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The electronic transport properties of graphene-like beryllium sulfide nanoribbons

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ABSTRACT

The electronic transport properties of zigzag beryllium sulfide nanoribbons (ZBeSNRs) are investigated by first-principles calculations. The results indicate that the electrons flow mainly through the two edges of ZBeSNRs. The electron transmission pathways are analyzed in detail. The ZBeSNRs show the remarkable negative differential resistance (NDR) properties, which are independent of the nanoribbon width due to their very similar band structures. The NDR behavior can be maintained by introducing a Be or S atom vacancy defect. The H-passivated ZBeSNR presents the interesting current-limited effect. The ZBeSNRs could be the promising candidates for the future nano devices, such as NDR devices.

1. Introduction

Since the discovery of graphene, the research effort on two-dimensional (2D) materials has rapidly increased, driven by their various intriguing mechanical and electrical properties [1–4]. Up to now, some graphene-like 2D crystals, such as hexagonal boron nitride (BN), BNC, SiC, and transition metal dichalcogenides, have been studied extensively to gain extraordinary properties beyond graphene [5–9]. For instance, BN sheet, one isoelectronic and isostructural analogue of graphene, can present several novel properties (such as superb thermal stability and chemical inertness, electrically-insulating properties, and extraordinary mechanical robustness) and great potential for high-quality nano devices (such as ultraviolet-light laser devices [10] and field emitters [11]). In addition, due to the quantum effects arising from the dimension and size reduction, their one-dimensional (1D) forms, such as nanoribbons, could offer electronic properties different from those of their 2D sheet counterparts [12–15]. For example, graphene sheet has a band structure following a linear dispersion relation at the Fermi level (E_F) in reciprocal space, forming the so-called zero-band-gap semimetal [12]. However, graphene nanoribbon can be either metallic or semiconducting, depending on the crystallographic direction (armchair or zigzag orientation) and ribbon width [13–15].

The 1D graphene-like nanoribbons have attracted great interest both from a fundamental point of view to understand their intrinsic properties and also from a practical point of view to explore their applications in future nano devices [16–23]. For instance, the high-quality BN nanoribbon recently was produced by unzipping during nanotube synthesis [16], and its band gap can be tuned by carrier doping or applying an external electrical field, thus offering unique opportunities for developing BN nano electronic devices [17,18]. 2D beryllium sulfide (BeS) sheet, a new graphene-like structure, recently was found to be a semiconductor with an indirect energy gap of 4.26 eV and outstanding thermodynamic stability up to 1000 K [24]. In addition, the 1D BeS nanoribbons (BeSNRs) were predicted to be the metals (with zigzag edges) or wide-band-gap semiconductors (with armchair edges).

In this report, we study the electronic transport properties of the BeS nanoribbons (as shown in Fig. 1(a)) with zigzag edges (ZBeSNRs) through the first-principles calculations. It is found that the metallic property of ZBeSNRs is mainly determined by the edge Be σ-dangling bonds, and the p_x orbitals of edge S atoms. When the bias voltages are applied to the two ends of the nanoribbons, the electrons mostly propagate along the two edges of nanoribbons through different transmission pathways. The ZBeSNRs display the interesting negative differential resistance behavior, which is not dependent of nanoribbon width due to their similar band structures. The defected and edge-passivated structures are also discussed.

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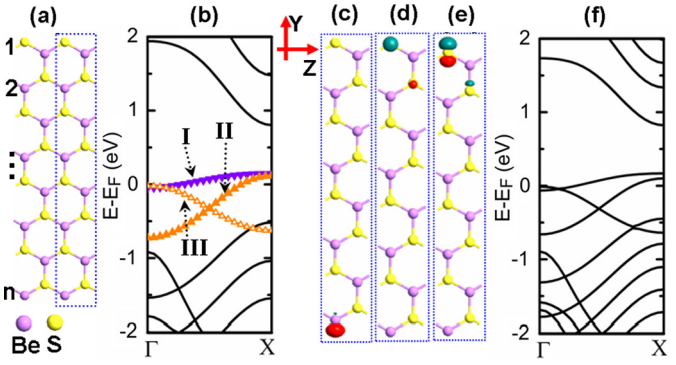

Fig. 1. The geometric and electronic structures of ZBeSNRs. (a) The geometric structure of ZBeSNRs. (b) Band structure of 8-ZBeSNR. (c)–(e) The wave functions of 8-ZBeSNR at Γ point for band **I**, **II**, and **III**, respectively. The red and green colors in (c) to (e) refer to the phase of wave functions. (f) Band structure of 12-ZBeSNR. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

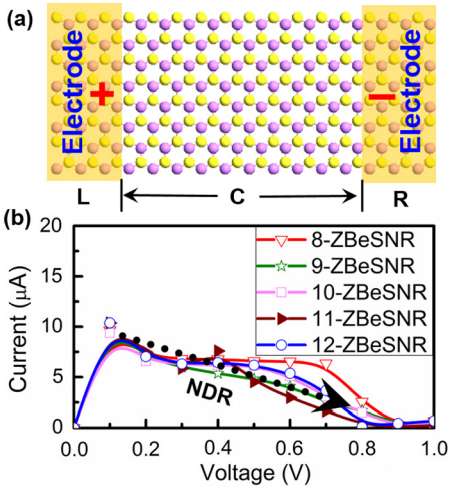

Fig. 2. The geometric structure (a) and calculated I–V curves (b) of the ZBeSNR-based devices. L, R, and C indicate the left and right electrodes, and the central scattering region, respectively. The dashed arrow shows the NDR behavior.

2. Computational methods

The electronic structure and transport calculations were carried out using the Atomistix Toolkit (ATK) code package based on density function theory (DFT) and non-equilibrium Green's functions (NEGF) [25–27]. We employ the Troullier–Martins norm-conserving pseudopotentials to describe the core of all atoms and linear combinations of atom orbitals (LCAO) to expand the valence states of electrons. The wave functions of all atoms are expanded by the double-zeta plus polarization. The local density approximation is used as the exchange-correlation functional. The Hamiltonian, overlaps, and electronic densities are evaluated in a real space grid defined with a plane wave cutoff of 150 Ry to achieve a balance between calculation efficiency and accuracy. The k-points grid ($1 \times 1 \times 100$) is used to sample the Brillouin zone of the left/right electrode in the x, y, and z direction, respectively, where the z is the electronic transport one. Open boundary conditions are used to describe the electronic and the transport properties of the ZBeSNRs. The geometric structures studied are optimized until all residual forces on each atom are smaller than 0.01 eV/Å.

3. Results and discussion

Fig. 1(a) shows the geometric structure of BeS nanoribbon with zigzag edges. We use the number of parallel zigzag chains n in a nanoribbon to describe the width of the nanoribbon. In the ZBeSNRs, all the outermost atoms at the Be edge are Be atoms while all the outermost atoms at the opposing edge (*i.e.*, the S edge) are S atoms. First, we focus on the electronic structure of BeSNR with 8 zigzag chains (labeled as 8-ZBeSNR). As shown in Fig. 1(b), the calculated band structure suggests that the 8-ZBeSNR is a metal with two bands (*i.e.*, **I** and **II**) crossing the E_F, consistent with the previously published result [24]. The two bands **I** and **II** are originated from the electronic states at the edge Be and S atoms, respectively. Intuitively, the bands **I** and **II** are ascribed to the σ-dangling bond states at the edge Be atom and the p_x orbital of edge S atom, respectively, according to the distributions of wave function space at Γ point (as shown in Figs. 1(c) and 1(d)). It is also noticed that another band (close to the Γ point, *i.e.*, **III**) approaches to the E_F level, which is from the σ-dangling bond states of the edge S atom (as shown in Fig. 1(e)). It demonstrates that the ZBeSNRs could have extensive applications in nano electronic devices due to the extraordinary edge states, like metallic graphene [28,29], B–N [7], and MoS_2 zigzag nanoribbons [30]. It is noted that the ferromagnetic and antiferromagnetic states of 8-ZBeSNR are the most energetically favored, but degenerated in energy in the accuracy of meV, namely, a spin glass state. What's more, our calculations confirmed that the energy of the spin-polarized state is ∼10 meV per edge atom lower than that of the spin-unpolarized state. However, the spin-polarized state would become unstable with respect to the spin-unpolarized state at finite temperature. Therefore, we focused our study only on the spin-unpolarized state of ZBeSNRs.

Next, we investigate the electronic transport behaviors of the 8-ZBeSNR and build the mode in Fig. 2(a). Such two-electrode system is composed of three regions: the left (L)/right (R) electrode, and the central scattering region (C). The electrode is described by a supercell composed of three repeated 8-ZBeSNR unit cells along z direction (*i.e.*, the transport direction). The current–voltage (I–V) curve is one important property in the research of electronic transport properties of nanomaterials. The current through the 8-ZBeSNR nanojunction can be obtained from Landauer–Büttiker formula [31]

$$I(V_b) = \frac{2e}{h}\int_{-\infty}^{\infty} T(E, V_b)\left[f_L(E-\mu_L) - f_R(E-\mu_R)\right]dE. \quad (1)$$

The I–V curve of 8-ZBeSNR is plotted in Fig. 2(b). It can be seen that 8-ZBeSNR shows the interesting negative differential resistance behavior. With the bias increasing, the current through 8-ZBeSNR reaches up to a peak at the bias of 0.1 V, while thereafter it drops down until to zero at a threshold voltage of about 1.0 V. In general, the electronic transport characteristics should be ascribed to the band structure of the 8-ZBeSNR under the applied biases. Fig. 3(a) gives the bias-dependent transmission spectrum and band structures of each electrode at the bias of 0.1 V. One can find that, under the positive bias voltages, the bands shift downward/upward for the L/R electrode, respectively. At 0.1 V bias, the bands **I** and **II** of the L electrode have the largest overlap with that of the R electrode, between which the electron transport is allowable and the probability is close to 2 from the bands **I** and **II** of the R electrode to those of the L electrode. It demonstrates that there exist at least two electron transmission channels in the 8-ZBeSNR nanojunction. While, it is noticed that the band **III** of the L electrode does not enter into the bias window (BW), thus then gives no contribution to the electron transmission.

Fig. 3(b) depicts the transmission pathways (local currents) [32] in the central region of 8-ZBeSNR nanojunction at the transmission peak **P** (shown in Fig. 3(a), here, local currents occur at 0.02 eV). The transmission pathways is an analysis option which splits the