Transport Properties of Nanostructured Graphene

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***Abstract* - Despite of its many wonderful properties, pristine graphene has one major drawback: it does not have a band gap, which complicates its applications in electronic devices. Many routes have been suggested to overcome this difficulty, such as cutting graphene into nanoribbons, using chemical methods, or making regular nanoperforations, also known antidot lattices. Theoretically, all these ideas lead to a reasonable band gap, but realizing them in the lab is very difficult because all fabrication steps induce disorder or other nonidealities, with potentially disasterous consequences for the intended device operation. In this talk I elaborate these ideas and review the state-of-the-art both from the theoretical and the experimental points of view. I also introduce two new ideas: (1) triangular antidots, and (2) nanobubbles formed in graphene. Both of these nanostructuring methods are predicted to yield novel transport signatures, which could form the basis of new types of devices. Our simulations show that it may be possible to generate very high quality spin- and/or valley polarized currents with these structures – something that has not yet been achieved in the lab. Importantly, our simulations involve millions of atoms which is necessary in order to address structures feasible in the lab.**

I INTRODUCTION

We pose the following question: is it possible to nanostructure graphene in a way that preserves the unique properties of the pristine material, and at the same time adds certain desired new features, such as an energy gap, spin-dependence, or valley sensitivity? There is a plethora of suggestions in the literature of how to achieve this: nanoribbons, perforations, bubbles, adsorbates, or periodic gates have been considered. But etching – which is invariably used as a fabrication step - always introduces damage, and the resulting edges are rarely smooth, which may ruin the otherwise good ideas. The modeler also faces the task of having to include millions of atoms in the simulations, and realistic models of disorder. I will use regular perforations of graphene as a paradigmatic example [1], but many of the considerations will apply to other nanostructuring methods as well.

II GAL – GRAPHENE ANTIDOT LATTICES

An atomically perfect triangular antidot lattice consisting of hexagonal unit cells (with the hexagon edge length of 7 lattice spacings) with circular holes with radius of 3 lattice spacings, gives rise to a band gap of 0.73 eV [1], of the order of magnitude needed in electronic applications. This lattice corresponds to a real-space pitch of a couple of nanometers, well beyond present etching techniques, where state-of-the-art is low tens of nanometers. Even worse, the used etching techniques (e-beam or block co-polymer masks) introduce substantial disorder, and until recently no unequivocal evidence of the GAL introduced band-gap has been observed. The mobility gaps seen in transport experiments are due to the disorder introduced by the fabrication steps. However, very recently it has been realized that using a protective hBN layer encapsulating the graphene layer [2,3], samples of much higher quality can be fabricated, and in magnetoresistance measurements features related to ballistic transport are clearly observed; the observations can be explained quantitatively with state-of-the art simulation tools [4]. We envisage many forthcoming experiments with these structures, since the combined effects of ballistic transport and a periodic potential with nanometer pitch allows one access many interesting experimental regimes.

III DUAL-PROBE MEASUREMENTS

The standard way to characterize nanostructured samples is to use scanning tunneling microscopy (STM), which provides a contactless and nondestructive way of obtaining important information. However, STM yields essentially the density of states (a one-particle Green's function), but the transport properties (which are encoded in a two-particle Green's function) are not accessible. Present technology allows, in fact, to do two-probe measurements, where two STM probes are brought to close vicinity – typically a few

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nanometers apart – and using them as an injector and collector, much valuable information can be extracted. During recent years we have developed a detailed theory of these spectroscopies [5,6], and in the following I discuss two recent applications.

IV TRIANGULAR ANTIDOTS

Consider a triangular antidot, with zig-zag edges. All the edge atoms belong to just one sublattice (recall that the graphene crystalline structure consists of two sublattices), and according to Lieb's theorem, a magnetic moment is formed whose magnitude is given by imbalance between A- and B-atoms. The magnetic moment of a triangular antidot can be used as a building block for many devices, and here we address the possibility to create spin-polarized currents, which are needed in spintronics applications. Consider the schematic device depicted in Fig. 1. A spin un-polarized current of electrons is incident from

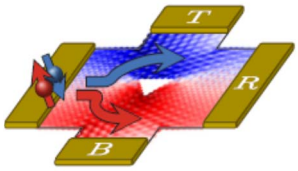

Fig. 1. A schematic of a device with an imbedded triangular antidot with zig-zag edges

left. The spin-up electrons are directed to the contact labeled B, while the spin-down electrons move to T. We have given a detailed explanation of this spin-splitting behavior in Ref.[7]: it is due to combined effects of geometry, and the magnetization profile. The efficency can be enhanced by an array of antidots [7]. Of course, an important question concerns the feasibility of fabrication of near-perfect triangular antidots with zig-zag edges. This has not been realized yet. However, hBN supports regular triangular holes, and these could perhaps be used as etch masks, thereby providing a route to triangular antidots in graphene.

V NANOBUBBLES AS VALLEY FILTERS

The band structure of graphene has two Dirac points located at the K and K'-points of the Brillouin zone. In a doped or gated graphene sheets the electrons reside in the neighborhood of either the K-point, or the K'-point (also called as the K-valley, and the K'-valley), and can be labeled accordingly. There is a strong analogy with the spin: the spin can be up or down – here the electron can either be in K- or K'-valley. The art of manipulating the valley index is called valleytronics, in analogy with spintronics. The literature has many theoretical suggestions of how to realize valleytronics in the lab, but they often involve complicated constructions involving either the spin-orbit interaction (which is intrinsically weak in graphene), or magnetic fields. We have recently realized that bubbles in graphene can achieve the same effect [8]. The physical mechanism is due to the so-called pseudomagnetic field, which occurs in graphene under strain, i.e., under situations where the distances between neighboring carbon atoms is varied, as is the case for a nanobubble. The pseudomagnetic field bends the electrons differently according to which valley they belong to. An example of such a behavior is shown in Fig. 2. The nanobubble is confined in the circle

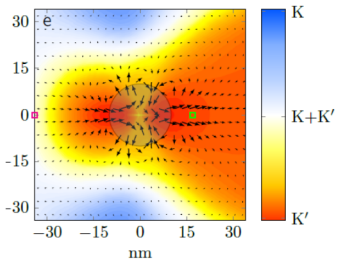

Fig. 2. Valley filtering for a Gaussian deformation of a graphene sheet.

at the center of the figure; white color indicates valley unpolarized electons, while red (blue) colors indicate K'-(K-) polarized electrons. Nanobubbles have been fabricated in the lab in a number of ways, and an experimental verification of our theoretical results appears quite feasible.

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