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Enhanced thermoelectric performance of defected silicene nanoribbons

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ABSTRACT

Based on non-equilibrium Green's function method, we investigate the thermoelectric performance for both zigzag (ZSiNRs) and armchair (ASiNRs) silicene nanoribbons with central or edge defects. For perfect silicene nanoribbons (SiNRs), it is shown that with its width increasing, the maximum of ZT values (ZT_M) decreases monotonously while the phononic thermal conductance increases linearly. For various types of edges and defects, with increasing defect numbers in longitudinal direction, ZT_M increases monotonously while the phononic thermal conductance decreases. Comparing with ZSiNRs, defected ASiNRs possess higher thermoelectric performance due to higher Seebeck coefficient and lower thermal conductance. In particular, about 2.5 times enhancement to ZT values is obtained in ASiNRs with edge defects. Our theoretical simulations indicate that by controlling the type and number of defects, ZT values of SiNRs could be enhanced greatly which suggests their very appealing thermoelectric applications.

1. Introduction

Thermoelectric materials which can convert dissipated heat into electric energy at nanoscale have attracted increasing attention from both theoretical and experimental research due to their potential technological applications [1–3]. The performance of thermoelectric materials is measured by the figure of merit $ZT = S^2GT/(\kappa_e + \kappa_p)$, where S, G, T, κ_e and κ_p represent the Seebeck coefficient, electronic conductance, absolute temperature, electronic and phononic thermal conductance, respectively. Explicitly, an optimal thermoelectric material should possess high Seebeck coefficient, high electronic conductance, and low thermal conductance.

Both experimental and theoretical research have indicated that nanoscale materials could exhibit much higher ZT values compared with those of bulk materials, which lead to a very important prospect of thermoelectric applications. Experimentally, in particular, it was found that the thermal conductivity of Si nanowires (SiNWs) can be 100 times smaller than that of bulk silicon, which suggests the possibility of using silicon-based nanostructures as efficient thermoelectric materials [4,5]. Theoretically, improved thermoelectric performance of SiNWs was predicated [6–9], as a result of reduced thermal conductivity caused by phonon surface scattering and enhanced power factor due to quantum confinement effect. Subsequently, other silicon-based nanostructures like nanotubes [10] and nanomembranes [11,12] have been suggested, and their interesting thermoelectric properties have also been reported.

Very recently, new two-dimensional materials like graphene and silicene, especially one-dimensional graphene (GNRs) and silicene (SiNRs) nanoribbons, have been attracting a great interest due to their unique properties [13–16]. Though the thermopower of pristine graphene is not very high, it can be considerably enhanced in GNRs, especially in nanostructures consisting of nanoribbons of various types. Indeed, in a properly designed nanoribbon with alternating zigzag and armchair sections, thermoelectric figure of merit exceeding unity at room temperature has been found [17]. The efficiency can be also enhanced by randomly distributed hydrogen vacancies in almost completely hydrogenated GNRs [18]. Furthermore, structural defects, especially in the form of antidots, also appear a promising way to enhance thermoelectric efficiency [19–21]. Meanwhile, giant spin related thermoelectric phenomena have been predicted for ferromagnetic ZGNRs with antidotes [22].

It is generally accepted that decreasing the characteristic size of nanostructures and introducing defects are two effective ways to further improve their ZT values. So higher thermoelectric performance can be expected for SiNRs with defects, which is due to lower thermal conductance than GNRs. In this paper, we investigate the thermoelectric performance for both ZSiNRs and ASiNRs

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with central or edge defects by using non-equilibrium Green's function method. For perfect silicene nanoribbons (SiNRs), it is shown that with its width increasing, the maximum of ZT values (ZT_M) decreases monotonously while the phononic thermal conductance increases linearly. For various types of edges and defects, with increasing defect numbers in longitudinal direction, ZT_M increases monotonously while the phononic thermal conductance decreases. Comparing with ZSiNRs, defected ASiNRs possess higher thermoelectric performance due to higher Seebeck coefficient and lower thermal conductance. In particular, about 2.5 times enhancement to ZT values is obtained in ASiNRs with edge defects. Our theoretical simulations indicate that by controlling the type and number of defects, ZT values of SiNRs could be enhanced greatly which suggests their very appealing thermoelectric applications.

2. Model and method

In order to enhance the ZT values of SiNRs, we introduce central and edge cavities in ZSiNRs and ASiNRs respectively, as shown in Fig. 1. Following a common convention, we refer to the SiNRs with N dimer lines in width as N-SiNRs. The system is composed of a central junction of length L and width W and two semi-infinite ideal leads of the same width. The central junction is formed by removing hexagonal carbon rings from perfect SiNRs, in which the numbers of hexagons along the transversal and longitudinal directions are denoted by index n and m.

For electronic transport, by using an atomistic p_z orbital basis, the silicene system can be described by the second-nearest-neighbor tight binding model [23]

$$H = -lE^z \sum_{i\alpha} c^{\dagger}_{i\alpha}\mu_i c_{i\alpha} - t\sum_{\langle i,j\rangle\alpha} c^{\dagger}_{i\alpha} c_{j\alpha} + \frac{i\lambda_{SO}}{3\sqrt{3}} \sum_{\langle\langle i,j\rangle\rangle\alpha\beta} c^{\dagger}_{i\alpha}\nu_{ij}\sigma^z_{\alpha\beta}c_{j\beta} \quad (1)$$

where ${c_{i\alpha}}^{+}$ and $c_{i\alpha}$ are creation and annihilation operators with spin polarization α on site i and the combinations $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ run overall the nearest and next nearest neighbo rhopping sites respectively. In Hamiltonian, the first term represents the staggered sublattice potential, where $l=0.23$ Å and $\mu_i = \pm 1$ for the A (B)site. It generates a staggered sublattice potential $\propto 2lE^z$ between silicon atoms at A and B sites. The second term is the usual nearest-neighbor hopping term with the transfer energy $t=1.6$ eV. The third term represents the effective SO coupling with $\lambda_{SO}=3.9$ meV, where $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ is the Pauli matrix of spin, with $\nu_{ij}=+1$ if the next nearest neighboring hopping is anticlockwise and $\nu_{ij}=-1$ if it is clockwise with respect to the positive z axis.

For incident electronic energy E, the electronic transmission per spin though junction region is calculated as $T_e(E)=Tr\left[\Gamma_L G^r \Gamma_R G^a\right]$, where the line width function $\Gamma_{L,R}(E)$ is defined as $\Gamma_{L,R}(E)=i[\Sigma^r_{L,R}-\Sigma^a_{L,R}]$, and the retarded (advanced) Green's function is given by $G^{r,a}(E)=\left[(E\pm i\eta)I-H_C-\Sigma^{r,a}_L-\Sigma^{r,a}_R\right]$, in which the retarded (advanced) self energy due to the coupling to all leads can be obtained numerically [24]. Define an intermediate function $L_n(\mu,T)$ as [25,26]

$$L_n(\mu,T)=(2/h)\int dET_e(E)(E-\mu)^n[-\partial f^{FD}(E,\mu,T)/\partial E] \quad (2)$$

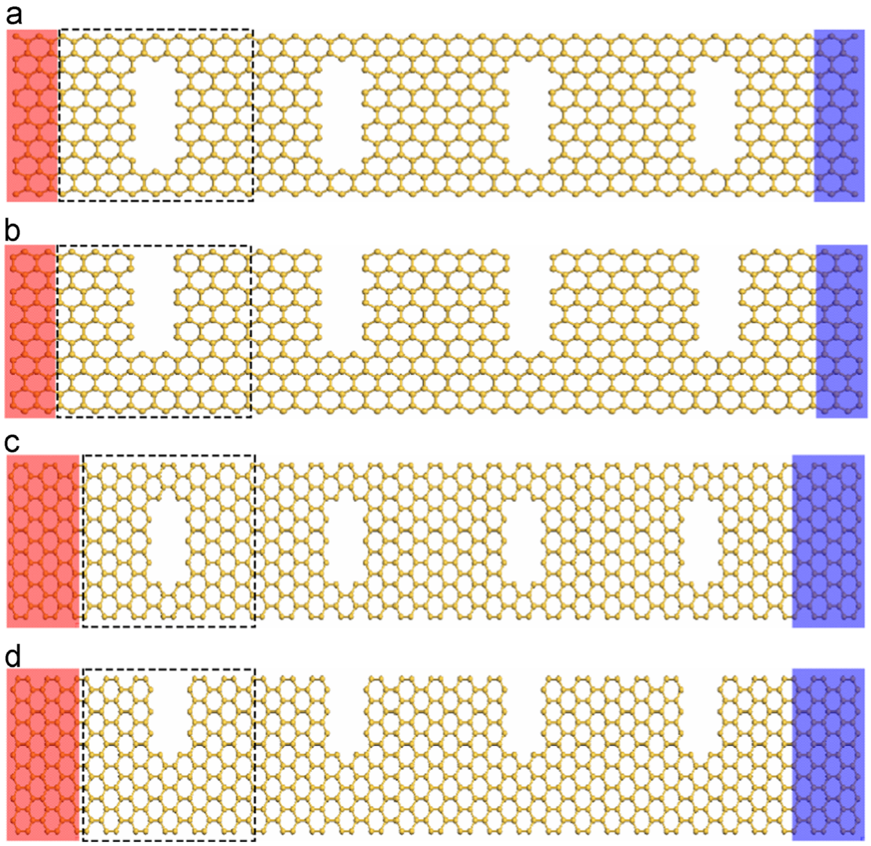

Fig. 1. (Color online) Schematic diagrams of defected SiNR atomistic structures with the length $L=15$ nm and width $W=3$ nm, for which the defect numbers are of $m=4$ and $n=3$. Figure (a–d) corresponding to 10-ZSiNR with central and edge defects and 15-ASiNR with central and edge defects, respectively.