Computational Materials Science 141 (2018) 353–359

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Investigation and comparison of the large-signal characteristics and dynamical parameters of silicene and germanene nanoribbon interconnects

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ARTICLE INFO

Article history:
Received 3 May 2017
Received in revised form 11 September 2017
Accepted 27 September 2017

Keywords:
Silicene
Germanene
Nanoribons
Kinetic inductance
Quantum capacitance

ABSTRACT

One dimensional materials such as nanotubes and nanoribbons are studied widely in the literature for their peculiar properties. In particular, zigzag graphene and silicene nanoribbons constitute an active research area for the possibility to use them as interconnects. Recently, it is exposed that asymmetric zigzag germanene nanoribbons also show similar metallic characteristics. In this work, the electronic transport properties and dynamical parameters of zigzag silicene and germanene nanoribbons (ZZ-SiNR and ZZ-GeNR) are investigated and compared. First-principles quantum mechanical simulations using density functional theory in conjunction with non-equilibrium Green's function formalism are utilized to extract the current-voltage behaviours and Fermi velocities of equivalent ZZ-SiNR and ZZ-GeNR samples. The results show that ZZ-SiNR and ZZ-GeNR samples show similar current-voltage characteristics with the ZZ-GeNR having slightly higher conductance. Then, dynamical parameters namely kinetic inductance and quantum capacitance values are obtained. The obtained values show that the kinetic inductance and quantum capacitance of the ZZ-GeNR are lower than those of ZZ-SiNR. It is concluded that both ZZ-SiNR and ZZ-GeNR can be used as nanoscale interconnects with the ZZ-GeNR having slightly higher linearity and lower kinetic inductance and quantum capacitance compared to its SiNR counterpart.

1. Introduction

Nanotubes and nanoribbons have taken great attention due to their peculiar characteristics and potential applications in the near future nanoelectronic technology. The research on one-dimensional (1-D) devices are also motivated by the fact that bulk silicon technology is approaching its physical limitations because of the unwanted effects such as tunnelling [1], leakage currents [2] and inelastic scattering [3]. Carbon-based 1-D materials such as carbon nanotubes (CNTs) and graphene nanoribbons (GNRs) are extensively studied both theoretically and practically in the literature [4,5]. CNTs and GNRs can be implemented as semiconductors or conductors depending on the cross-sectional and edge configurations [6–8]. While semiconductiong CNTs and GNRs are used as the channel regions in CNTFETs and GNRFETs [9,10], their metallic counterparts have no less importance because they can be used as interconnect components in nanoelectronic circuits [11,12]. Metallic 1-D materials are shown to have better promise compared to their bulk counterparts [13,14]. While these research is mainly on carbon-based materials, it has been argued that silicon-based nanotubes and nanoribbons also have the potential to offer versatile conductance properties [15–18].

It has recently been demonstarted that germanene nanoribbons (GeNRs) also have conducting properties prompting their use in nanoelectronic circuits as interconnects [19–21]. These studies are motivated by the fact that germanene sheets have a carrier mobility on the order of 10^5 cm^2 V^{-1} s^{-1} which is comparable to that of the graphene sheet [21]. Moreover, it has also been shown that asymmetric zigzag GeNRs have an almost linear current-voltage behaviour independent of their spin-polarization in a wide voltage range permitting their utilization as interconnects [19]. It is worth noting that this behavious is similar to those of SiNRs [22]. Therefore, asymmetric zigzag nanoribbons of both silicene and germanene seem suitable for use as metallic interconnect components. Considering the expertise in silicon and germanium processing in electronics technology, it is obviously worth studying the conduction properties of metallic SiNRs and GeNRs extensively from various viewpoints.

In this work, the electronic transport properties and dynamical parameters of metallic zigzag silicene and germanene nanoribbons (ZZ-SiNR and ZZ-GeNR) are investigated and compared. First-principles quantum mechanical simulations using density func-

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https://doi.org/10.1016/j.commatsci.2017.09.050
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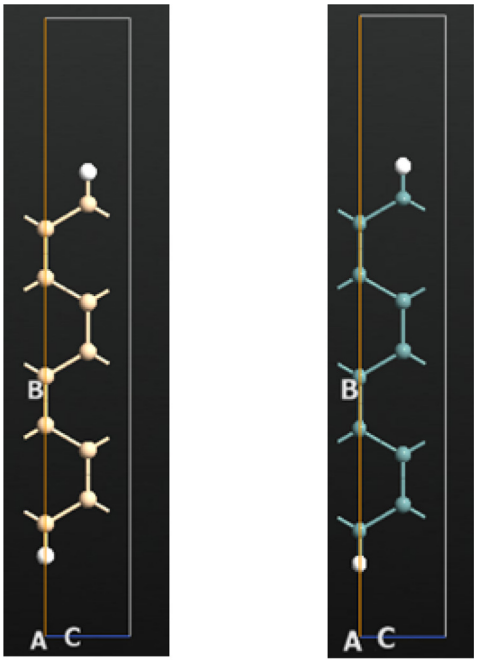


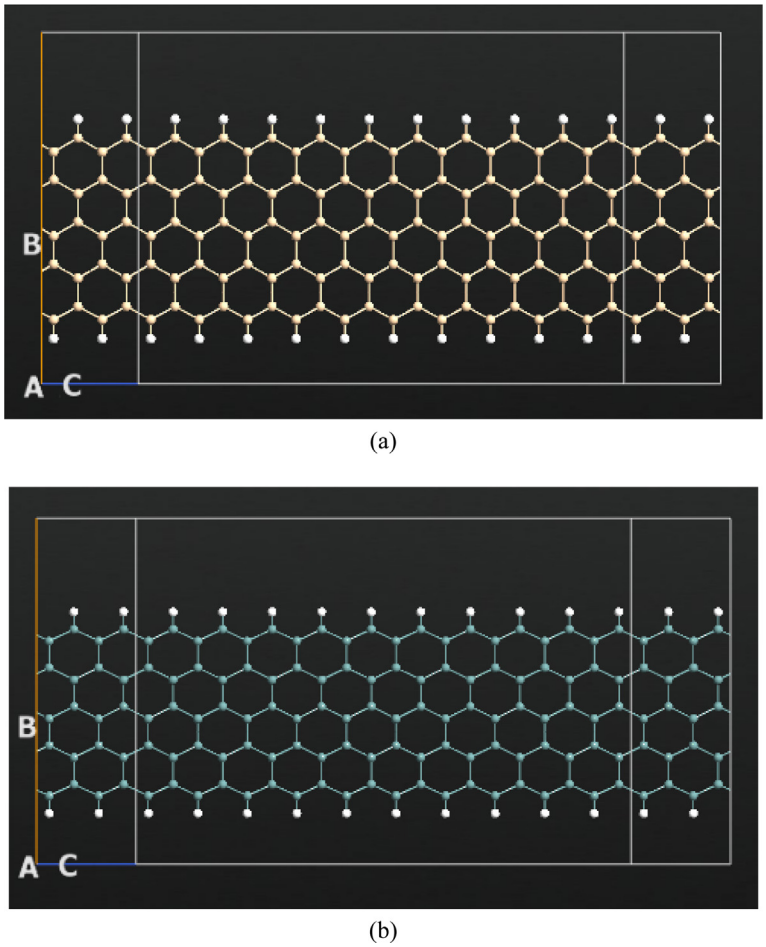
(a) (b)

Fig. 1. Considered asymmetric zigzag SiNR and GeNR unit cells.

tional theory in conjunction with non-equilibrium Green's function formalism are utilized to extract the current-voltage behaviours and Fermi velocities of equivalent ZZ-SiNR and ZZ-GeNR samples. Then, the dynamical parameters namely kinetic inductance and quantum capacitance values of these samples are obtained. Finally, the current-voltage curves, kinetic inductances and quantum capacitances of the investigated identical ZZ-SiNR and ZZ-GeNR samples are compared and the origins of their differences are thoroughly discussed considering the transmission eigenstates and carrier mobilities of these devices.

2. Material and methods

It has been demonstrated in the literature that ab initio simulations of nanoelectronic materials provide accurate insights to the electrical behaviours of various materials including GNRs [23], SiNR [24] and GeNRs [25]. Density functional theory (DFT) is a prominent method among various first-principles strategies [26,27]. In this method, the electronic interactions are modelled using a generalized exchange-correlation functional which is then used for solving the Schrodinger equation numerically. A three-dimensional electron density matrix is obtained from DFT and various electrical parameters can be extracted from this matrix [28]. Furthermore, DFT can also be combined with non-equilibrium Green's function formalism (NEGF) to obtain the electrical transport properties from the transmission spectrum data [29]. In this study, Atomistix Toolkit (ATK®), which implements DFT in con-



(a)

(b)

Fig. 2. Simulated metallic SiNR (a) and GeNR (b) interconnect samples.