Engineering the Thermoelectric Power Factor of Metallic Graphene Nanoribbons

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ABSTRACT

In this work we engineer the thermoelectric (TE) properties of metallic zigzag graphene nanoribbons by the introduction of extended line defects and positively charged substrate impurities. We show that, in such a way, an asymmetry in the transmission of electrons and holes can be created, which allows separation of hot and cold carriers and will provide a very high TE power factor.

METHOD

Zigzag graphene nanoribbons (ZGNRs) are metallic conductors. As such, they have a small Seebeck coefficient (S) and therefore a poor TE power factor GS^2. In this work, we demonstrate how the Seebeck coefficient can be increased by bandstructure engineering after incorporating two types of defects: i) extended line defects (ELDs) and ii) positively charged impurities. To calculate the bandstructure and transport coefficients, we use a standard tight-binding model and the quantum mechanical non-equilibrium Green's function method, respectively. The long-range substrate impurities with the density of one impurity per 100 nm are introduced only in the channel of length L. The effect of impurities is described by a potential $V(r)=V_0 \exp(-r^2/2R^2)$, where V_0 is its strength and R its variance [1]. We use V_0=+/-0.5eV for negative/positive impurities.

DISCUSSION

In addition to impurities, extended line defects (ELD) are introduced in the channel. The geometrical structure of the ZGNR with ELD [2], denoted as ELD-ZGNR(n_1,n_2), is shown in Fig. 1a. The bandstructures of the ELD-ZGNR(10,10) and the ELD-ZGNR(15,5) are shown in Fig. 1a and c, respectively. The thick-red lines show a new band that is introduced in the conduction band near the Fermi energy due to the ELD. Figure 2 shows the asymmetry of the transmission around the Fermi level. With introduction of one ELD the conduction band (E>0) has now two bands, whereas the valence band (E<0) remains as before. The effect of positive impurities and channel length is shown in Fig. 3. A positive impurity is a barrier for holes and degrades hole transport more than electron transport, therefore increasing the asymmetry between hole and electron transport. By increasing the impurity spread R (Fig. 3a) and the channel length L (Fig. 3b), respectively, we can further increase the asymmetry between electrons and holes. On the other hand, as shown in Fig. 4a the introduction of negative impurities (barriers for electrons) reduces the electron transmission and therefore the electron hole asymmetry, a case which needs to be avoided. We also examined the effect of ELD position in Fig. 4b, and found it to be not significant

Figure 5 shows the effect of ELD on the TE coefficients. The electrical conductance (Fig. 5a) and Seebeck coefficient (Fig. 5b) are increased compared to the pristine ZGNR value (dotted lines). Although positive impurities decrease the electrical conductance, they largely improve S. This results in a high TE power factor (Fig. 5c). Assuming a value of k_l=0.1 W/Km for the lattice thermal conductance of substrate supported graphene nanoribbons [3], a value of ZT=0.5 can be achieved as shown in Fig. 6.

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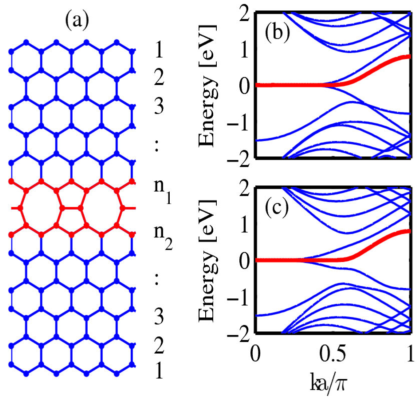

Fig. 1. (a) The geometrical structure of the ELD-ZGNR(n_1,n_2). The bandstructure of ELD-ZGNR(10,10) (b) and ELD-ZGNR(15,5) (c)

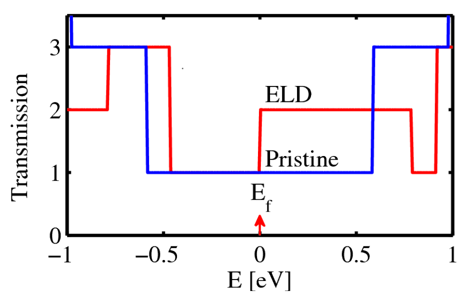

Fig. 2. The transmission function for ZGNR(20) and ELD-ZGNR(10,10)

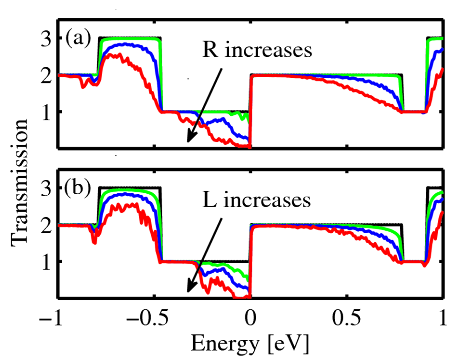

Fig. 3. The effect of positive impurities on the transmission function of ELD-ZGNR(10,10). (a) The channel length L is assumed to be 300 nm and the impurity spread R takes values 0.1, 0.3, and 0.5 nm. (b) R is 0.3 nm and L takes values 100, 300, and 1000 nm

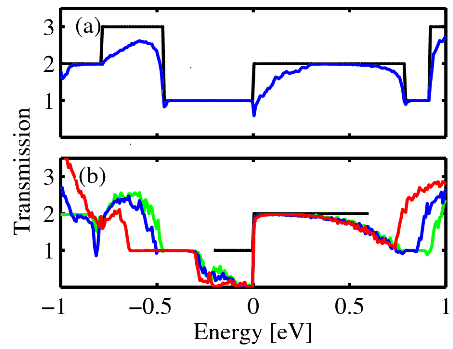

Fig. 4. The transmission function. (a) Negative impurities with R=0.3 nm are introduced in a ELD-ZGNR(10,10) channel of the length 300 nm. (b) The effect of ELD's position. L = 1000 nm. Positive impurities are considered.

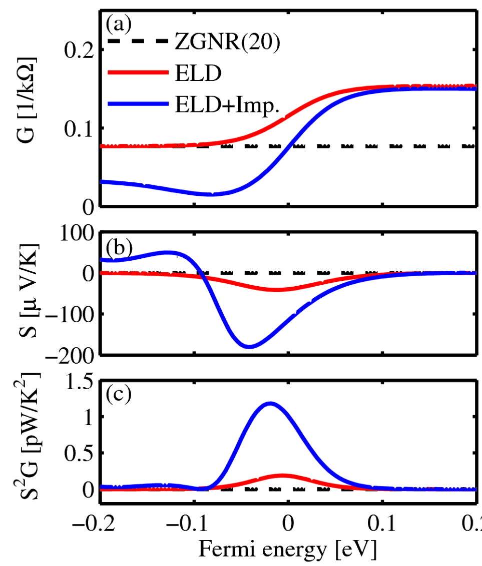

Fig. 5. (a) Electrical conductance, (b) Seebeck coefficient, and (c) power factor of ZGNR(20) and ELD-ZGNR(10,10) with and without impurities (R=0.3 nm). L = 1000 nm

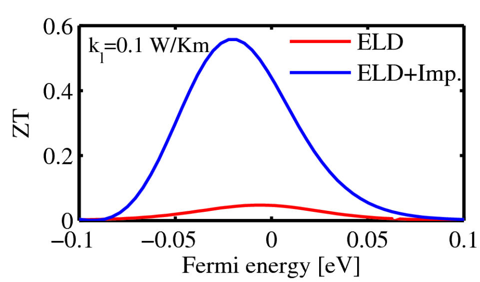

Fig. 6. The figure of merit for ELD-ZGNR(10,10) with and without impurities (R=0.3 nm). The channel length is assumed to be L=1000 nm