Strain modulated electronic properties of silicon nanoribbons with armchair edges

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ABSTRACT

The electronic properties of silicon nanoribbons (SiNRs) with strain are studied by ab initio and tight-binding calculations. The strain modulated band gap variations of N_A-ASiNRs depend on the family types categorized according to $N_A = 3p$, $3p + 1$ and $3p + 2$ and could be tuned over several hundreds meV. For $(3p + 2)$-ASiNRs, the band gaps are proved to be linear as a function of strains and exactly closed under small tensile strains. Meanwhile, the structure of the lowest conduction and highest valence bands are Dirac-type dispersion. These results suggest that the strain modulated SiNRs may have potential applications in the field effect nanodevice.

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1. Introduction

Silicon is the most important material in the semiconductor industry. In recent years, the nanoscale forms of silicon, such as nanowires [1–5] and nanotubes [6–10] have attracted great scientific interests due to their fascinating physical properties. Besides these sp^3 nanowires and nanotubes, the more attractive sp^2 silicene sheet also has been obtained by epitaxial growth on close-packed silver surface [11–16]. The one-dimensional silicon nanoribbon (SiNR) has also been precisely synthesized on the silver surface with a unique structure [17–19]. The angle-resolved photoelectron spectroscopy (ARPES) measurements suggest that the band dispersion of the nanoribbons are Dirac-type [20]. The Dirac dispersion means the band across the Fermi level is linear and the effective masses of the electrons near the Dirac point are massless. The carriers in Dirac electronic system have ultra high mobilities and therefore a great potential in high-speed electronic devices. The silicon-based nanoelectronics will be compatible with the integrated circuit technology for bulk silicon. With a much smaller size than the building units in-use today, the silicon nanomaterial is the most promising one of building a circuit with higher integration. The Dirac type dispersion in silicene and silicon nanoribbons indicates a high mobility of electrons near the Fermi level. It is demonstrated that the silicon nanoribbons with armchair edges (ASiNR) are semiconductors with small gaps [21–23], recognized as a suitable material. To realize the function of field effect devices, a variation of the conductivity of ASiNRs will be needed, which is traditionally tuned by a gate voltage. However, a quite large gate voltage should be applied to open a small gap in silicene [24]. Other methods such as hydrogenation will open a gap but meanwhile break the linear dispersion near the Fermi level [25].

It is important to find a method to tune the band gaps with the dirac-type dispersion maintained. Considering the strain is an important method to tune their electronic properties [26–30], we investigate the electronic properties of SiNRs with strain by ab initio calculations. We find that under the small strains, the dispersion of the lowest conduction and the highest valence bands for $(3p + 2)$-ASiNRs are linear, meanwhile, the band gaps can be tuned over several meV.

2. Method

The total energies and electronic structures are calculated by the VASP code [31]. The approach is based on the density functional theory in a plane-wave basis set with the projector augmented-waves method [32]. We use the exchange–correlation with the generalized gradient approximation in the form of Perdew–Burke–Ernzerhof (PBE) [33]. The plane-wave cutoff energy is set to be 350 eV and the convergence of the force on each atoms is less than 0.01 eV/Å. The vacuum space is larger than 15 Å, which is sufficient for making the system isolated. The Monkhorst–Pack scheme [34] is used to sample the Brillouin zone. All the structures are relaxed with a mesh of $10 \times 1 \times 1$ and the mesh of k space is increased to $20 \times 1 \times 1$ in the static calculations.

3. Results and discussion

The SiNRs are constructed from the buckled silicon hexagonal sheet. In accordance with the previous convention [23,35], the ASiNR with N_A dimer lines across the ribbon width is named as N_A-ASiNR. The outmost atoms of SiNRs are passivated by hydrogen atoms. The equilibrium lattice constant without strain is obtained from the fitted curve of the total energy as a function of lattice parameter. The strain is given by changing the unit cell size along the ribbon stretched direction. The atoms are allowed to relax

Figure 1. The band gaps E_g of (3p + 2)-ASiNRs as a function of strain.

et al. have demonstrated the band gaps of ASiNRs periodically change alongside the width N_A with a period of three [23]. Thus these ASiNRs can be categorized into three families with $N_A = 3p$, $3p + 1$ and $3p + 2$, where p is a positive integer. We discuss the ASi-NRs in different families separately because they also behave distinctly with the effect of strains. We find that the curves between band gap and strain show a zigzag behavior. The band gap depends on the strain almost linearly at each side of the band gap extremum. Except for these common features, the three types of ASiNRs have individual characters. Since the experimentally grown nanoribbon is the 8-ASiNR as shown in our previous work [36], we focus on (3p + 2)-ASiNRs because their applications are more realizable than 3p-ASiNRs and (3p + 1)-ASiNRs. For the nanoribbons with the width $N_A = 3p + 2$, there is a little difference in band gap under the same strain for p = 2,3,4, as shown in Figure 1. The band gaps initially decrease with the increase of ε. After the turning points, the band gaps increase with the increase of ε. The band gaps of (3p + 2)-ASiNRs (p = 2,3,4) without strain are 56, 39, 33 meV, respectively.

In our calculations, the band gaps of 8-ASiNR, 11-ASiNR and 14-ASiNR are closed within 1 meV when the corresponding strains of $\varepsilon_0 = 1.70\%, 1.24\%$ and 1.00% are applied, respectively, meanwhile, the energy dispersion of the highest valence and the lowest conduct bands remain linear. Figure 2 exhibits the band structures and partial charge densities of the highest occupied crystal orbital (HOCO) and the lowest unoccupied crystal orbital (LUCO) of 11-ASiNRs under different strains.

From the detailed band structures of 11-ASiNR near the Γ point in Figure 2, it is worth to notice that the linear dispersions still hold except for the Γ point when the strain is around the ε_0. The band

when the strain is applied. The strain is expressed as $\varepsilon = (r - r_0)/r_0$, where r is the lattice constant for the strained SiNR and r_0 is the equilibrium lattice constant. Negative ε value corresponds to the compressive strain and positive ε value corresponds to the tensile strain.

For the ASiNRs with different widths, the perpendicular buckled heights are almost the same under the same strain value ε. The buckled height becomes larger when the compressive strain is applied, and it gets smaller with the tensile strain. For the different ASiNRs without strain, the buckled height is calculated to be 0.46 Å, which is consistent with the previous study [21]. Ding

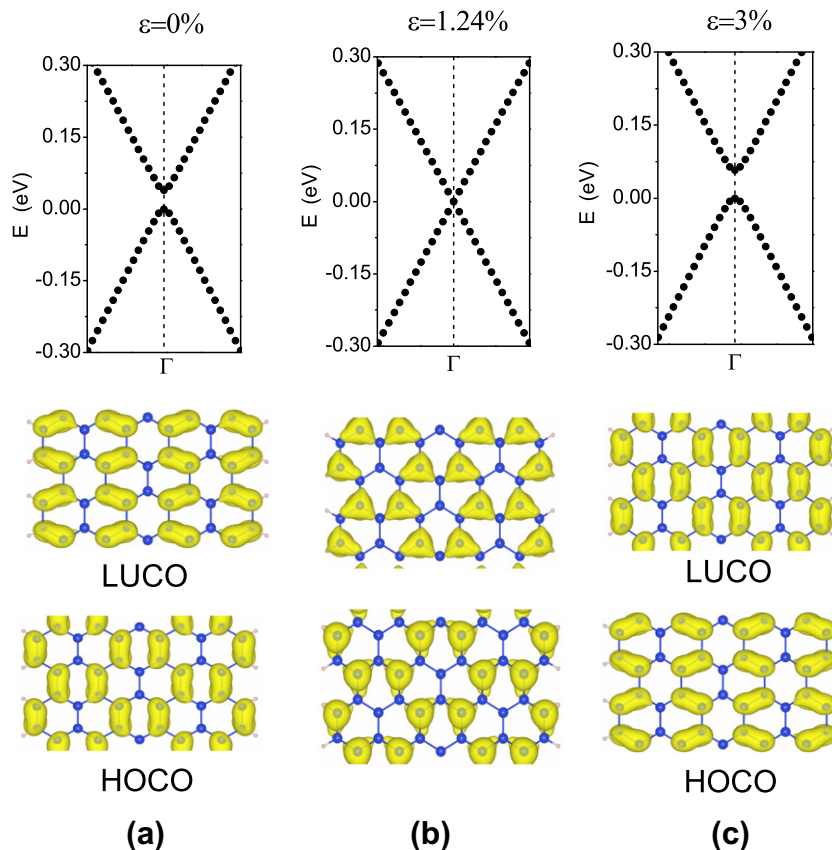**Figure 2.** (Top) The detailed band structures of 11-ASiNRs near the Γ point with the strain of (a) $\varepsilon = 0\%$, (b) $\varepsilon = 1.24\%$ and (c) $\varepsilon = 3\%$. The highest occupied energies are set to zero. (Middle and Bottom) The partial charge densities of the lowest unoccupied crystal orbital (LUCO) and the highest occupied crystal orbital (HOCO) for 11-ASiNR with the strain of (a) $\varepsilon = 0\%$, (b) $\varepsilon = 1.24\%$ and (c) $\varepsilon = 3\%$. The isosurface of partial charge densities is $0.005e/Å^3$. With the strain of $\varepsilon = 1.24\%$, the LUCO and HOCO are degenerate.