

# Semiconducting graphene nanostrips with edge disorder

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(Dated: January 24, 2007)

We present a study of semiconducting armchair-edge graphene nanostrips in the presence of edge disorder. Our tight-binding calculations show that edge disorder could transform long semiconducting nanostrips into Anderson insulators. In contrast, we show that short nanostrips allow current to tunnel through the band gap. Therefore, we prescribe a method for how to find an intermediate regime, in which the nanostrips retain a semiconducting band gap. To find that regime, we have calculated half amplitude localization lengths using different widths and degree of disorder. Our numerical results indicate that the maximum localization length is approximately proportional to the square of the width of the nanostrip and inversely proportional to the disorder concentration.

PACS numbers: 73.50.-h, 73.23.Ad, 73.61.Wp

Recent progress in isolating single sheets of graphite [1–5] has sparked interest in graphene-based nanoelectronics. Experiments have already demonstrated anticipated physics such as electron-hole symmetry and half-integer quantum Hall effect [3, 4]. By further confining the electrons in the graphene plane one can obtain new one-dimensional structures which we refer to as graphene nanostrips (GNS's). These GNS's may offer attractive features such as room-temperature ballistic transport [6, 7], which has also been demonstrated in the closely related single-walled carbon nanotubes (SWNT's) [8]. Compared to SWNT's, in-plane GNS's may well be easier to pattern, which would make them more versatile for large-scale nanoelectronics.

Most of the features of the GNS and SWNT energy dispersions can be directly derived from graphene. However, unlike SWNT's, GNS's have edges. In zigzag-edge GNS's, these edges give rise to edge states which are located near the Fermi level [9]. Armchair-edge GNS's, on the other hand, do not exhibit these edge states, and have therefore, in analogy with zigzag SWNT's, been predicted to be metallic or semiconducting depending on their widths [9–11]. The condition (ignoring curvature effects) for a zigzag nanotube with circumference  $na$  ( $a$  is the graphene lattice spacing) to be a semiconductor is  $n \neq 3l$  for all integers  $l$ . The corresponding condition for an armchair-edge GNS is

$$N + 1 \neq 3l, \quad (1)$$

where  $(N + 1)a/2$  is the effective width of the GNS. The factor of a half follows from the Dirichlet boundary condition which quantizes the wavefunction in half periods. The semiconducting band gap in the GNS is also nearly inversely proportional to the width of the confined in-plane dimension and could be approximated by

$$E_g = \frac{2\pi|\gamma|}{\sqrt{3}(N + 1)}, \quad (2)$$

where  $\gamma \approx -2.7$  eV is the nearest-neighbor hopping in-

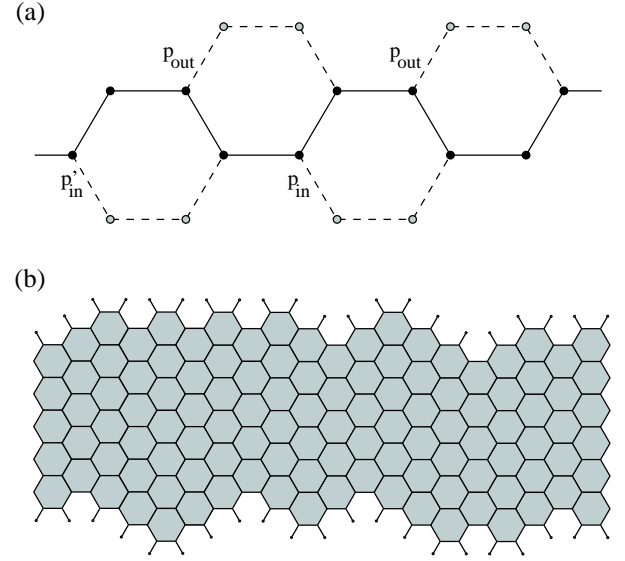


FIG. 1: Armchair-edge nanostrip with imperfect edges. **(a)** A single perfect edge (solid lines) is deformed by adding or removing pairs of carbon atoms with different probabilities, thereby generating an imperfect edge with defects (dashed lines). **(b)** An example of a nanostrip with imperfect edges.

tegral. We emphasize that Eqs. (1) and (2) are derived using perfect edges. To achieve perfect edges in experiments based on any present lithography technique, however, is a practically hopeless challenge.

In this letter, we present a study of armchair-edge GNS's with imperfect edges. The edges are assumed to be terminated with hydrogen atoms. Adding or removing single carbon atoms is energetically unfavorable because it would require that two hydrogen atoms are spatially too close together. Therefore, we only allow pairs of carbon atoms to be added or removed as illustrated in Fig. 1(a). The edges are initially assumed to be perfect. Then, we start from the left and remove a pair of atoms with probability  $P'_{in} \equiv P/(1 + P)$ . Follow-

ing the edges to the right, we continue to add or remove pairs of atoms with probabilities  $P_{out} = P_{in} = P$ . In the process, we ensure that the edges return to their neutral position after each added/removed pair to again avoid tight hydrogen atoms. An example of an armchair-edge GNS with edges following the devised scheme is shown in Fig. 1(b).

To find out how the imperfect edges affect the transport properties of semiconducting armchair-edge GNS's, we employ a recursive self-energy method. Our model is based on nearest-neighbor  $\pi$ -orbital Slater-Koster tight-binding and uses two semi-infinite GNS's with perfect edges as leads. We obtain the self-energies for the leads by transforming the  $\pi$ -orbital states  $|\psi_{m,n}\rangle$ , where  $m$  and  $n$  index the transverse zigzag chains and the positions along those chains. First, we use

$$|\phi_{p,m}\rangle = \sqrt{\frac{2}{N+1}} \sum_{n=1}^N \sin \frac{np\pi}{N+1} |\psi_{m,n}\rangle, \quad (3)$$

where  $p = 1, 2, \dots, N$ . Then, we let  $p = 1, 2, \dots, N_L$  with  $N_L$  the largest integer  $\leq N/2$  and apply

$$|\chi_{p,m}^\pm\rangle = \frac{1}{\sqrt{2}} (|\phi_{p,m}\rangle \pm |\phi_{(N+1-p),m}\rangle). \quad (4)$$

If  $N$  is odd, we also use  $|\chi_m^{(0)}\rangle = |\phi_{(N+1)/2,m}\rangle$ . In the transformed representation, electron transport occurs along independent linear chains for which the self-energies can be calculated analytically. We solve the scattering problem by dividing the scattering region into narrow slices  $s$  (four per unit cell) and then iterating the left self-energies from the left lead towards the right lead using

$$\Sigma_s^L = H_{s,s-1}(E - H_{s-1,s-1} - \Sigma_{s-1}^L)^{-1} H_{s-1,s}. \quad (5)$$

This equation simplifies somewhat by the fact that  $H_{s,s} = 0$  in our model. Immediately before the right interface, we calculate the surface Green functions  $g_{L,R} = (E - \Sigma_{L,R})^{-1}$  which are needed to calculate the conductance of the GNS. We use a general conductance expression obtained by Todorov et al. [12] which we have simplified to:

$$G = \frac{2e^2}{h} 4\text{Tr} \left[ \text{Im}\{g_L\} t_{LR} \text{Im}\{g_R\} t_{LR}^\dagger \right], \quad (6)$$

where  $t_{LR} = \left( I - H_{LR} g_R H_{LR}^\dagger g_L \right)^{-1} H_{LR}$  and  $H_{LR}$  is the interaction connecting the last slice in the scattering region with the first slice in the right lead.

The conductances of two semiconducting ( $N = 85$ ) GNS's with  $P = 0.3$  and different lengths,  $L$ , are shown in Fig. 2(a). In the longer sample ( $L = 2048$ ), the conductance is strongly suppressed by Anderson localization which arises due to the random scattering potential experienced by the conduction particles. This effect has

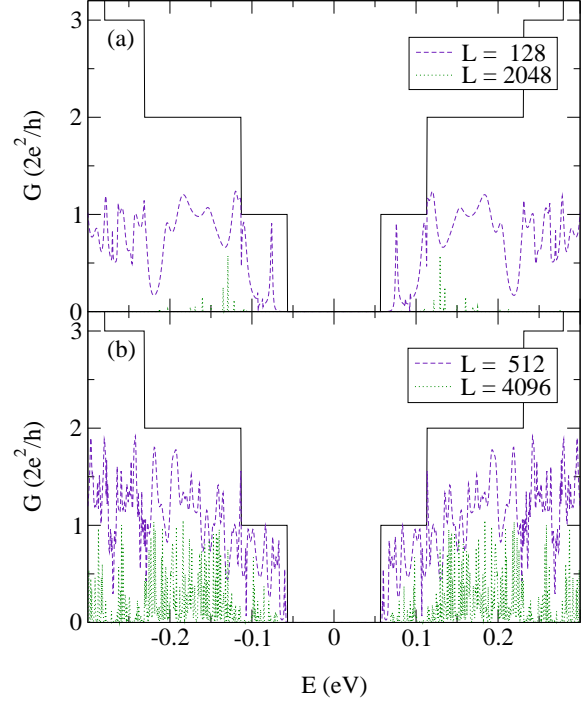


FIG. 2: Conductance of semiconducting armchair-edge graphene nanostrips with edge defect probability: (a)  $P = 0.3$  and (b)  $P = 0.05$ . The widths of the nanostrips are approximately 10.6 nm ( $N = 85$ ). The lengths of the samples are specified in unit cells (1 unit cell =  $3d \approx 0.426$  nm) and are approximately 54.5 nm and 872 nm in (a) and 218 nm and 1740 nm in (b). The conductance of the samples can be compared to a nanostrip without defects, shown as solid.

been reported in metallic armchair-edge GNS's but not in zigzag-edge GNS's which appear to be relatively robust against edge disorder [6]. The number of scattering centers is roughly proportional to the defect probability  $P$ , and consequently, the localization effect is less pronounced in the dotted curve in Fig. 2(b) which uses  $P = 0.05$ , despite that sample being twice as long. In spite of the localization effect, it is still possible to use the GNS's in semiconducting devices by choosing appropriate lengths. The semiconducting behavior is evident from the dashed curves in Fig. 2, which represent shorter GNS's.

A requirement for semiconducting behavior of a nanostrip of a desired width is that the length is short enough so that states in the vicinity of what was the semiconducting band edges remain extended over its length but long enough that most of the states introduced into the semiconducting band gap by the edge disorder are strongly localized. The transition between localized and extended states should also occur over a reasonably small energy range with the localized states of insufficient measure to strongly pin the Fermi level. To better quantify the length requirement, we recall that all

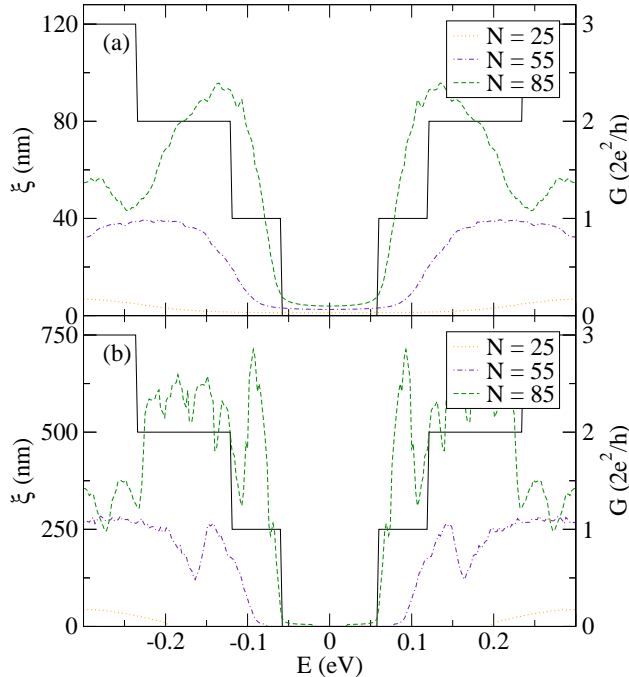


FIG. 3: Half amplitude localization lengths of armchair-edge graphene nanostrips with edge defect probability: (a)  $P = 0.3$  and (b)  $P = 0.05$ . The solid curves represent the conductance of a defect-free nanostrip ( $N = 85$ ) and exhibit a band gap that can be estimated by Eq. (2).

states in one-dimensional wires ultimately become localized as the length is increased. Deep within the localization regime the conductance is expected to behave as  $G(L) \propto \exp(-L/\xi)$ , where  $\xi$  is half the wavefunction localization length [13]. We obtain  $\xi$  for a fixed energy  $E$  by applying a least squares fit to the slope of  $-\langle L/\ln G \rangle$ , where the ensemble average includes 1000 random disordered configurations. Also note that for a single channel the mean free path for disorder-induced backscattering should be of the same order as  $\xi$ . Therefore, we expect the conductance to be fairly robust for  $L \ll \xi$ .

Figure 3 shows  $\xi$  as a function of energy, and has been calculated using metallic linear-chain contacts. These contacts should not affect  $\xi$ , which is an intrinsic property of the disorder, other than that they allow for conductance within the band gap of the GNS's by providing a non-zero density of states. As expected,  $\xi(E)$  is relatively small within this energy range, suggesting that the requirement of localized and extended states could be met. The figure also confirms that GNS's with less defects have a longer localization length. We have, in addition, found that the maximum localization length scales approximately inversely with the defect concentration and quadratically with the width of the GNS, the latter suggesting that wider GNS's are less affected

by edge disorder.

Semiconducting nanostrip devices should not be too short, as particles could then tunnel through the band gap. In a defect-free sample with perfect contacts, the tunneling conductance decays as  $G = (2e^2/h) \exp(-2\kappa L)$ , where  $\kappa = \sqrt{(E_g/2)^2 - E^2}/\hbar v$  has been estimated by expanding the energy dispersion ( $\hbar v \equiv 3|\gamma|d/2 \approx 0.575 \text{ eV nm}$ ). Direct tunneling contributes to the calculated localization length and can be expressed as

$$\xi_t(E, N) \approx \frac{3d}{4} \frac{1}{\sqrt{\frac{\pi^2}{3(N+1)^2} - (E/\gamma)^2}}, \quad (7)$$

where we have applied Eq. (2). Therefore, a semiconducting nanostrip device requires that  $L \gg \xi_t$ .  $\xi_t \approx 5.0 \text{ nm}$  in the middle of the gap of an  $N = 85$  GNS.

In conclusion, we have shown that edge disorder in armchair-edge graphene nanostrips could cause short localization lengths which could make expected semiconducting nanostrip devices insulating. This problem can be overcome by using appropriate lengths of devices with specific widths and degree of disorder.

DG acknowledges support from the National Academies Research Associateship Programs. This work was also supported by the Office of Naval Research both directly and through the Naval Research Laboratory.

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