About Nanometer Sized Analogues of Basic Electronic and Optical Components

Alexander Quandt, Cem Özdoğan*, Maurizio Ferrari, Giorgio Speranza*****
Institut für Physik der Universität Greifswald, Felix-Hausdorff Str. 6, 17489 Greifswald, Germany
** Department of Computer Engineering, Çankaya University, Balgat, 06530 Ankara, Turkey*
*** CNR-IFN Trento,CSMFO Group, Via Alla Cascata 56/c, 38050 Povo-Trento, Italy*
**** Fondazione Bruno Kessler, Via Sommarive 18, 38050 Povo-Trento, Italy*
Tel: ++49-3834-864772, Fax: ++49-3834-864701 , e-mail: alexander.quandt@physik.uni-greifswald.de

ABSTRACT
We discuss a downsizing of optical components into the nanometer range. It presupposes the substitution of photons by ballistic electrons, but it also requires a simple and robust concept to assemble the analogues of basic electronic and optical components on such a tiny length scale. Here, one of the most promising candidate schemes employs graphene as a basic nanosubstrate. We elucidate the suggested behaviour of graphene as an electronic metamaterial [1], and show that other desired electronic or optical functionalities may be obtained through a patterning with sub-nanometer sized boron clusters [2].
Keywords: nanotechnology, electronic devices, photonic devices, metamaterials, graphene, clusters.

1. INTRODUCTION

Compared to the minuscule sizes of state of the art integrated electronic or magnetic devices, optical components are rather bulky. Of course, it is well known that an optical component, which ought to interact quite strongly with light of a certain wavelength, must dispose of at least one similar physical dimension. But unfortunately, there is only a limited range of optical frequencies available for manageable and affordable optical technologies, where the most promising wavelengths might be located in the near infrared. Therefore the sizes of suitable optical components ought to be in the micrometer range, which is about 10000 times the diameter of a hydrogen atom, and far from *writing small* in the sense of Feynman's legendary proposal [3].

One promising strategy to overcome an anticipated division between electronic and optical technologies, caused by incompatible length scales of their basic devices, is a subwavelength optical approach based on surface plasmons [4-5], called *plasmonics*. Here the interaction of light with the electrons of a metal/dielectric interface leads to the excitation of surface waves with combined electromagnetic and surface charge character, and the plasmonic wavelengths are shorter than the wavelengths of the incident light. Various efforts to manipulate these surface plasmons, in a fashion similar to optical waves, are already under way [4-5]. But a lot of work remains to be done to rejoin optics with a rapidly shrinking electronics by means of an intermediate plasmonic technology. And not just disturb one functionality by the other.

In the following, we will suggest a somewhat different approach, and an extended version of our discussion may be found in [6]. It is well known since the time of De Broglie [7] that electrons are of a similar dual wave-particle nature like photons. Furthermore elementary solid state physics shows that electrons in a solid usually behave like noninteracting pseudoparticles [8], which allows for their linear superposition, analogous to optical waves. Note that those kinds of resonances are also an essential ingredient of our modern picture of the chemical bond [9]. The naive model of electrons being charged bullets bouncing through a solid is the picture of classical transport, where system sizes are much larger than the length scales, over which electrons wave will retain their momentum and phase coherence [10].

Within a reasonably clean nanosystem, however, the system sizes will be much smaller than those length scales, over which the electrons will decohere. Therefore the electronic wave character will dominate, and transport is mostly ballistic [10]. Furthermore, in a collective electron model characterized by Z electrons per atom and marked by a Fermi energy E_F, we can estimate the wave lengths λ_F of electrons at the Fermi level according to the relation [8]:

$$\lambda_F = \frac{2\pi}{k_F} \sim \left(\frac{2}{Z}\right)^{\frac{1}{3}} 2 \cdot 6 r_S \qquad (1)$$

Here r_S is the radius of the Wigner-Seitz sphere, which is about half the interatomic distance within a Bravais lattice [8]. Therefore the electron wavelengths are in the range of interatomic distances, and in principle, suitable small cluster units might be used to manipulate ballistic electronic wave functions, similar to optical components operating on light. Those analogies should at least hold for optical phenomena that may be treated within a scalar wave approach, where the remaining differences between spin-1/2 spinor waves (electrons) and spin-1 vector waves (light) may be neglected. We will elaborate on this idea in the following two sections.

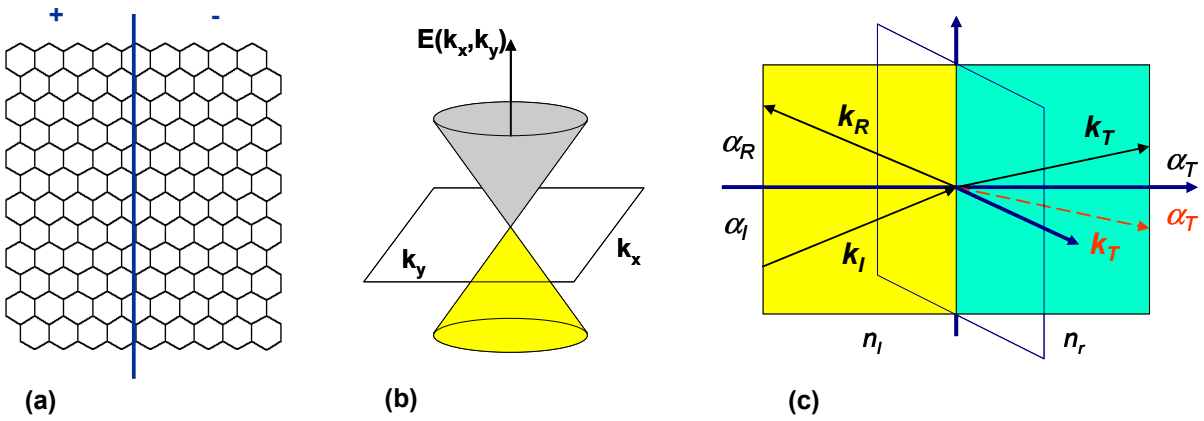

Figure 1. (a) Single sheet of graphene may be turned into interface by applying an external voltage, (b) linear dispersion relation around K point, (c) refraction at an interface between two (dielectric) materials.

2. GRAPHENE AND ELECTRONIC METAMATERIALS

The ultimate goal of extending optical or electronic functionalities into the nanometer range would be the development of a simple and robust scheme to synthesize functional networks of integrated basic components. For electronic functionalities, we would need a semiconducting substrate, whereas for electronic analogues of optical components, we would need a metallic substrate. A basic substrate chameleon that might supply both functionalities are long stripes of carbon called graphene nanoribbons. They may be obtained in a disarmingly simple fashion, for example by thinning out bulk graphite using adhesive tape, until little more than one atom thick flakes of carbon remain attached to that tape [11].

The basic atomic structure of those flakes derives from a two-dimensional honeycomb lattice shown in Fig.°1(a), where carbon atoms are sitting at the corners of the honeycombs. Graphite itself consists of an ABAB-stacking of infinite two-dimensional honeycomb layers called graphene [10]. Therefore carbon nanoribbons may be pictured as large rectangular stripes carved out of graphene. In order to understand their basic electronic properties, we may employ a basic tight-binding model [10], with just one π-electron per atomic site. We then observe that graphene is metallic, and that the conductivity just stems from overlapping bands in the corners of the reciprocal unit cell (the so-called K points). Around these K points, the corresponding electronic energy dispersion relation is mainly linear, which may be approximated by:

$$E(\vec{k}) \approx \pm \nu k \tag{2}$$

where $\vec{k}$ is measured from the corners of the reciprocal unit cell. This is indicated in Fig.°1(b). The Fermi energy E_F is located at a single point separating the yellow cone from its grey counterpart. If we apply a voltage across a graphene monolayer, as indicated in Fig.°1(a), that Fermi level will be shifted upwards and downwards, depending on the sign of the applied field. The applied voltage will thus create an electronic interface [1].

In order to understand the path that an electron will take once it crosses such an interface, we have to briefly recapitulate some features of optical metamaterials. It has been noticed by Veselago some time ago [12], that there is a certain asymmetry in the optical behaviour of materials, as indicated in Fig.°1(c). Light that shines on an interface between two homogeneous materials of refractive index n_l and n_r will be partially reflected, and most likely transmitted along the (black) upper path. What are the preconditions to observe the lower (red) path? We suppose that a general wavefunction at a point $\vec{r}_0$ on the interface may be described in the following fashion:

$$\vec{U}(\vec{r}_0,t) = \begin{cases} \vec{U}_I(\vec{r}_0,t) = \vec{U}_I(t - \dfrac{\vec{e}_I \cdot \vec{r}_0}{v_I}) + \vec{U}_R(t - \dfrac{\vec{e}_R \cdot \vec{r}_0}{v_R}) \\ \vec{U}_r(\vec{r}_0,t) = \vec{U}_T(t - \dfrac{\vec{e}_T \cdot \vec{r}_0}{v_T}) \end{cases} \text{ with phase velocity } v = \frac{\omega}{k}. \tag{3}$$

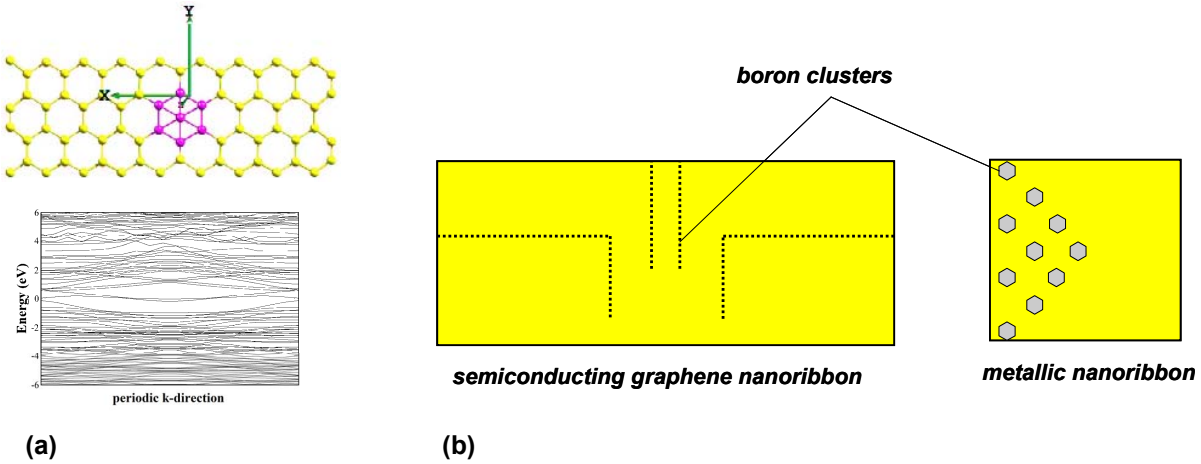

Figure 2. (a) B_7-cluster embedded into graphene nanoribbon opens a conducting channel in a semiconducting substrate, (b) blueprint for graphene-based transistor (left) and analogue of optical diffraction element (right).

If we assume that the arguments of the incident, reflected and transmitted wavefunctions should be the same for all times at all points on the interface (consistency condition), we recover the following relations:

$$\sin\alpha_I = \sin\alpha_R \Leftrightarrow \alpha_I = \alpha_R \text{ (Snell's law), and } \sin\alpha_I = \frac{v_I}{v_T}\sin\alpha_T = \frac{n_r}{n_l}\sin\alpha_T \text{, as } v = \frac{c}{n} \tag{4}$$

Therefore, in order to observe the lower (red) path, which corresponds to a *negative* value of α_T, either n_l or n_r should be negative, which is characteristic of a metamaterial [12].

It must be noted that the vector or scalar nature of the optical wave amplitudes were completely irrelevant in our previous reasoning. Therefore, we may as well try to apply our reasoning to idealized electronic De Broglie waves [1], [6] crossing the electronic graphene interface described above. We only have to take into account, that the angular frequencies ω entering equation°(3) are directly related to the electron energies at the conducting Fermi levels on both sides of the interface, via the de Broglie relation $E = \hbar\omega$ [7]. But those energies, and thus the corresponding frequencies, have different signs according to equation°(1). Therefore, also the corresponding phase velocities in equation°(4) will have different signs, and the electron will take a path similar to the red one indicated in Fig.°1(c). In summary, the electronic interface will act like an optical interface between a metamaterial and a regular material, which is known to re-focus diverging waves [1]. Other peculiarities of these electronic interfaces, and of related optical interfaces, have recently been analyzed in some detail by Pendry [13].

3. FUNCTIONALIZED GRAPHENE NANORIBBONS

Now that we familiarized ourselves with the peculiar electronic nature of graphene, we would like to describe the electronic properties of graphene nanoribbons. It turns out that the electronic properties of graphene nanoribbons or nanoflakes will strongly depend on the nature of their borders. This follows from the tight binding model described above, as well as from advanced *ab initio* band structure calculations, as shown in [2]. Therefore, carbon nanoribbons should be an ideal substrate to host functional nanometer sized networks, made from analogues of microelectronic and optical components.

However, it is not immediately clear how to engrave those basic electronic or optical components into the underlying substrate. But quite obviously, it will be necessary to use another material compatible with carbon. In the last decade, it became clear that boron, which is carbon's immediate neighbour in the periodic table, has a similar potential to from complex nanomaterials. And that boron based nanomaterials have a strong affinity to bind to carbon [14]. Based on such fundamental chemical compatibility, one of the most promising strategies of stamping a certain functionality into the graphene substrate could be the implantation of small boron clusters [6].

At first sight, the end result might look like a speckle pattern of boron islands inside the graphene matrix. *Ab initio* results for a simple model system to describe those embeddings [14] are shown in Fig.°2(a). A model nanoribbon has been chosen, which is periodic (and thus infinite) in the y-direction, and finite in the x-direction. It is marked by so-called armchair borders, and it has just the right width to be semiconducting [14]. The simulations show that the embedding of a model B_7-clusters is quite stable, and that the electronic properties of the underlying substrate will be modified quite dramatically by the implanted boron islands: in the corresponding band structure of Fig.°2(a), conducting channels appear around the Fermi level located at zero.

Quite surprisingly, the boron clusters are not directly connected, as shown in Fig.°2(a). Together with the underlying substrate, they form some kind of dotted lines, which are nevertheless able to conduct electrons. On the left side of Fig.°2(b), we sketched the layout of a basic transistor, whose wiring consists of these dotted lines of boron clusters, and which is supposed to operate on the underlying semiconducting graphene substrate. This layout is several orders of magnitude smaller than any conventional functionalization of graphene using microelectronic wiring.

For a metallic substrate, like graphene nanoribbons with so-called zigzag borders (see [14]), we can infer the same basic stability of the embedding of boron clusters. Furthermore, an electron propagating through such a material will be scattered by boron islands just a few atoms thick, and the sizes of theses islands will be in the range of the wavelength of such an electron, as estimated from equation°(1). On the right part of Fig.°2(b), we sketched a simple analogue of a basic optical component within the nanometer range. If we should somehow be able to directly manipulate the borders of the nanoribbon substrate, and thus succeed in changing its electronic properties, we might even be able to switch between electronic and optical functionalities. Let us focus on the right part of Fig.°2(b): for an underlying metallic substrate, the structure might act like a diffraction element, where scalar electrons that impact from the left will be scattered by the prismatic speckle pattern. But as soon as we switch to a semiconducting substrate, that pattern will just act like some bulky nanowire, which should nevertheless conduct electrons along the vertical direction.

4. CONCLUSIONS

We illustrated a proposal to extend optical and electronic functionalities into the nanometer range: Light will be substituted by ballistic electrons, dielectric or semiconducting substrates will be substituted by graphene, and patterning will be carried out by embedding boron clusters. Such a strategy, or a somewhat similar approach, might offer the possibility to create analogues of standard optical and microelectronic devices within the nanometer range. And it might also offer the possibility to invent novel types of devices, which utilize the particularities of nanosystems [15].

ACKNOWLEDGEMENTS

A.Q. would like to thank the CNR-IFN Trento for their hospitality and support during a sabbatical leave in 2007/2008.

REFERENCES

[1] V.V. Cheianov, V. Fal'ko, B.L. Altshuler: The focusing of electron flow and a Veselago lens in graphene p-n junctions, *Science,* vol. 315 pp. 1252, 2007.
[2] A. Quandt, *et al.*: Functionalizing graphene by embedded boron clusters, *Nanotechnology,* vol. 19 pp. 335707, 2008.
[3] R.P. Feynman: There's plenty of room at the bottom, *J. Microelectromech. Sys*., vol. 1 pp. 60, 1992.
[4] W.L. Barnes, A. Dereux, T.M. Ebbesen: Surface plasmon subwavelength optics*, Nature*, vol. 424 pp. 824, 2003.
[5] S.A. Maier, H.A. Atwater: Plasmonics: Localization and guiding of electromagnetic energy in metal/dielectric structures, *J. Appl. Phys.*, vol. 98 pp. 011101, 2005.
[6] A. Quandt, M. Ferrari: Low Dimensional composite nanomaterials: Theory and applications, *Adv. Sci. and Tech.*, vol. 55 pp.74, 2008.
[7] L.V. De Broglie: Nobel lecture, *in Nobel Lectures in Physics 1922-1941*, Amsterdam: Elsevier, 1965.
[8] J.M. Ziman: *Principles of the theory of solids*, Cambridge: Cambridge University Press, 1972.
[9] L. Pauling: *The nature of the chemical bond*, Ithaca: Cornell University Press, 1960.
[10] R. Saito, G. Dresselhaus, M.S. Dresselhaus: *Physical properties of carbon nanotubes*, London: Imperial College Press, 2004.
[11] K.S. Novoselov, *et al.*: Electric field effect in atomically thin carbon films, *Science*, vol. 306 pp. 666, 2004.
[12] V.G. Veselago: The Electrodynamics of substances with simultaneously negative values of ε and μ, *Soviet Physics Uspekhi*, vol. 10 pp. 509, 1968.
[13] J.B. Pendry: Time reversal and negative refraction, *Science*, vol. 322 pp. 71, 2008.
[14] A. Quandt, I. Boustani: Boron nanotubes, *ChemPhysChem*, vol. 6 pp. 2001, 2006.
[15] G. Fasol: Interference rules the waves, *Nature*, vol. 338 pp.464, 1989.