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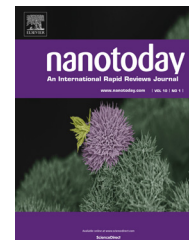
NEWS AND OPINIONS

Can a silicene transistor be realized?

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Summary   In the past decade a new exciting class of materials has been developed, which is not three-dimensional, but only two-dimensional in nature. Graphene is by far the most famous example of this new class of materials. Graphene exhibits a wealth of exotic and intriguing properties, which has resulted in a myriad of scientific breakthroughs. However, graphene also suffers from a severe drawback: it is gapless, implying that a graphene based field-effect transistor is not within reach. Silicene, the silicon analog of graphene, is in many aspects very similar to graphene, but in contrast to the planar graphene lattice, the silicene lattice is slightly buckled and composed of two vertically displaced sub-lattices. By breaking the sub-lattice symmetry a band gap can be opened, which would in principle allow the realization of a silicene field-effect transistor. This piece introduces the various band engineering options for silicene as well as additional hurdles that will need to be overcome before the door can be opened to a silicene transistor.
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Introduction

Modern semiconductor-based electronics is in essence two-dimensional since the functionality of electronic devices is mainly governed by what occurs at the interface of the semiconductor. The manipulation of charge carriers and transport at the semiconductor interface/surface is often far from trivial since we have to use bulk semiconductors for the realization of electronic devices. The usage of semiconductors that are two-dimensional in nature would not only make things much easier, but it would also open the door to exciting new physics and applications. However, the Mermin and Wagner theorem [1] states that a two-dimensional (2D) crystal cannot be stable since it does not exhibit long-range order and therefore the crystal should melt at any, non-zero, temperature. Fortunately, recent detailed and thorough theoretical studies have revealed that these critical fluctuations can be suppressed by an anharmonic coupling between stretching and bending modes [2,3]. This means that a 2D crystal can, in principle, exist at non-zero temperatures, but it should be rippled.

In 2004 Novoselov et al. [4] ignited a revolution in materials science by preparing graphene, a single layer of sp^2 hybridized carbon atoms. The unique electronic structure of this archetypal 2D material has led to numerous exciting and

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breathtaking physical discoveries [4—7]. Despite its exciting properties graphene suffers from a severe drawback: it is gapless making it useless for field-effect applications. Electrons propagating through graphene effectively lose their mass and are described by the Dirac equation rather than the Schrödinger equation. At the *K* points of the surface Brillouin zone the cone-shaped valence and conduction bands (Dirac cones) touch. A bilayer of graphene is gapless too, but in contrast to a single layer graphene the energy bands are parabolic near the *K* points. Many scientists have attempted to realize a band gap in graphene by chemical modification, applying strain or biasing bilayer graphene. The opening of a band gap in graphene by the interaction with a substrate or adsorbed molecules has proven to be ineffective, and band gap opening by chemical modification of graphene seriously degrades its carrier mobility. It has been predicted [8] and experimentally confirmed [9,10] that graphene nanoribbons have a band gap that is inversely proportional to the width of the nanoribbons. However, even the smallest disturbance or roughness of the nanoribbon armchair or zigzag edges severely affects the band gap.

Ten years earlier Takeda and Shiraishi [11] performed quantum mechanical ab initio calculations on planar silicon and germanium structures that have the graphite structure. They found that the lowest energy configuration was obtained if the two atoms of the honeycomb are slightly displaced with respect to each other in a direction normal to the planar structure. Their calculations also revealed that these materials exhibit semi-metallic properties. However, they did not pay any attention to the exact *k*-dependence of the energy dispersion relations in the vicinity of the Fermi level. In a pivotal paper in 2007 Guzmán-Verri and Lew Yan Voon [12] proved, using analytical tight binding calculations, that silicon with the graphite structure has Dirac cones. In addition, they also pointed out that the presence of Dirac cones is robust against the buckling of the silicene lattice. Hence the electrons in flat as well as buckled silicene are described by the Dirac equation and behave as massless particles (Dirac fermions). Guzmán-Verri and Lew Yan Voon called this exciting material 'silicene'.

The structure of silicene is more flexible than that of graphene, because of the absence of strong π-bonds that enforce planarity. It is, therefore, easier to create a band gap in silicene than in graphene. For instance, interactions with a substrate can strongly affect the silicene structure, and open a band gap by breaking the sub-lattice symmetry in the honeycomb lattice. Ideally, in order to realize an on—off current of 10^4—10^7 at room temperature, a band gap of at least 0.4 eV is required. In silicene, various routes to band gap opening and tuning are being explored, including the application of an electric field perpendicular to the silicene sheet [13—15], coupling to a substrate, and chemical [16] or structural modification [18,41,42]. But there are several hurdles that will have to be overcome first: (1) The relevant electronic states of silicene, i.e. the electronic states in the vicinity of the Fermi level, should be decoupled from the underlying substrate. Therefore a wide band gap material is an ideal template for silicene, however to date the vast majority of silicene layers have been grown on metallic substrates. (2) In contrast to graphene, which

is stable under ambient conditions, silicene is expected to oxidize easily. Hence the silicene layer will need to be covered with a capping layer that does not affect the relevant electronic states of silicene.

Structural and electronic properties of silicene

Unlike graphene, silicene does not occur in nature. The tight binding calculations of Guzmán-Verri and Lew Yan Voon [12] of free-standing silicene indicated that electrons in the vicinity of the *K* points of the Brillouin zone should behave as massless Dirac fermions with a Fermi velocity of $\sim 10^5$ m/s. Silicene and silicene nanoribbons have been synthesized on Ag(1 1 0), Ag(1 1 1), ZrB$_2$(0 0 0 1) and Ir(1 1 1) surfaces, and have been characterized with a broad range of surface science techniques, such as scanning tunneling microscopy, photoemission electron spectroscopy and low energy electron diffraction [17—22,28,29,31]. The usage of silicene for electronic device applications is, however, severely limited by the fact that all aforementioned substrates are metallic. Fortunately, theoretical calculations by Cahangirov et al. [23] have revealed that free-standing silicene is metastable, implying that it is in principle possible to transfer silicene onto another substrate.

In order to verify the presence of massless Dirac fermions it is most straightforward to measure the dispersion of the energy bands with for instance photoemission spectroscopy or scanning tunneling spectroscopy. There are, however, a few pitfalls. Firstly, the observation of only a part of the dispersion curve is not always sufficient to discriminate between a linear and a quadratic dispersion relation since parts of a parabolic band can be well approximated by a linear band. Secondly, substrate-related and silicene-related bands are sometimes hard to distinguish (at least in angle-resolved photoemission), since both bands are affected by hybridization.

Another, more conclusive, way to discriminate between a 2D electron gas where the electrons are described by the Schrödinger equation, and a 2D system of massless Dirac fermions where the electrons are described by the Dirac equation, is the energy spectrum of Landau levels. For a conventional 2D electron gas the Landau levels are equidistantly spaced, whereas the Landau levels of a massless Dirac fermion system are proportional to $\sqrt{B_z(n + (1/2) \pm (1/2))}$, where $n = 0, 1, 2, \ldots$ is the quantum number and B_z is the magnetic field. The chirality of the Dirac electrons (the $\pm\frac{1}{2}$ term) is a direct consequence of the symmetry of the crystal. A massless Dirac fermion system exhibits a zero-energy state ($n = 0$ and the minus sign in the equation). The existence of a zero-energy Landau level results in an anomalous quantum Hall effect with half-integer quantization of the Hall conductivity rather than an integer quantization.

Opening of a band gap in silicene via an applied external electric field

As pointed out above silicene has a buckled structure. The silicene honeycomb lattice is composed of two hexagonal sub-lattices that are, in a direction normal to the silicene sheet, slightly displaced by about 0.044 nm [23,24] with respect to each other (see Fig. 1). Silicene has a sizeable