Robustness of topologically protected transport in graphene–boron nitride lateral heterostructures

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Received 9 November 2016, revised 16 November 2016
Accepted for publication 30 November 2016
Published 29 December 2016

Abstract
Previously, graphene nanoribbons set in lateral heterostructures with hexagonal boron nitride were predicted to support topologically protected states at low energy. We investigate how robust the transport properties of these states are against lattice disorder. We find that forms of disorder that do not couple the two valleys of the zigzag graphene nanoribbon do not impact the transport properties at low bias, indicating that these lateral heterostructures are very promising candidates for chip-scale conducting interconnects. Forms of disorder that do couple the two valleys, such as vacancies in the graphene ribbon, or substantial inclusions of armchair edges at the graphene–hexagonal boron nitride interface will negatively affect the transport. However, these forms of disorder are not commonly seen in current experiments.

Keywords: graphene, heterostructures, transport, topological protection

Online supplementary data available from stacks.iop.org/JPhysCM/29/075303/mmedia
(Some figures may appear in colour only in the online journal)

1. Introduction
Attempts to utilise the remarkable electronic properties of monolayer graphene [1, 2] by incorporating it into devices are ongoing [3]. For example, tunnelling field effect transistors [4], photocurrent generators [5], and high frequency transistors [6] have all been demonstrated in the laboratory. However, if graphene devices are to be integrated into circuits with multiple components, it will be highly convenient to have graphene connectors to allow electronic current to move between different devices. Zigzag graphene nanoribbons (ZZGNRs) are known to host metallic edge states, and are attractive candidates for such current-carrying wires. This idea has been investigated previously, but it was found that the transport properties of the ZZGNRs were highly fragile against edge roughness [7–11]. This is a crucial issue, since any growth-based fabrication method for will necessarily introduce lattice scale disorder into the ZZGNRs. Lateral heterostructures are monolayers where two or more 2D materials are ‘stitched’ together to form 1D interfaces. It is possible to grow lateral heterostructures of graphene and insulating hexagonal boron nitride (hBN) [12–18], and much theoretical work, especially using ab initio methods, has been done to investigate their electronic properties [19–23]. However, the topological properties of these lateral heterostructures has received only very limited attention [24]. Jung et al suggested that by engineering hBN ‘cladding’ on either side of the ZZGNR, then the topological properties of the combined system can ensure that there are always conducting channels in the graphene [24]. This topological protection is akin to the Jackiw–Rebbi states that are predicted to exist at mass-inversion boundaries in hexagonal crystals [25], and is described by a valley Chern number [24, 26].

The atomic-scale precision required to produce these lateral heterostructures does currently exist [17, 18], but the graphene-hBN interfaces defined by such techniques are
still rather disordered. This issue is crucial in the context of
topological protection because, as explained in [24, 26] the
topological protection described by the valley Chern number
only persists as long as the two valleys in the graphene are
not coupled to each other. However, the edge roughness may
constitute short-range disorder that is strong enough to scatter
electrons between the two valleys, breaking the topological
protection, and allowing backscattering which reduces the
conductance.

In this manuscript, we present a full analysis of the role
of atomic-scale disorder on the transport properties of
ZZGNR-hBN lateral heterostructures. We find that only
certain types of lattice disorder break the topological pro-
tection and couple the valleys, allowing the backscattering.
Specifically, inclusion of substantial regions of armchair inter-
face and graphene vacancies will do this, but rough edges and
inclusions of random boron or nitrogen atoms in the graphene
ribbon will not. We contend that the explanation for this is
that the latter types of disorder are smooth enough in the sense
that they can be reached from the original Hamiltonian by an
adiabatic transformation, and therefore they do not modify the
overall topological properties of the system and hence do not
couple the valleys. This is a surprising result, since atomic
substitutions typically allow large momentum scattering
by virtue of the short associated length scale. This analysis,
combined with recent advances in fabrication techniques, reo-
opens the issue of ZZGNRs clad with hBN as a highly suitable
method of providing chip-scale conducting channels.

2. Methods
To demonstrate the robustness of the predicted low bias trans-
port channel, we compute the 1D charge conductance using the
Landauer–Buttiker scattering formalism within the Kwant
package [27]. We use a ZZGNR with width 5.0 nm and length
10.0 nm, corresponding to chip-scale dimensions, and we take
the hBN width to be 3.0 nm, which is wide enough to ensure
the topological properties are manifested whilst still being
small enough to ensure reasonable computation time. This
configuration is shown in figure 1(a). To compute the spectrum
and wave functions in the leads and in the scattering region,
we use a nearest-neighbour tight binding model. The tight
binding parameterisation requires the onsite energies $U_i$
for each chemical species, and the hopping elements $t_{ij}$ between
them, where $i,j \in \{C,B,N\}$ denote the chemical species.
Throughout, we use $U_C = 0$, $U_B = 3.6$ eV, $U_N = -1.0$ eV,
$t_{CC} = 2.7$ eV, $t_{CB} = 2.1$ eV, $t_{CN} = 2.3$ eV, and $t_{BN} = 2.5$ eV
[21]. We stress that so long as $\text{sign}(U_C) = \text{sign}(U_B)$, the
precise values of the tight binding parameters do not make any
difference to the overall topological properties of the system,
and merely give small quantitative changes to the band struc-
ture and hence the exact positions of the conductance steps.

In principle, a more accurate description of the band
structure of the ribbons is given by a third-nearest neighbour
tight binding theory [28, 29], but this additional complexity
changes none of the qualitative features of the results, or the
considerations about the topology of the system. Therefore,
we restrict our discussion to the nearest neighbour model
for clarity. In the supplementary material (stacks.iop.org/
JPhysCM/29/075303/mmedia), we show data which justifies
this assumption further.

To create randomly disordered ribbons, we keep track of
the two boundaries between the ZZGNR and the hBN. For
each lattice unit cell along the length of the wire, we allow
the $y$ coordinate of the boundaries to change relative to the
previous unit cell $y'_i = y_{i-1} + \delta y$ where $\delta y = 2 \tan \theta_i$ and $\theta$
is the lattice constant. The deflection angle $\theta_i$ is a random vari-
able characterised by a Gaussian distribution with variance $\theta$
so that higher values of $\theta$ correspond to a higher propensity
towards rough edges.

3. Results and discussion
Figure 1(a) shows the non-disordered ZZGNR with hBN clad-
ing that forms the basis of the ribbons we consider in this
manuscript. In the ‘same’ topology configuration, sketched in
figure 1(b), the $\alpha$ and $\beta$ sublattices of the two regions of hBN
cladding have the same chemical orientation. (Throughout,
we use the notation $\alpha$ and $\beta$ for the two sublattices of the
hexagonal crystal to avoid confusion between the ‘B’ sublat-
tice and the chemical symbol for boron atoms.) In this case,
there are no topologically protected states in the graphene
because the mass gap generated in the hBN has the same sign
in both hBN regions and hence there is no difference in the
valley Chern number across the system. However, when the
chemical orientation is ‘opposite’, sketched in figures 1(a) and
(c), the mass term has opposite sign in the two hBN regions,
and therefore their valley Chern number is different. The
bulk-boundary correspondence then ensures that there are
topologically protected states in the graphene, which forms
an extended boundary between the two topologically distinct
regions of hBN [24].

The band structures and conductance of the ZZGNR are
shown in figures 1(d) and (e), respectively, where the blue lines
correspond to the ZZGNR with no cladding and the black lines
are for cladding in the ‘opposite’ topology configuration with
nitrogen termination. These are fully consistent with the results
of [24]. The units on the vertical axis are $2e^2/h$ to account for
the spin degeneracy of each of the bands. We see that the cladding
causes the flat band edge states to be removed and instead there
are dispersing modes at zero energy. These are the topologi-
cally protected Jackiw–Rebbi-like modes, and they manifest
in the conductance by a finite minimum conductance plateau
$-0.35$ eV $< E < 0.35$ eV. This is the feature that we are most
interested in, since it defines the conducting channel that may
be used to direct current between different graphene devices
on a chip. The sharp increase in the conductance at roughly
$E = -1$ eV is caused by conduction through modes located
mainly on the nitrogen atoms which can be seen in the band
structure in figure 1(d). Modes located mainly on the boron
atoms are located at approximately $E = 3.6$ eV and so do not
appear in the conductance plot. The presence of the cladding
also slightly reduces the gap between the first non-topologically
protected modes in the conduction and valence bands.
Our central result is shown in figure 2, where we plot the conductance of ZZGNRs with random edge disorder and hBN cladding. Figure 2(a) shows a typical example ribbon with $\theta = 15^\circ$, and we stress that the shape of the upper and lower boundaries are independent of each other. For each value of $\theta$ we compute the conductance of 200 ribbons with random disorder, calculate the mean conductance at each value of energy, and show the result in figure 2(b). For even high values of edge roughness, on average, the finite minimum conductance at low energy remains intact, indicating that the topologically protected modes in the graphene are resilient against edge disorder. The reduction in the conductance at higher energy (i.e. away from the finite minimum conductance plateau) is caused by backscattering in the non-topologically protected states as would be expected in ZZGNRs without hBN cladding [9]. To confirm the effect of the cladding, the red dotted line shows the averaged conductance for the exact same 200 ZZGNRs with $\theta = 5^\circ$ but with the hBN cladding removed, and therefore with no topological protection. In this case, the finite minimum conductance plateau at low energy is completely absent. In figure 2(c) we show the fifth percentile conductance at each energy, i.e. the level at which 190 of the 200 disorder realisations have better conductance than the line shown. This shows that for the vast majority of randomly disordered ZZGNRs, the finite minimum conductance plateau remains intact. The narrow dip in conductance at $E \approx -0.3$ eV for some ribbons is caused by small boron impingements into the ZZGNR (see below).

We now examine some more controlled forms of disorder to determine which contribute to the breakdown of the topological protection. Figure 3 shows the calculated conductance for carbon vacancies and boron substitution in the ZZGNR. In principle, since this type of disorder has the shortest associated length scale, it should scatter electrons between states separated by a momentum of the order of the Brillouin zone size, and therefore couple the $K$ and $K'$ valleys the most strongly, leading to breakdown of the topological protection of the low energy modes. In figure 3(b), we show the conductance of our standard ZZGNR with a single carbon atom removed from the $\beta$ sublattice of a unit cell near the lower edge. The location of the vacancies are shown in panel (a), where the colour of the dot corresponds to the colour of the line in the conductance plot. If it is removed from the first unit cell (blue line), then a sharp decrease in the conductance at the top of the low energy finite conductance plateau is seen. As the vacancy is moved into the ZZGNR (red, green, and orange lines) the position of the resonance moves towards zero energy. When the vacancy is in the center of the ZZGNR (black line), the conductance

Figure 1. (a) The non-disordered ZZGNR with hBN cladding. Atomic sites are colour-coded as follows. Carbon: blue; nitrogen: red; boron: green. (b) Sketch of the ‘same’ topology configuration. Notice that the $\alpha$ site both above and below the ZZGNR hosts a boron atom. (c) Sketch of the ‘opposite’ topology configuration. In this case, the $\alpha$ site below the ZZGNR hosts a boron atom, while above the ZZGNR, the $\alpha$ site hosts a nitrogen atom. (d) Band structures of non-disordered 5nm ZZGNR without (blue) and with (black) hBN cladding. (e) Conductance of non-disordered 5nm ZZGNR without (blue) and with (black) hBN cladding.

Figure 2. (a) Typical disordered wire with $\theta = 15^\circ$. (b) Averaged conductance, and (c) fifth percentile conductance of 200 disordered wire realisations.
The mirror symmetry of the opposite topology configuration insists that vacancies on the \( \alpha \) sublattice at the upper edge have their conductance dip at the same energy. Swapping either the sublattice or the edge makes the sign of the energy at which the conductance dip occurs change.

In contrast, figure 3(c) shows that substitution of a carbon atom with a boron atom has very little effect on the conductance. We have verified that nitrogen substitution gives even smaller changes to the conductance. This explains the small dip in the conductance in figure 2 at the low energy side of the finite minimum conductance plateau, since mild edge roughness is replicated by many boron or nitrogen substitutions.

In figure 4 we demonstrate the crucial difference between zigzag and armchair protrusions of hBN into the ZZGNR. It is well known that armchair edges strongly couple the two valleys, since the projection of the 2D Brillouin zone of bulk graphene onto the 1D Brillouin zone of a ribbon in the armchair direction projects the \( K \) and \( K' \) valleys to the same point. In contrast, the zigzag ribbon projects the \( K \) and \( K' \) valleys to different points in the 1D Brillouin zone and so the two valleys are not strongly coupled (see the supplementary material). Figures 4(a) and (b) show a triangular protrusion of hBN into the ZZGNR with width \( R \) with zigzag and armchair edges, respectively. Figure 4(c) shows the calculated conductance for the zigzag protrusion up to \( R = 4 \) nm (i.e. 80% of the ZZGNR width). The finite conductance minimum associated with the topological states is perfectly intact for all zigzag protrusions, indicating that there is no backscattering induced in this case. However, backscattering is induced in the high energy non-topologically protected states by the zigzag protrusion. Figure 4(d) shows the equivalent data for armchair protrusions. In this case, the valley coupling manifests as substantial and apparently uncontrolled oscillations in the conductance as a function of energy in the finite minimum conductance plateau. This indicates that substantial inclusions of armchair edges in the ZZGNR lead to sub-optimal low energy transport properties.

4. Conclusions

We have shown highly promising results for the use of hBN-clad ZZGNRs as chip-scale interconnects with perfect ballistic conductance. In particular, we have systematically investigated the impact of lattice disorder of various types on the transport properties of such ZZGNRs. Our conclusion is that only atomic-scale disorder which strongly couples the
$K$ and $K'$ valley of the bulk graphene—thus invalidating the Valley Chern number construction and lifting the topological protection of the low energy modes—is effective at inducing backscattering between the topological states and weakening the transport. Other types of disorder, such as edge roughness and chemical substitution, do not impact the transport. This is because, at least within a tight binding model, atomic substitution amounts only to changing the onsite energy and hopping elements by a finite amount. This is a only a small change in the theory from the ‘clean’ case, or, in the language of topology, it is an adiabatic transformation and hence retains the same topological properties. This is a very encouraging result, since zigzag interfaces are energetically favourable to armchair interfaces, and have been shown to dominate in fabrication by a ratio of better than 3:1 [17], and carbon vacancies are very rare [18]. However, devices do exhibit substantial edge roughness. Therefore, topologically protected transport may be expected in such devices even with contemporary growth techniques.

One issue that has so far not been addressed is that of the 1.8% lattice mismatch between graphene and hBN. However, the results presented here are enough to justify that this should not present a problem for short interconnects. For ZZGNRs which are less than approximately 50 unit cells in length (NB, the one we have modelled here is 40 unit cells long), the strain buildup in the hBN due to the mismatch should result only in a few rows of BN lattice sites and the first few rows of carbon lattice sites. However, our results indicate that small modifications in the hopping parameters do not result in changes in the topological properties of the system and hence there should be no impact on the topologically protected transport channels. For longer wires, we have explicitly calculated the conductance with a missing nitrogen atom at the edge (see supplementary material), and found that there was no impact on the topological modes in the graphene because there is essentially no wave function weight in the hBN for energies $U_R < E < U_B$. Hence, the strain induced by the lattice mismatch for chip-scale ZZGNRs should have minimal impact on the transport properties.

Acknowledgments

This work is supported by Nordita and by ERC project DM-321031.

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