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ScienceDirect
Physica E 40 (2008) 2635–2638
PHYSICA E
www.elsevier.com/locate/physe

Wave packet dynamical simulation of electron transport through a line defect on the graphene surface

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Available online 18 September 2007

Abstract

Formerly, we proposed an approach to construct new graphene-based elements for nanoelectronics with different properties using "lines" of chemisorbed H atom pairs on a graphene surface. According to band structure calculations these H–C "lines" change the electronic spectrum of pure graphene, forming quasi-one-dimensional electronic waveguides. The periodic "line" superlattices have semiconductor or metallic electronic structures according to their geometry, similar to the case of carbon nanotubes. We calculated the propagation of electronic wave packets parallel to the H–C line. The results make it possible to gain insight into the details of electron transport in nanoelectronic devices made of line superlattices.

PACS: 73.63.−b; 84.40.Az; 71.15.Dx

Keywords: Graphene nanoribbon; Waveguide; Transport properties; Wave packet dynamics; Nanoelectronics

1. Introduction

Planar optical waveguides have successful applications in current technologies, e.g. in sensors. Similar electronic waveguides are used in microelectronics. However in nanotechnology we have no two-dimensional (2D) analogues. So a great deal of attention has been focused recently on a new class of 2D materials—graphenes [1].

Graphene ribbons, with atomic structure as if cut from planar graphene sheets, has been shown to hold unusual electronic properties, depending on their edge shape and width, as shown by theoretical calculations [2,3] and STM measurements [4]. Ribbons with armchair edges—corresponding to (*n*,0) zigzag nanotubes—can be either metallic or semiconducting depending on their width [5], an armchair ribbon of width N_a is metallic only if $N_a = 3k+2$ and semiconducting otherwise, where k is an integer. By joining graphene stripes of different electronic properties, metal–semiconductor junctions can be formed, which can be the building blocks of graphene-based nanoelectronics.

We proposed formerly to use monoatomic graphite sheets "ruled" by adsorbed hydrogen lines [6] as nanosize electronic waveguides. It has been shown that superlattices of the (*n*,0) graphene stripes with linearly arranged pairs of H atoms have band structures similar to the spectra of (*n*,0) zigzag carbon nanotubes. In contrast to pure graphene stripe preparation [1] for which special cutting methods would be necessary, we proposed a simple method of fabricating such electronic waveguides using the bending of graphene which leads to increasing probability of hydrogen adsorption on its surface in the form of a "line" [7].

If we want to use graphene nanoribbons as elements of nanoelectronic devices, a detailed understanding of the electron transport through such systems is necessary. Owing to the characteristic lengths of nanoelectronic devices, comparable to λ_f, the Fermi wavelength of the electrons and to the large electronic coherence lengths in carbon nanosystems quantum interferences and multiple scattering are important ingredients to account for in a realistic model of transport through carbon stripes.

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1386-9477/$ - see front matter © 2007 Published by Elsevier B.V.
doi:10.1016/j.physe.2007.09.016

Formerly, we developed a wave packet dynamical simulation package [8] for transport through carbon nanosystems and this helped in understanding a number of problems arising in STM experiments on such systems. Wave packet dynamics [9] is an effective and conceptually simple method to study electron tunnelling through nanostructures. First we utilized this method for jellium models of tunnelling through STM tip–nanotube–support tunnel junctions [10–12], later we were able to incorporate the atomic structure [13] into our model by the use of a local one-electron pseudopotential [14].

In this paper, we study the transport of a three-dimensional (3D) electronic wave packet in the central stripe of a 2H (5,0)+(6,0)+(5,0) waveguide, modelled by the one-electron pseudopotential.

2. Calculation method

If we attach lines of H atoms to a graphene surface, this causes a slight elevation of the carbon atom rows below the H lines. The atomic positions are shown in Fig. 1, the geometry optimalisation was performed by the Brenner potential [15]. The one-electron density of states (cf. Fig. 2) shows a gap of 0.2 eV. The (6,0) stripe was modelled by a local one-electron pseudopotential [14] matching the band structure of graphite and graphene sheet. It was shown to be well suited to carbon nanotubes [16]. Its expression is given by $V(\vec{r}) = \sum_{j=1}^{n}\sum_{i=1}^{3} A_i \, e^{-a_i|\vec{r}-\vec{r}_j|^2}$, where the $\vec{r}_j$ denote the atomic positions and n is the number of atoms. The A_i, a_i coefficients are given in Ref. [14]. Fig. 3 shows the -2.7 eV equipotential surface calculated for the (6,0) stripe by the pseudopotential. The potential forms low value "channels" between the nearest neighbour C atoms and has a large value at the centres of the hexagons. This effectively prevents the electron to enter the centre region; most of the probability current has to flow along the bonds—as is really seen in the wave packet dynamical simulation. The C atoms in the armchair edges—shown by dashed lines in Fig. 3—have H atoms attached to them. This changes the sp^2 character of these atoms into sp^3, which can be taken into account within the framework of the local π electron pseudopotential model by simply removing the potential well from these atomic sites.

The geometry of the wave packet transport calculation is shown in Fig. 4. The incoming wave packet is approaching the (6,0) stripe from a jellium electrode, with Fermi energy $E_F = 5$ eV and work function $W = 4.81$ eV. The jellium electrode is coupled with the (6,0) stripe with a thin (0.2 A) tunnelling interface. To prevent the reflection of the wave packet from the far end of the stripe we calculated for a system which models a half-infinite stripe. This was accomplished by closing the edges of the calculation space by an imaginary drain potential and the pseudopotential modelling the (6,0) stripe was continued into the drain potential region. Fig. 4 shows the cross-section of the real- and imaginary parts of the potential used in the wave packet scattering calculation in composite colours and with contours in the plane crossing the nuclear positions. The cyan colour component correspond to the real part, a darker shade mean a lower potential value. The red component and the black contour lines show the imaginary part.

The incoming wave packet was launched with $E_k = E_F = 5$ eV kinetic energy (relative to the $V_0 = -9.81$ eV

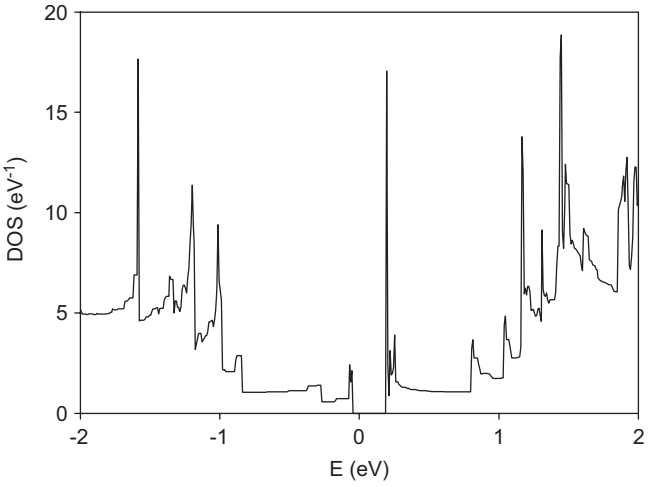

Fig. 2. One electron density of states per eV for the superlattice with clearly shown band gap $E_g = 0.2$ eV.

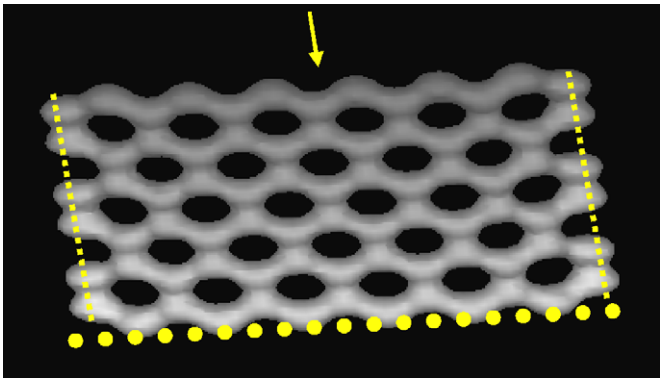

Fig. 3. (Colour online) -2.7 eV equipotential surface of the (6,0) waveguide shown in 3D. The upper arrow shows the incoming wave packet and the lower dotted line indicate the absorbing boundary condition. The dashed lines show those atoms in the armchair edges whose potential well was removed (see the text for details).

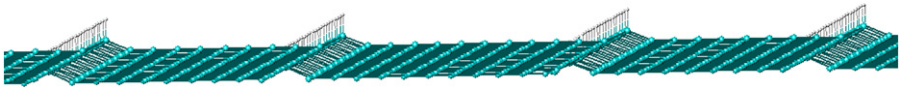

Fig. 1. (colour online) Atomic structure of a 2H (5,0)+(6,0)+(5,0) waveguide (grey circles denote the C atoms, open circles are the H atoms).

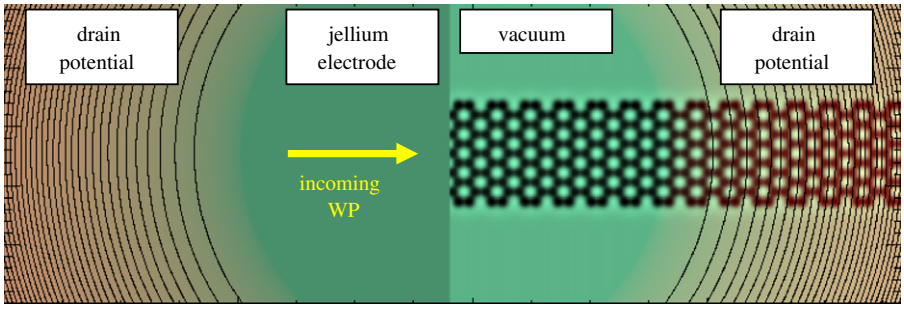

Fig. 4. (Colour online) Potential model used in the transport calculation. Darker shades correspond to lower potential values. The wave packet is approaching the nanoribbon from the left jellium electrode. The left- and right side of the calculation box is closed by the drain potential (shown by red shading and contour lines).

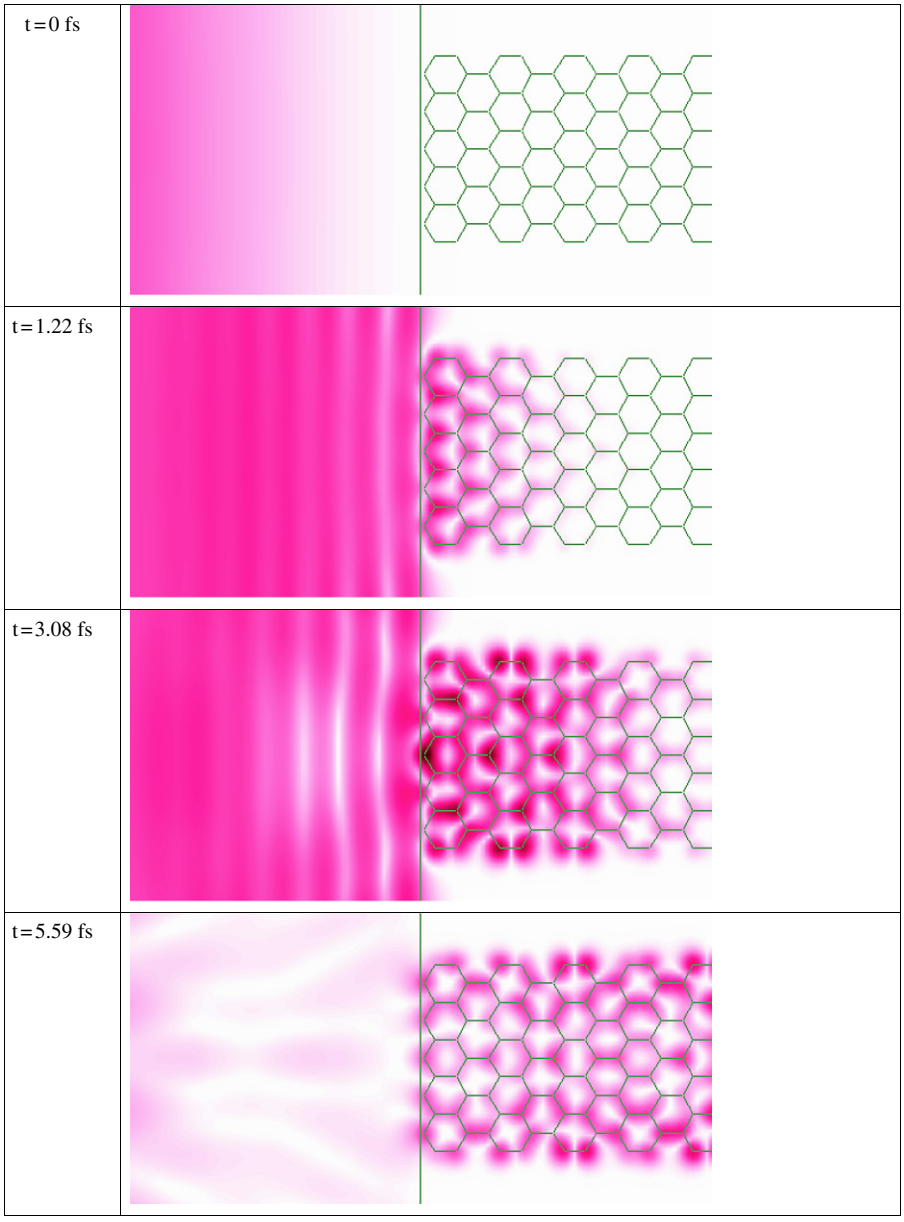

Fig. 5. (Colour online) Snapshots of the probability density in the plane of the nanoribbon. White means zero probability; darker shades denote larger probability. A common colour scale was used for all frames. The edge of the jellium electrode and the graphene network is shown by thin lines.

potential of the jellium electrode) and had a spatial width of $\Delta x = 0.74\,\mathrm{nm}$, $\Delta y = \Delta z = \infty$. This corresponds to a width of $\Delta k_x = 0.66\,\mathrm{nm}^{-1}$ in momentum space and a $\Delta E = 0.6\,\mathrm{eV}$ energy spread.

3. Results and discussion

Fig. 5 shows snapshots of the time development of the probability density of the wave packet. The first frame ($t = 0\,\mathrm{fs}$) is the initial state, the wave packet is still in the jellium electrode. At $t = 1.22\,\mathrm{fs}$ the wave packet already tunnelled into the nanoribbon. The incoming- and reflected wave packet parts form interference patterns inside the jellium electrode. By $t = 3.08\,\mathrm{fs}$ the wave packet already advanced seven zigzag lines in the nanoribbon, which corresponds to a 0.41 nm/fs group velocity. This is smaller than the $v_g^K = \mathrm{d}\omega/\mathrm{d}k = 0.94\,m\mathrm{m/fs}$ value calculated from the graphene dispersion relation at the K point, because the incoming wave packet excites several eigenstates of the nanoribbon, due to its finite energy spread. By $t = 5.59\,\mathrm{fs}$ the incoming wave packet already left the part of the jellium electrode shown in the presentation window—partly it was reflected and absorbed by the drain potential at the left side, partly it tunnelled into the nanoribbon. The wave packet already went through the part of the nanoribbon shown in the presentation window. Pronounced edge states [4] are seen and the interference of the eigenstates of the nanoribbon causes different patterns to appear along the C–C bonds.

In conclusion, the 3D wave packed dynamical simulation is a useful tool in predicting the likely behaviour of nanodevices built by joining graphene waveguides. Further calculations are underway for several device configurations.

Acknowledgements

The work was partly supported by the Hungarian OTKA grant nos. 049131 and 049182 and by the Russian Foundation for Basic Research (Grant no. 05-02-17443). GIM and LPB gratefully acknowledge a grant from the Belgian FNRS.

References

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov, Science 306 (2004) 666; M.I. Katsnelson, Mater. Today 10 (2007) 20.
[2] K. Wakabayashi, M. Fujita, H. Ajiki, M. Sigrist, Phys. Rev. B 59 (1999) 8271.
[3] K. Nakada, M. Fujita, G. Dresselhaus, M.S. Dresselhaus, Phys. Rev. B 54 (1996) 17954.
[4] Y. Kobayashi, K. Fukui, T. Enoki, K. Kusakabe, Y. Kaburagi, Phys. Rev. B 71 (2005) 193406.
[5] Y. Son, M.L. Cohen, S.G. Louie, Phys. Rev. Lett. 97 (2006) 216803.
[6] L.A. Chernozatonskii, P.B. Sorokin, E.E. Belova, J. Brüning, A.S. Fedorov, JETP Lett. 85 (2007) 77.
[7] L.A. Chernozatonskii, P.B. Sorokin, J. Brüning, Appl. Phys. Lett., in press.
[8] G.I. Márk, L.P. Biró, Ph. Lambin, Modeling and interpretation of STM images of carbon nanosystems, in: NATO Science Series II: Mathematics, Physics and Chemistry, vol. 57, Kluwer, 2002, p. 43.
[9] B.M. Garraway, K.-A. Suominen, Rep. Prog. Phys. 56 (1995) 365.
[10] G.I. Márk, L.P. Biró, J. Gyulai, Phys. Rev. B 58 (1998) 12645.
[11] G.I. Márk, L.P. Biró, J. Gyulai, P.A. Thiry, A.A. Lucas, Ph. Lambin, Phys. Rev. B 62 (2000) 2797.
[12] G.I. Márk, L.P. Biró, Ph. Lambin, Phys. Rev. B 70 (2004) 115423.
[13] G.I. Márk, L.P. Biró, L. Tapasztó, A. Mayer, Ph. Lambin, Atomic pseudopotential model for wave packet tunneling through a carbon nanotube, in: Electronic Properties of Syntetic Nanostructures, AIP Conference Proceedings, vol. 723, 2004, p. 389.
[14] A. Mayer, Carbon 42 (2004) 2057.
[15] D. Brenner, Phys. Rev. B 42 (1990) 9458.
[16] A. Mayer, Carbon 43 (2005) 717.