

Electronic properties of zigzag silicene nanoribbons with single vacancy defect

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ABSTRACT

Silicene is envisaged as one of the two-dimensional (2D) materials for future nanoelectronic applications. In addition to its extraordinary electronic properties, it is predicted to be compatible with the silicon (Si) fabrication technology. By using nearest neighbour tight-binding (NNTB) approach, the electronic properties of zigzag silicene nanoribbons (ZSiNRs) with single vacancy (SV) defects are modelled and simulated. For 4-ZSiNR with $L=2$, the band structures and density of states (DOS) are computed based on SV incorporated ZSiNRs at varying defect locations. The results show that the SV defect will shift the band structure and increase the peak of DOS while the bandgap remain zero. This work provides a theoretical framework to understand the impact of SV defect which is an inevitable non-ideal effect during the fabrication of silicene nanoribbons (SiNRs).

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1. INTRODUCTION

The success of mechanically exfoliated graphene has driven the rigorous explorations of two-dimensional (2D) materials [1-3]. Silicene is the silicon (Si) counterpart of graphene-like 2D materials which has recently become an interesting research topic [4, 5]. Besides sharing similar Dirac cone properties [6-8] with graphene, silicene has the potential to be compatible with the semiconductor fabrication processes which depend primarily on Si technology [9]. In 2015, silicene field-effect transistor (FET) was fabricated using grow-transfer-fabrication technique [10], but the electronic properties are greatly degraded by the silver substrate. Hence, it is important to perform computational study on silicene while fabrication researchers are searching for other breakthroughs in silicene fabrication technique.

Vacancy defect is an unpreventable non-ideal effect during fabrication process which can significantly affect the electronic properties of the fabricated material [11, 12]. Although defects are undesirable events, they can sometimes enhance the electronic properties of the material for specific application [13]. In this paper, the effects of single vacancy (SV) defect on the electronic properties of zigzag silicene nanoribbons (ZSiNRs) were modelled using nearest neighbour tight-binding (NNTB). Figure 1 illustrates the schematic atomic arrangement of a ZSiNR. This work has considered only zigzag edge because ZSiNRs possess semi-metallic properties for all nanoribbon widths while finite gap opening has been observed in certain widths of armchair silicene nanoribbons (ASiNRs) [6].

2. MODELLING IMPLEMENTATION

For the ease of description, nanoribbon of width, N_z is denoted as N_z -ZSiNR where N_z is defined as the number of zigzag chains across the N_z -ZSiNR. Furthermore, the length of N_z -ZSiNR is denoted by L which represents the number of unit cells along the nanoribbon length direction. Both N_z and L are positive integers. Figure 2 depicts the structural model of defective ZSiNR. In this work, we focus on 4-ZSiNR with $L=2$ while varying the SV defect locations (A, B, C and D). The structure in Figure 2 is assumed to be perfect planar hexagonal and stable despite the SV defect. The following subsections discuss the mathematical models to compute band structures and density of states (DOS).

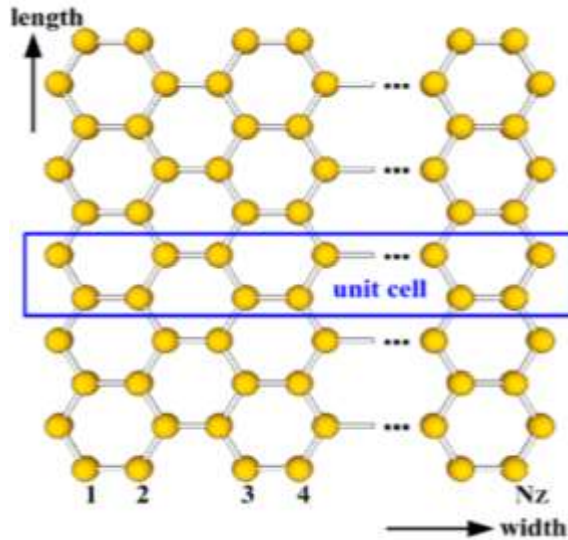


Figure 1. The schematic diagram for the atomic structure of ZSiNR [14]. The length, is defined as the number of unit cell in the SiNR and the width is denoted as N_z

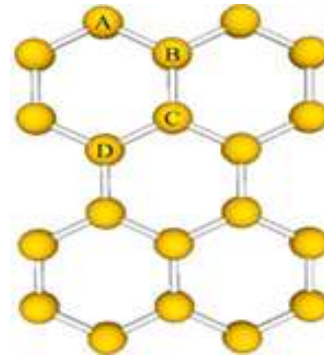


Figure 2. The schematic diagram for the SV defect locations (A, B, C and D) for 4-ZSiNR with =2

2.1. Band structures

The band structures of the defective ZSiNRs are plotted by using the dispersion relation from the solutions of energy eigenvalues from the Hamiltonian matrices. The defective ZSiNRs are modelled using the NNTB approach based on the time-independent Schrödinger in matrix form [15-17]:

$$E\{\phi_0\} = [h(\vec{k})]\{\phi_0\}, \quad (1)$$

where $h(\vec{k})$ is the Hamiltonian matrix, ϕ_0 is the time-independent wave function and E is the energy. In this work, the Hamiltonian matrix is divided into the α -matrix and β -matrix which describes the interactions of silicon atoms in the zigzag unit cell chain and the interactions among the zigzag unit cell chains respectively. Therefore, the complex model is now reduced to a form similar to one-dimensional (1D) problem which can be solved using the simple, given by [18, 19]:

$$h(k) = \beta' e^{-ika} + \alpha + \beta e^{+ika}, \quad (2)$$

where β' is the transverse matrix of β -matrix, k is the wave vector and $a=0.382$ nm [20] is the lattice constant of silicene, but the lattice constant is negligible in this work because the x-axis of the band structure is ka/π .

The bonding energy, t used in this study is -1.03 eV adapted from previous study [21]. The standard eigenvalue problem solution, $\det[h(k) - \epsilon(k)I] = 0$ is employed to evaluate the $h(k)$ to obtain the energy eigenvalues, where I is an identity matrix of the same size as $h(k)$ and $\epsilon(k)$ is the energy eigenstates.

2.2. Density of states

DOS determines the number of available states in a semiconductor material for the carriers to flow, which is essential to obtain the current flow in the system [22]. The numerical solution of DOS for a system can be obtained using delta, δ function [13], given as:

$$DOS(E) = \sum_{i=1}^N \int_{-\infty}^{+\infty} \delta[E - \varepsilon(k)] dk , \tag{3}$$

where $\varepsilon(k)$ is the energy eigenstates as described in previous subsection. By applying the spectral function identity [23] as shown in (4) and the integration rule for δ function, the numerical solution for DOS as a function of energy, E can be simplified as (5). The are given as:

$$\delta[E - \varepsilon(k)] = \frac{1}{2\pi} \left[\frac{2\eta}{[E - \varepsilon(k)]^2 + \eta^2} \right]_{\eta \rightarrow 0^+} , \tag{4}$$

$$DOS(E) = \sum_{i=1}^N \frac{1}{2\pi} \sum_{all\ k} \frac{2\eta}{[E - \varepsilon(k)]^2 + \eta^2} , \tag{5}$$

where η is a very small positive value to prevent the inverse matrix from diverging. The DOS is calculated by iterating E from the minimum to the maximum value of (k) .

3. RESULT AND DISCUSSION

In this section, the NNTB model is benchmarked with a more sophisticated computational study (first-principle study) to ensure the parameters are accurate. Then, the results for the pristine and defected 4-ZSiNRs are shown and discussed. The band structures and DOS of pristine and defected 4-ZSiNRs are plotted in the same graph to examine the effects of SV defect to the electronic properties.

3.1. Benchmark of pristine zigzag silicene nanoribbons

The parameters of NNTB model is benchmarked with the same structure of 6-ZSiNR with $L=1$ from Figure 3(a) in [6]. This step is done to ensure the accuracy of the NNTB model. Figure 3 depicts the comparison between the proposed model and published result. The graph in Figure 3(a) shows that NNTB is consistent with the more computationally expensive calculations.

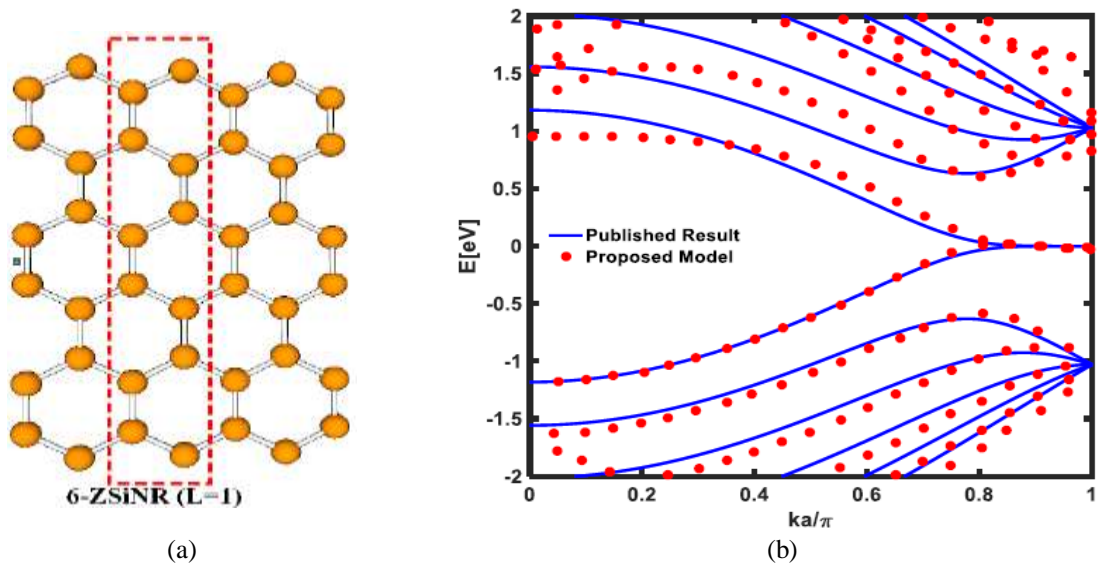


Figure 3. The benchmark of band structure for pristine 6-ZSiNR with $L=1$. Blue solid lines show the band structure of present work and red dots show the band structure adapted from first-principle calculations (a) Lattice Structure, (b) Band Structure [6]

3.2. Pristine zigzag silicene nanoribbons

Figure 4 depicts the band structures and DOS for pristine 4-ZSiNR with $L=2$. The band structure shows that the valence band maximum (VBM) and the conduction band minimum (CBM) touches at $E=0$ eV and the extracted band gap is zero by calculating the difference between VBM and CBM.

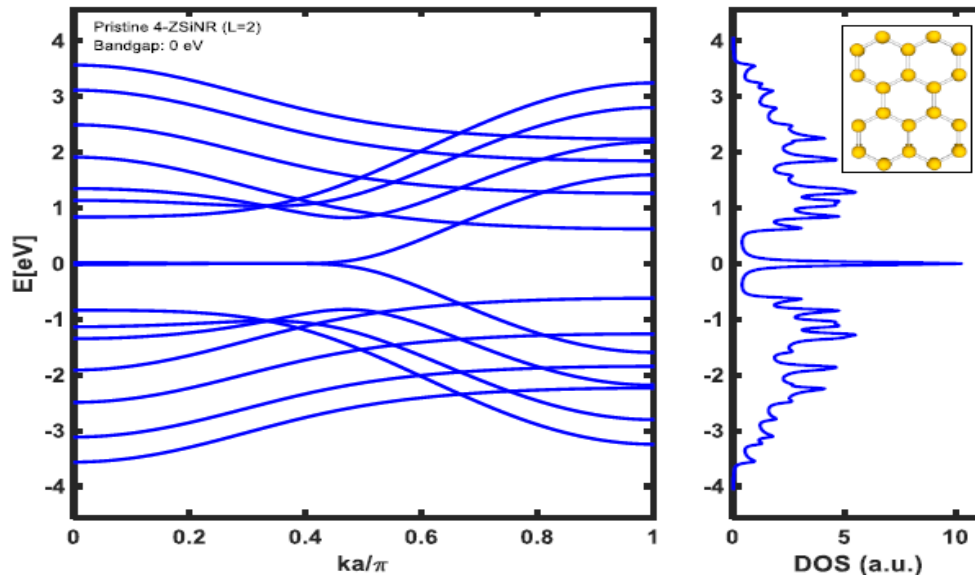


Figure 4. The band structure and DOS for pristine 4-ZSiNR with $L=2$

3.3. Defective zigzag silicene nanoribbons

Figures 5(a) to (d) depict the band structures and DOS for defective 4-ZSiNR with $L=2$ for SV locations of A, B, C and D respectively. For all the simulated SV locations, the extracted band gaps are zero. Moreover, all the SV locations affect shapes of the band structures and DOS when compared to the band structures and DOS of the pristine 4-ZSiNR. Figures 5(a) and (b) show that the CBM and VBM touches at $E=0$ eV and Figures 5(c) and (d) show that the CBM and VBM overlaps at $E=0$ eV (or in other words, the conduction band is below Fermi level and valence band is above Fermi level).

3.4. Discussions

By comparing Figure 3 to Figures 5(a) to (d), it is shown that the SV defect does not have significant effects to the bandgaps for 4-ZSiNR with $L=2$ for all the simulated SV defect locations (A, B, C and D). Similar results were also shown by previous study on zigzag graphene nanoribbons (ZGNRs) where the study had concluded that SV defect does not bring significant effect to the bandgaps of ZGNRs [24]. On the other hand, there are interesting points to notice from the band structures. For SV locations at A and B, the defected 4-ZSiNRs show semi-metallic properties. In addition, the overlapping of conduction and valence bands for SV locations at C and D indicates metallic properties [25].

The shapes of the band structures are distorted in different ways when the SV defect locations are varied. The peaks of DOS at $E=0$ eV for defected 4-ZSiNR increase significantly compared to pristine 4-ZSiNR. The peaks in the DOS are crucial for transport properties which can affect the current versus voltage characteristics of electronic devices [26]. The DOS is a quantity of the material that indicates the number of available states for conduction [27]. Higher peaks of DOS at $E=0$ eV for defected 4-ZSiNRs imply that there is more number of available states for carriers to flow around the Fermi energy level compared to pristine 4-ZSiNR.

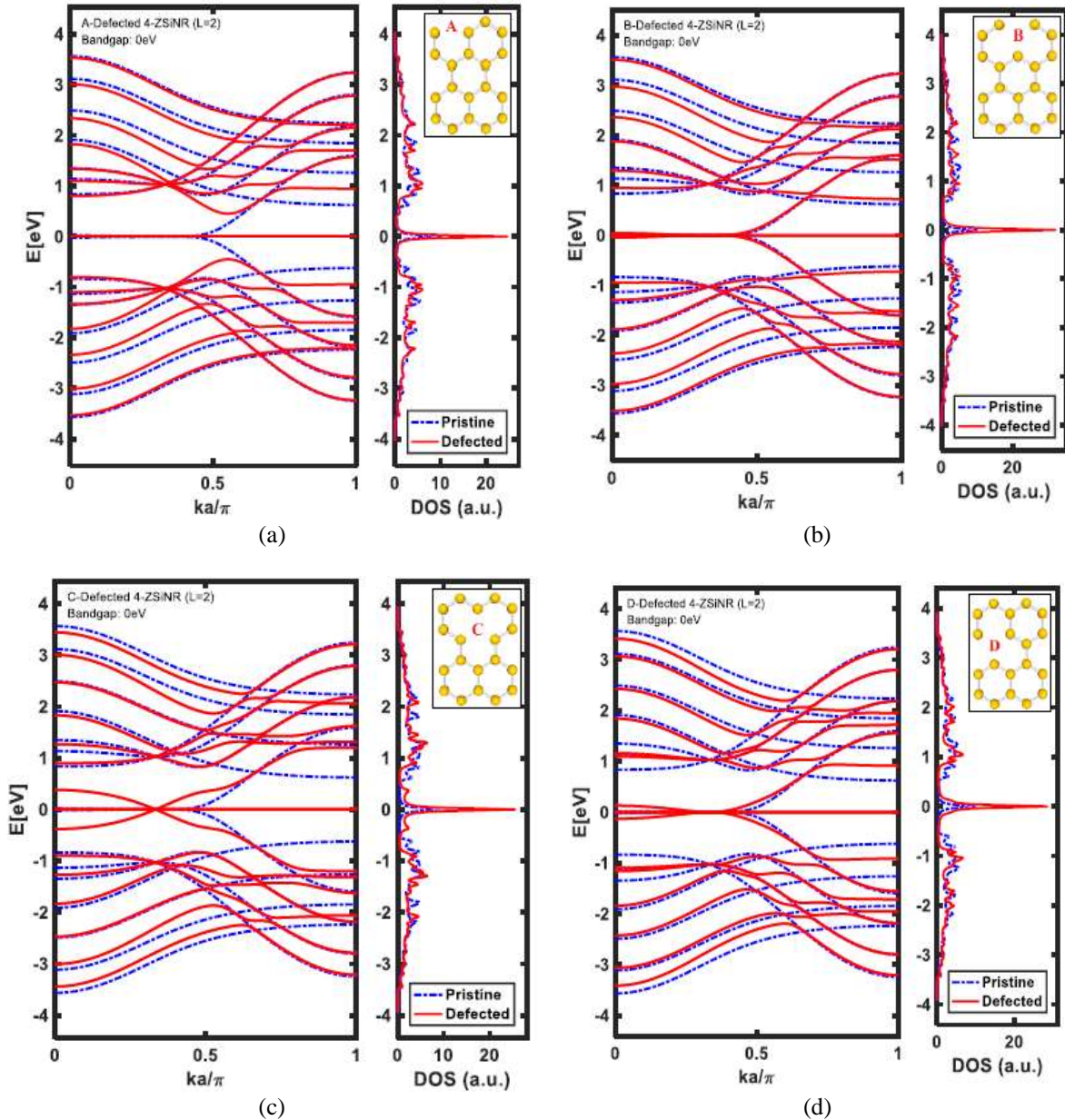


Figure 5. The band structures and DOS for defected 4-ZSiNR with $L=2$ for various SV locations. Blue dotted lines represent the results for pristine nanoribbons and red solid lines represent the results for defected nanoribbons. The schematic diagram for each defected 4-ZSiNR is shown at the top right corner of each result, (a) Defected (SV Location=A), (b) Defected (SV Location=B), (c) Defected (SV Location=C), (d) Defected (SV Location=D)

4. CONCLUSION

The electronic properties, namely band structures and density of states of pristine and defective ZSiNRs of various lengths have been modelled and simulated using NNTB. The results show that SV defect does not have significant impact on the bandgaps of 4-ZSiNR with $L=2$ when the locations of SV defects are varied. However, the SV defect can shift and distort the band structures and increase the peak of DOS. This work can be extended by investigating the electronic properties for ZSiNR by varying the vacancy concentrations or widths and lengths of nanoribbons.

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