The recent discovery of free state graphene has generated great interest in the scientific community. Remarkably, experimentalists have succeeded in isolating individual graphene sheets freely suspended on a microfabricated scaffold in vacuum or air. Despite being only one atom thick, these sheets still display long-range crystalline order.

Graphene ribbons are obtained by cutting a graphene sheet along a straight line. Since there are two types of graphite edges, the ribbons can be classified either as zigzag (Fig. 1, top) or of armchair (Fig. 1, bottom) type. The ribbon width \( N \) in Fig. 1 denotes the number of zigzag lines (\( N = 8 \)) for zigzag ribbons and the number of dimer lines (\( N = 14 \)) for armchair ribbons. The zigzag ribbons are conducting for all \( N \), while the armchair ribbons can be either conducting or semiconducting depending on their width \( N \). The ribbons with width \( N = 3m - 1 \), \( m \) being an integer, are conducting. Otherwise, the armchair ribbon is semiconducting. These features give us the possibility of constructing various graphene structures in a plethora of combinations of conducting and semiconducting parts. Defect-free straight graphene nanoribbons of infinite length and uniform width have been studied extensively for their electronic properties.

The fact that single wall carbon nanotubes (SWCNs) are formed from graphene ribbons by appropriate rolling, it can be expected that most of the transport properties of SWCN junctions to have a noticeable correspondence with those of the graphene junctions. However, graphene ribbons exhibit some exotic and unique features which make them very promising candidates for future device applications. For example, introducing a constriction in an armchair graphene ribbon can result in a metal-semiconductor junction (see Fig. 2, top). We call this structure arm-constrict-arm (ACA) ribbon. The band structure for this type of constriction exhibits unusual valley shaped features with no analogue in silicon based electronics. This feature is so unique that it creates by itself a unique type of electronics, the so called valleytronics. Another way to generate a metal-semiconductor junction in a graphene ribbon would be to connect an armchair ribbon to a zigzag ribbon via pentagon-heptagon defect chain (Fig. 2, bottom). We denote this structure arm-zig-arm (AZA). Correspondingly, we denote by ZAZ the structure with the zig-arm-zig configuration. The electronic and transport properties of these heterostructures could reveal many interesting features not previously known.

We investigate the conductance of various ACA and AZA structures. For the ACA ribbons we vary the lengths of the middle constricted regions while keeping the wider por-

---

**Strong dependence of transport properties of metal-semiconductor-metal graphene ribbons on their geometrical features**

Antonis N. Andriotis\(^a\)

\(\text{Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, Heraklio, Crete 71110, Greece}\)

Ernst Richter\(^b\)

\(\text{DaimlerChrysler AG FT3/SA, Wilhelm-Runge-Str. 11, 89081 Ulm, Germany}\)

Madhu Menon\(^c\)

\(\text{Department of Physics and Astronomy and Center for Computational Sciences, University of Kentucky, Lexington, Kentucky 40506, USA}\)

(Received 23 August 2007; accepted 23 September 2007; published online 8 October 2007)

The conducting properties of various finite graphene ribbons and their junctions are investigated. These were found to depend strongly on their size and geometric features. Small arm-chair ribbons, when connected through tapered geometries, are found to exhibit very narrow conducting windows. No conductance is found through small armchair zigzag armchair ribbon junctions when connected via pentagon-heptagon defect lines. However, the conducting windows become broader as the size of the ribbons increases. © 2007 American Institute of Physics. [DOI: 10.1063/1.2798593]

---

\(^a\)Electronic mail: andriot@iesl.forth.gr

\(^b\)Electronic mail: ernst.richter@daimlerchrysler.com

\(^c\)Electronic mails: super250@pop.uky.edu and madhu@ccs.uky.edu

---

**FIG. 1.** (Color online) Figure showing graphene ribbons of zigzag type (top) with \( N = 8 \) and armchair type (bottom) with \( N = 14 \). The red lines mark the dimers for determining the length index \( L \).
tions at the two ends the same. This allows us to study the conductance of metal-semiconductor-metal ribbons containing different lengths of the semiconductor portions. Similarly, for the AZA ribbons we vary the lengths of the zigzag portions. All the structures studied are fully relaxed without any symmetry constraints using the generalized tight-binding molecular dynamics (GTBMD) method. The structural relaxations were carried out within periodic supercells incorporating a constant pressure ("movable wall") ensemble. This allows for a simultaneous relaxation of lattice and basis degrees of freedom. A uniform grid consisting of 126 \( k \) points was used in the calculation of forces. In the case of the ACA ribbons the lengths of the middle semiconductor portion are measured in terms of the number of carbon dimers \( L \) along the length of the ribbon (indicated by red colored bonds in Fig. 1). For the ACA ribbon in Fig. 2, \( L=9 \) and \( N=15 \). Similarly, for the AZA ribbon in Fig. 2, \( L=9 \) and \( N=11 \).

The electronic band structure analysis is carried out using the scheme in Ref. 12. In Fig. 3 we show the band structures for the ACA and AZA ribbons of Fig. 2.

The quantum conductivity of graphene ribbons are calculated using the surface Green’s function matching method. This formalism is based on the theory proposed by Datta. The tight-binding Hamiltonian used in the conductivity calculations is the same as that used in the GTBMD scheme for obtaining structural relaxation, ensuring consistency in the calculations. The formalism has been extensively used in the calculations of the electronic transport of various types of SWCN junctions. Conductivity calculations are performed on graphene ribbons of finite length. These are extracted from structures fully relaxed within the supercell formulation described above. The finite ribbon structures shown in Figs. 1 and 2 as well as in all subsequent calculations performed in this work are obtained in this manner. For the band structure calculations shown in Fig. 3, however, we use the full supercell with periodic boundary conditions.

We use the conductivity formalism to first investigate the transport properties of armchair graphene ribbons of finite length. We characterize these ribbons by indices \( (L,N) \), where \( L \) and \( N \) represent integers for the length and width, respectively. Our aim is to determine the dependence of conductivity on the geometric features (length, width, and atomic configuration) of the ribbons. With this in view, we consider armchair \( (8,8) \), \( (16,8) \), \( (24,8) \), \( (24,17) \), and \( (24,23) \) ribbons. These are all metallic since, \( N=3M-1 \), with \( M \) an integer. Our results are presented in Fig. 4. As seen in the figure, the transmission coefficient \( T(E) \), of the ribbons exhibit resonances at energies \( E\approx -2.25 \), \(-2.50 \), and \( 0.00 \) eV (Fermi level is set to 0 eV). However, the strength of the resonant peaks appears to depend on both the length and the width of the ribbon. As general trends we notice (i) the decrease of the resonant peak at \( E=0.00 \) eV and the increase of the peaks at the energies \( E\approx -2.25 \) and \(-2.50 \) eV as the width of the ribbon increases, and (ii) the decrease of the peak at \( E=0.00 \) eV as length of the ribbon increases. The latter trend is reminiscent of analogous property observed in SWCNs attributed to finite size effects.

We next investigate the transport properties of ACA ribbons. In particular, we study the length dependence of conductivity by considering \( (7,15) \), \( (9,15) \), \( (11,15) \), \( (13,15) \), \( (15,15) \), and \( (17,15) \) graphene ribbons (all semiconducting) sandwiched between two tapering armchair ribbons of \( N=23 \) (both metallic). A representative ACA where \( a=9,15 \) graphene ribbon connected at the two ends with tapering \( N=23 \) armchair ribbons is shown in Fig. 2 (top). In Fig. 5 we plot \( T(E) \) as a function of energy. As can be seen in the figure, \( T(E) \) exhibits two pronounced peaks at \( E\approx -2.25 \) and \(-2.50 \) eV that vary depending on the length of the constrictions.
The highest $T(E)$ peak was found for $L=9$ followed by that for $L=13$ at $E = -2.50$ eV. These two ribbons exhibited negligible peaks at $E = -2.25$ eV. The ribbon with $L=7$ exhibits a small peak at $E = -2.25$ eV but no peak at $E = -2.50$ eV. The ribbons with $L=11, 15,$ and $17$ did not show any $T(E)$ peaks, i.e., these ribbons are not conducting. By increasing the width of the ribbon (width of ends and constriction $N=37$ and $29$, respectively) we find that the resonance peaks at $E = -2.25$ and $-2.50$ eV evolve to a broad resonance peak while a narrower peak appears at $E = +3.0$ eV.

Transport properties of AZA ribbons are investigated next. As can be seen in Fig. 2 (bottom), the heptagon-pentagon line defect transforms the arm-type ribbon to the zigzag type and vice versa. The dependence of conductivity on the geometry and atomic configuration of the ribbon is studied by calculating the transmission function $T(E)$ of the $(10,11), (13,11)$, and $(16,11)$ zigzag ribbons sandwiched between two armchair ribbons of width $N=20$. The results are shown in Fig. 6. As can be seen in the figure, all these structural ribbon configurations are nonconducting; their $T(E)$ exhibits a negligible peak [$T(E) = 0.01$ in units of $2e^2/h$] at $E = -2.25$ and $-2.50$ eV. However, when the width of the arm-type parts is increased, we find (not shown) an increase in the resonances of $T(E)$ at $E = -2.25$ and $-2.50$ eV [$T(E) = 0.20$]. It is thus clear that the $T(E)$ peaks depend strongly on the geometrical features of the zigzag part. Nonconductive behavior as found for the $L=10$ ribbon was also found for the corresponding ZAZ configuration.

To summarize, there is no conductance for small AZA or ZAZ ribbons. Small ACA ribbons are found to exhibit very narrow conducting windows in comparison to the wider and longer ones which exhibit the valley structure. More importantly, the transport properties of the small ACA ribbons show strong dependence on their geometric features (length, width, and atomic configuration) and can range from semiconducting to metallic type.

The present work is supported through grants by USARO (W911NF-05-1-0372) and DOE (DE-FG02-00ER45817).

16. After the preparation of the manuscript we became aware of a just published paper reporting the length dependence on the energy gap of straight armchair graphene ribbons of uniform width (Ref. 17). Their results are in agreement with our results showing length dependence on conducting properties shown in Fig. 3 for straight armchair ribbons.