-substrate interactions.[17-20,22,23,46] The buckled height is about 1 Å for silicene on Ag(111) surface. As discussed above, some insulating substrates with appropriate work function can preserve the Dirac cone of silicene and thus the outstanding electronic properties. In the case of metal substrates, there is a fierce debate about whether the Dirac cone can be preserved on Ag(111) surface.[16,26-30] In 2012, using angular-resolved photoelectron spectroscopy (ARPES) measurements, linear dispersion was observed in the (3 × 3) silicene on (4 × 4) Ag(111) superstructure (refer as (4 × 4) superstructure hereafter) with the Dirac cone about 0.3 eV below the Fermi level.[16] It was proposed that the linear dispersion came from silicene and a Fermi velocity of $1.3 \times 10^6$ ms$^{-1}$ was estimated. However, combining spectroscopic signatures of quantum Hall effect by the Landau quantization under a magnetic field and density functional theory calculations, Takagi and co-workers proposed that silicene would no longer be a two-dimensional Dirac fermion system when synthesized on the Ag(111) surface due to substrate-induced symmetry breaking.[27] Figure 4a shows the scanning tunneling microscopy (STM) image of a (4 × 4) superstructure. The amplificatory STM image is shown in Figure 4b. Scanning tunneling spectroscopy (STS) spectra was used to measure the Landau levels. For the magnetic field perpendicular to the sample between zero and 7 T, characteristic structures due to the Landau quantization were not found (Figure 4c), which implies the silicene loses its characteristic of Dirac fermion system. In contrast, Landau levels appear in the highly-oriented
pyrolytic graphite (HOPG) (Figure 4d), which can be reasonably rationalized by a combination of massless and massive Dirac fermions.[62-66]

Figure 4. (a) STM image of large area of silicene (sample bias voltage $V_S = -0.70$ V and tunneling current $I_t = 0.19$ nA. The image size is $35 \times 35$ nm$^2$). (b) High resolution STM image of the $4 \times 4$ silicene ($V_S = +0.50$ V and $I_t = 0.30$ nA, $3.65 \times 3.65$ nm$^2$). The unit cell is shown by the white rhombus. (c) STS spectra of silicene for various magnetic fields perpendicular to the sample surface, $B_Z$. (d) STS spectra of HOPG for various $B_Z$. The purple triangles and green circles show the peaks originating from the LLs of massless and massive Dirac fermions, respectively. The LL with $n = 0$ is marked by the yellow bar and the LL with $n = 1$ of massive Dirac fermions is not clearly resolved in 3 T due to low magnetic field.[27]

Detailed analysis of Kohn-Sham orbitals from first-principles calculations of the $(4 \times 4)$ superstructure along the $\Gamma$–K direction showed the linear band observed by ARPES experiment may correspond to the sp band of Ag substrate.[26] Almost at the same time, another group independently demonstrated that the Dirac cone in silicene on Ag(111) surface was destroyed due to the distortion of silicene on Ag surface and strong band hybridization at silicene/Ag(111) interface, by unfolding bands.
from supercell calculations.[28] They proposed that the linear dispersion observed in angular-resolved photoemission spectroscopy[16] indeed comes from the Ag substrate, instead of silicene. Very recent first-principles calculations show that the linear dispersion observed in experiment originates from the hybridization states between silicene and Ag(111) surface, neither from silicene nor from Ag sp bands.[29] The reconstructed (3 × 3) silicene without Ag substrate opens a 0.3 eV band-gap at the pristine Dirac cone (red dots in the left panel of Figure 5) due to structural modification induced by the Ag substrate. Comparing the unfolded band of reconstructed (3 × 3) silicene (red dots in the left panel of Figure 5) with the unfolded band of silicene/Ag (red dots in the right panel of Figure 5), no one to one correspondence can be found between them. Thus, a strong hybridization occurs between silicene and Ag substrate. The surface states of Ag have no contribution to the linear dispersion in absence of silicene (Figure 6b). When silicene is present, however, the linear band appears again (Figure 6c). This coincides with the experiment observation.[16] Moreover, the linear dispersion from bulk Ag states is absent at the band structure of surface Ag states. Therefore, Cahangirov et al. proposed that it is more reasonable to attribute the observed linear bands to the hybridized states of silicene and Ag rather than bulk Ag state.[29] On the contrary, Avila and the co-workers recently revisited the electronic structures of the 3×3 silicene phase on Ag(111) surfaces by using a compiled set of LEED, CLs and ARPES data, pronouncing that the linear dispersion still comes from silicene rather than Ag substrate.[30]

Figure 5. Left panel: bands of reconstructed (3 × 3) silicene in the absence of Ag substrate (unsupported silicene) unfolded to BZ of (1 × 1) silicene are shown by red dots. The radii of dots correspond to the weight of unfolding. The band structure of ideally buckled silicene is shown by green lines. Right panel: unfolded band structure of silicene on Ag. Red dots correspond to states with significant contribution from silicene.[29]
Besides the characteristics of electronic band structures, understanding the interaction mechanism between silicene and metal surface is crucial for growth of high quality silicene. Among these metal substrates, Ag(111) surface is widely used. Hence, it may serve as a representative to explicate the interaction mechanism between silicene and metal substrates. A silicon clusters Si_{24} composed of seven hexagonal rings, which can be viewed as a small patch of silicene, was constructed to explore the interaction between silicon atoms and Ag(111) surface.[21] Upon relaxation, Si_{24} cluster retains its geometry on Ag(111) surface (Figure 7a). The local density of states (LDOS) for Si_{24}@Ag(111) (Figure 7b) shows that the 3p states of Si atoms couple with the 4d states of Ag atom in the vicinity of the Fermi level, implying the hybridization between Si p_z electrons and Ag 4d electrons. Such hybridization may also explain why silicene loses its Dirac fermion characteristics on Ag(111) surface. The charge differential densities of Si_{24}@Ag(111) shown in Figure 7d illustrate that all Si atoms at both periphery and inner regions of Si_{24} cluster interact evenly with Ag(111) surface. Moreover, the on-site charges of Si atoms in Si_{24}@Ag(111) system (Figure 7c) are nearly homogeneous (range between $-0.13$ |e| and $-0.08$ |e|). This finding coincides with the small difference of adsorption energies for Si atom on different sites of Ag(111) surface (less than 0.031 eV).[21] Thus, the local tensions in Si_{24} cluster and other silicene patches induced by the Ag(111) surface should be small, which is surely beneficial for continuous growth of high-quality silicene. In contrast, the difference of adsorption energies for Si atom on different sites of Rh(111) surface is calculated to be 0.306 eV[21], much larger than that for Ag(111) surface. In short, moderate and homogeneous interaction between Si atoms and Ag atoms makes Ag(111) surface a suitable substrate for epitaxial growth of silicene.
Due to the moderate silicene-substrate interaction, silicene sheets can be rather stable on Ag(111) surface and form some superstructures, including (3×3) silicene on (4×4) Ag(111) surface, (\(\sqrt{7} \times \sqrt{7}\)) silicene on 2\(\sqrt{3} \times 2\sqrt{3}\) Ag(111) surface, (\(\sqrt{13} \times \sqrt{13}\)) silicene on \(\sqrt{13} \times \sqrt{13}\) Ag(111) surface.\cite{21} The atomic structures and simulated STM images of these silicene@Ag(111) superstructures are shown in Figure 8. Note that the simulated STM images agree well with experimental ones.\cite{16-20} After geometry optimization, silicene sheets retain the honeycomb structure with a buckled height of about 1 Å. Only the topmost silicon atoms in the silicene sheets (highlighted by red balls) can be seen in the STM images. The stability of different silicene superstructures is characterized by the binding energy, defined as

\[
E_b = E_{si} + E_{sub} - E_t
\]

(1)

where \(E_{si}\) is the energy of silicene, \(E_{sub}\) is the energy of Ag substrate, \(E_t\) is the energy of silicene/Ag system. According to the computed binding energy, we can compare the stability of three types of silicene superstructures on Ag(111) surface. The type I, i.e., (3×3) silicene on (4×4) Ag(111) with a binding energy of 0.368 eV per silicon atom, is the most stable one. The binding energies of other two silicene phases ((\(\sqrt{7} \times \sqrt{7}\)) silicene on (2\(\sqrt{3} \times 2\sqrt{3}\)) or (\(\sqrt{13} \times \sqrt{13}\)) Ag(111) surface) are very
closed, which are 0.336 eV and 0.332 eV per Si atom, respectively. This may help understand why the type I is the most frequently observed phase of silicene on Ag(111) surface in experiments.[30]

![Figure 8. Atomic structures and simulated STM images of three types of silicene@Ag(111) superstructures. (a), (c), (e) are geometry of silicene@Ag(111) superstructures with topmost Si atoms highlighted by red balls; (b, d, f) are the STM images with a constant height of 2 Å to the topmost Si and a bias voltage of -1.5 V.[21]]

Ab initio molecular dynamics (AIMD) simulations were also carried out to assess the thermal stability of (3 × 3) silicene superstructure on (4 × 4) Ag(111) surface.[21] The snapshots from AIMD simulation of this superstructure are shown in Figure 9. At 500 K (which is about the growth temperature of silicene), no topological defect was ever generated during the entire simulation time up to 7.5 ps, indicating high thermal stability of silicene on Ag(111) surface. At 900 K, some defects arose in silicene after 0.8 ps (Figure 9c), but were spontaneously recovered very quickly.

For comparison, a silicene@Rh(111) superstructure ((4 × 4) silicene on (6 × 6) Rh(111) surface) was constructed. After DFT relaxation, silicene keeps its honeycomb geometry on Rh surface (Figure 9d). However, after AIMD simulation of only 0.7 ps at 500 K, two Si-Si bonds were broken (Figure 9e). Afterwards, the silicene sheet became amorphous after 2.3 ps at 500 K (Figure 9f). As discussed above, the diffusion barrier of silicon monomer on Rh(111) surface is about ten times of that on Ag(111) surface. Therefore, the thermal instability of silicene monolayer on Rh(111) surface can be ascribed to the larger local energy difference of Si atom on Rh surface. Again, comparative AIMD simulations demonstrate that the superiority of Ag as a substrate for silicene growth originates from the intermediate and homogeneous interaction between Si atoms and Ag atoms.
Figure 9. Snapshots from AIMD simulation of (5 \times 5) silicene monolayer on (7 \times 7) Ag(111) surface with 3.8\% lattice mismatch: (a) initial configuration, (b) structure after 5.0 ps at 500 K, (c) structure after 0.8 ps at 900 K. Snapshots from AIMD simulation for (4 \times 4) silicene on (6 \times 6) Rh(111) surface with 3.7\% lattice mismatch: (d) initial configuration, (e) structure after 0.7 ps at 500 K, (f) structure after 2.3 ps at 500 K.[21]

3. Growth behavior of silicene

Typically, the process for epitaxial growth of silicene on metal surface involves three stages: (i) silicon clusters are deposited on metal surface; (ii) silicon monomers or dimers aggregate into many small silicon clusters, but most of them dissociate into monomers, dimers and small pieces again; (iii) continuous growth of silicon clusters beyond nucleation size to cover the whole metal surface. Among the three stages, stage (ii), the nucleation of silicene, is crucial for understanding and controlling silicene growth on metal surface. Thus, it is important to explore the geometries and energies of small silicon clusters on metal surface in order to understand the growth mechanism of silicene, similar to the case of graphene.[67-69]

In vacuum, small silicon clusters prefer supercluster configuration composed of Si_{6}, Si_{9}, and Si_{10} subunits (Figure 10a).[70-72]. For comparison, we have also considered small planar Si_{N} clusters (N=6, 10, 13, 16, 19, 22, 24) as aggregates of six-membered rings (6MRs). Upon relaxation, these Si_{N} clusters can’t keep planar in vacuum and transform into severely buckled configurations (see Figure 10b). This is because silicon atom doesn’t like sp^2 hybridization in vacuum. Therefore, homogeneous nucleation in vacuum is impossible for synthesis of silicene and a completely wet substrate (such as Ag) is needed.

During the epitaxial growth of silicene on Ag(111) surface, a silicene sheet forms by the continuous growth of small silicon cluster. Thus, elucidating the behavior of small silicon clusters on Ag(111) surface is significant for the growth of silicene. Figure 10c shows silicon monomer, dimer
and 6MR-based silicene-like 2D clusters on Ag(111) surface. Except for Si₆ and Si₁₃, the planar honeycomb structures can be preserved on Ag(111) surface, which may act as the nucleation center during the growth of silicene.

Figure 10. (a) Ground state structures and their formation energies (eV per atom) for Siₙ clusters (N=6, 10, 13, 16, 19, 22, 24) in vacuum; (b) planar Siₙ clusters composed of hexagonal rings (left) and the corresponding structures after relaxation in vacuum (right); (c) geometries and formation energies (eV per Si atom) of 2D Siₙ clusters on Ag(111) surface.[21]

Due to metal passivation effect (Figure 11), the formation energies of clusters decrease after they are adsorbed on Ag(111) surface. More interestingly, on Ag(111) surface, the planar Siₙ clusters have lower formation energies than the corresponding ground state Siₙ cluster in vacuum (Figure 11). Thus, on Ag surface, silicon clusters prefer 2D planar structures to 3D structures, which implies that Ag(111) surface is a wet substrate. Moreover, the formation energy for silicene-like 2D cluster decreases as the number of hexagonal ring increasing (Figure 11), which means that the aggregation of silicon atom is energetically favorable.

Another important factor for the growth of silicene is the diffusion barrier for silicon atom on Ag(111) surface. NEB calculation showed that the diffusion barrier for silicon monomer on Ag(111) is as low as 0.031 eV, implying easy diffusion of silicon atom on Ag surface.[21] As a consequence, after depositing silicon atoms on Ag(111) surface, these silicon atoms would quickly aggregate into small planar clusters, overcoming a small barrier. Small patches of silicene will occur at some critical cluster size and grow into large silicene sheet by continuously adsorbing silicon atoms on the Ag surface.
In the fabrication of silicene or during the process of device manufacture, defects are almost inevitable. Here we briefly discuss the geometry and stability of some point defects in silicene monolayer, such as Stone-Wales rotation, single and double vacancies (abbreviated as SW, SV and DV, respectively, hereafter) and Si adatom. The formation energy of a defect in silicene $\varepsilon_F$ is defined as:

$$\varepsilon_F = \varepsilon_T - N \times \varepsilon_{Si}(2),$$

where $\varepsilon_T$ is the total energy of defective silicene, $N$ is the number of silicon atoms in the supercell of defective silicene, $\varepsilon_{Si}$ is the energy per silicon atom in a perfect silicene sheet. There are two types of single and double vacancies as shown in Figure 12. The formation energy for a DV is smaller than two isolated SVs, implying that two SVs may coalesce into a DV by overcoming a migration barrier (0.12 eV for SV-1). The diffusion of a DV is much difficult. The barrier for creating a SW defect is 2.64 eV, while the reverse transition barrier is as low as 0.5 eV. Therefore, SW defects may be eliminated by annealing at appropriate temperature for a short time to achieve high-quality silicene. Surprisingly, adsorption of a Si adatom on silicene sheet is exothermic with negative formation energy of $-0.03$ eV. The Si adatom prefers the top site of silicene and the original lattice Si atom is pressed down (Figure 12f). Due to the negative formation energy, the influence of Si adatom needs to be carefully considered to produce high-quality silicene.

Moreover, the influence of electronic properties by defects must be taken into account. SW and DV-1(585) defects would introduce small band gaps of 33 meV and 161 meV in silicene respectively. SV-1(556) defect will transform semi-metallic silicene to metallic. DV-2(555777) will destroy the Dirac cone, but keep the semimetal characteristic of silicene. Most interestingly, Si adatom not only opens a noticeable band gap of 91 meV, but also induces a magnetic moment of 2 $\mu$B in silicene.
4. Summary and prospect

In this minireview, substrate effects on silicene including insulating and metal substrate and the growth behavior of silicene on Ag were discussed. Some insulating substrates with appropriate work functions, such as h-BN monolayer and hydrogenated Si-terminated SiC(0001) surface, can preserve the Dirac cone of silicene. Thus, these substrates can provide effective supports for the applications of silicene in future microelectronic devices without destroying its geometry and electronic properties. Recently, there is an intense debate about whether Ag surface would preserve the linear dispersion of silicene, which is crucial for the possible application of silicene fabricated on metal substrates.

Moderate and homogeneous interaction between Si and Ag makes silicene very stable on Ag(111) surface even at a high temperature of 900 K. Thus, Ag(111) or other metal surface that has similar interaction with silicene may be good substrate for silicene growth. On Ag(111) surface, small 6MR-based silicene-like clusters are more stable than the ground state supercluster structures in vacuum. The reduction of formation energy with increasing cluster size and the easy diffusion of Si atom on Ag(111) surface ensure the facilitatory synthesis of silicene on Ag(111) surface. Some point defects may arise in silicene during the growth or fabrication process and greatly affect the electronic properties of silicene. Particular attention should be paid to Si adatom with negative formation energy and local magnetic moment.

At this moment, two major obstacles still obstruct in the middle of the road towards practical application of silicene in microelectronic devices. One is the competition and transformation between different silicene superstructures on Ag(111) surface. Deeply understanding the relationship between silicene reconstruction and substrate temperature is no doubt helpful to synthesize homogeneous large-scale silicene of high quality. Another important issue is to peel silicene from metal substrate. For microelectronic applications such as field effect transistors, silicene must be placed on insulating substrate. However, the epitaxial growth of silicene on insulating substrate has not realized yet. Therefore, how to peel silicene from metal surface and then transfer to inert substrate is vital for silicene application and is an urgent problem in silicene research. Alternatively, it is also desirable to directly synthesize silicene on insulating substrates.

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