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Energy band gaps in periodic bent graphene



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ABSTRACT

Based on the first-principles calculations, we studied the energy bandgaps of the two kinds of periodic bent graphenes: smooth-bent graphene and stepped graphene. In the smooth-bent graphene, the sinusoidal type of graphene superlattice is a gapless semiconductor as the flattened graphene. The periodic smooth bending is unable to open the bandgap of graphene. Although the bandgap can be larger than 100 meV in stepped graphene, it is sensitively dependent on the details of structure. Band gap can only be opened in a certain range of tilt angle. The localized states greatly influence the bandgap opening in stepped graphene.

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1. Introduction

Graphene as a novel two-dimensional electronic system has attracted extensive attention in recent years due to its unique and remarkable electronic properties [1–3]. The construction and exploration of artificial graphene structures have raised more concerns and brought great interests [4–7]. Switching electronic properties by controlling the bandgap of graphene is crucial for many practical applications [8–12]. It was studied that the bandgap opening in lithographically patterned graphene nanoribbons in many works [13–16]. Recent studies found that steady substrates can be used to construct commensurate and controllable graphene geometries [17–20], and semiconductor–metal transition [12,13] can be realized in graphene. These scalable geometry-dependent structures may be used to design new electronic devices [21,22]. It is well-known that silicon carbide (SiC) is an attractive substrate to grow high quality graphene [5,6]. In experiment [20], large bandgap can be produced by growing graphene nanoribbons on sidewall facets of SiC. The bandgap is related to a finite size effect which is caused by 1–2 nm wide bent miniribbons with ordered edges bonded to the substrate. In addition, graphene grown on the SiC (0001) surface with a graphene-like buffer layer is quasi-free-standing, which may support rational design of graphene-based systems at nanoscale [23–25].

It was reported that one-dimensional metallic–semiconducting–metallic junction can be made entirely from a single graphene layer above the buffer graphene-like sheet on the SiC (0001) [19,23]. The band structure of graphene is altered when it is bent

along armchair direction and over steps. In the semiconducting graphene region, the bandgap can be greater than 0.5 eV with a width of few-nanometer (~ 1.4 nm) [19]. The weak interaction [23], between graphene and the SiC (0001) surface with a graphene-like buffer layer, seems to be impossible to well understand the large bandgap in graphene. Although the large bandgap may be concerned with the finite size effects in graphene nanoribbon and the local distortion or strain induced by bending [19,26,27], it is unclear that the exact understanding of this phenomenon.

In this work, we focused on the bending effect on the energy bandgap of graphene. It was considered that two kinds of periodic bending: smooth bending and stepped bending. Smooth bending has little influence on the band structure of graphene near Fermi level. It is unable to open a nonzero bandgap of graphene. In comparison, the local distortion in stepped graphene, which may be induced by substrates, greatly changes the band structure of graphene. However, stepped bending can only induce a nonzero bandgap in some specific structures within certain range of tilt angle. Although the nonzero bandgap can be larger than 100 meV, it is much smaller than the reported bandgap in narrow graphene ribbons (~ 1 nm) with armchair edges [8,13,14]. The bandgap in stepped graphene is sensitively dependent on the localized states induced by local distortion near Fermi level.

2. Computational details

The band structures were calculated on the basis of density-functional theory (DFT) at the level of local density approximation (LDA) [28,29]. Although there may be some limitations within LDA method, most of the early DFT results based on LDA about the

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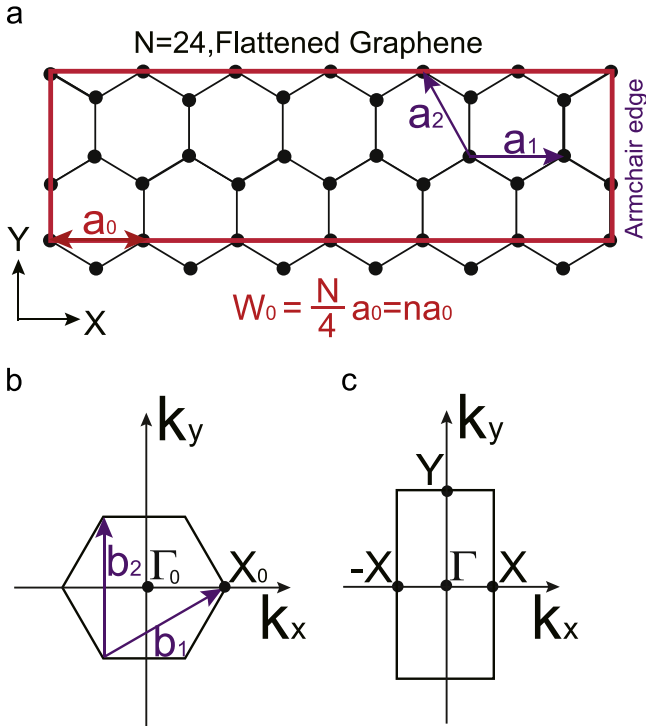


Fig. 1. (Color online) (a) The supercell of flattened graphene with 24 C atoms. The zigzag edge is in the x-direction, and the armchair edge is along the y-direction. The length of the superlattice vector in x-direction is denoted as ' W_0 '. $W_0 = N/4a_0 = na_0$, where N is the number of atoms in each supercell, a_0 is the lattice constant of graphene unit cell ($a_0 = 2.46 \text{ \AA}$) and n is an integer. The lattice vectors of graphene unit cell are denoted as \vec{a}_1 and \vec{a}_2 . The lattice constant of the supercell in y-direction is set to be 4.26 \AA . (b) The Brillouin zone of the graphene unit cell. The reciprocal lattice vectors are denoted as \vec{b}_1 and \vec{b}_2 . (c) The Brillouin zone of the graphene superlattice. Some high symmetry points are marked in (b) and (c).

interface formed between graphene and substrate have been confirmed by experiments [24,25,30,31]. LDA is usually used in the calculations about graphene and/or graphene-based structures [32–35]. Therefore, LDA is used in all our calculations. The projector-augmented wave (PAW) pseudopotentials method [36] implemented in the VASP package [37] were employed to describe the effect of core electrons. The energy cutoff in calculations was set to be 400 eV , and the total energy was converged to better than 10^{-5} eV . The structures were modeled by a periodic slab geometry, with a vacuum of at least 15 \AA between two neighboring slabs [8]. The Γ -centered k -point grid of $5 \times 25 \times 1$ was employed to sample the Brillouin zone in our calculations.

The lattice constant of graphene is set to be 2.46 \AA , and the C–C bond length is about 1.42 \AA . The supercell of flattened graphene is shown in Fig. 1(a). The superlattice vector in y-direction is along the armchair direction, and its length is set to be 4.26 \AA . The superlattice vector in x-direction is along the zigzag direction, its length can be expressed as $W_0 = N/4a_0 = na_0$, where $a_0 = 2.46 \text{ \AA}$, N is the number of carbon atoms in each supercell and n should be an integer. The Brillouin zones of the graphene unit cell and the supercell are shown in Fig. 1(b) and (c), respectively. Some high symmetry points are marked in Fig. 1(b) and (c) for the benefit of expression.

As for the periodic bent graphene, graphene is bent along armchair direction [19], since graphene nanoribbons with armchair edges are predicted to open a bandgap whereas zigzag edges should not [14,15]. Fig. 2 shows the supercell of the periodic bent graphene: the smooth-bent graphene and the stepped graphene. The superlattice vector in y-direction is along the armchair direction, and its length is set to be 4.26 \AA as that in the flattened

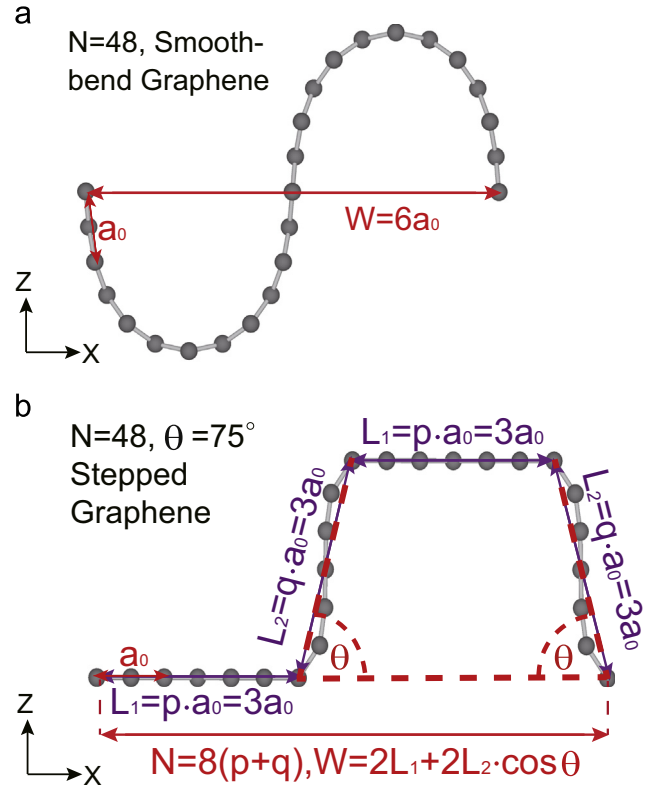


Fig. 2. (Color online) Side view of the supercell of periodic bent graphene: the smooth-bent graphene (a) and the stepped graphene (b). Graphene is bent along the armchair direction (Fig. 1(a)). The number of atoms in each supercell is denoted as ' N ', and the length of the superlattice vector in x-direction is denoted as ' W '. The lattice constant of the supercell in y-direction is set to be 4.26 \AA . The atomic structure of the smooth-bent graphene can be indexed by (N,W) . In the stepped graphene, the tilt angle is denoted as ' θ ', and the atoms in horizon are fixed in plane. The horizontal length is denoted as ' L_1 ', and the length of slope is denoted as ' L_2 '. $L_1 = p \cdot a_0$, and $L_2 = q \cdot a_0$, where both p and q are set to be integers, and $a_0 = 2.46 \text{ \AA}$. The atomic structure of the stepped graphene can be indexed by (p, q, θ) .

graphene superlattice. In the smooth-bent graphenes, the equilibrium structures were obtained through structural relaxation until Hellmann–Feynman forces were less than 0.02 eV/\AA . As for the stepped graphenes, the atoms in horizontal plane were fixed in the z-direction and free in the xy horizontal plane. The Hellmann–Feynman forces on free atoms were less than 0.02 eV/\AA .

The atomic structure of the smooth-bent graphene can be indexed by (N,W) , where N is the number of atoms in each supercell, and W is the length of the superlattice vector in x-direction. In order to simplify the calculations in stepped graphene, its horizontal length is set to be $p \cdot a_0$ and the length of slope is set to be $q \cdot a_0$, where p and q are set to be integers. The number of atoms in each supercell $N = 8(p+q)$, and the length of the superlattice vector in x-direction $W = 2(p \cdot a_0 + q \cdot a_0 \cdot \cos \theta)$, where θ is the tilt angle marked in Fig. 2(b). Therefore, the stepped graphene can be indexed by (p, q, θ) . In our calculations, $N = 48, 56, 64$; $p = 3, 4, 5$; $q = 2, 3, 4, 5$; and θ is considered from 45° to 85° . Although the structures studied are small ($\sim 2 \text{ nm}$), the size is comparable to the width of the semiconducting graphene region reported in the experiment [19].

3. Results and discussion

Fig. 3 shows the band structures of the flattened graphene and the smooth-bent graphene. Although the smooth bending induces some flat bands (localized electronic states in x-direction [38])

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