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Tight-binding calculation of conductance and magnetoresistance in disordered FM/graphene/FM junctions

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1. Introduction

Graphene is a two dimensional honeycomb lattice made of carbon atoms. Although the carbon is the well known element, the graphene is a novel material which attracts much interest recently because of its characteristic features [1, 2]. The graphene is a gapless semiconductor, and electrons in the graphene behave as massless Dirac fermions. The massless electrons give rise to distinguished features of electrical transport properties, such as the quantum spin Hall effect, from those in conventional metals and semiconductors. Furthermore, the graphene is expected to be an alternative to silicon in the contemporary electronics, because of its high mobility, long spin diffusion length [3] and planer structure. When two electrodes attached to the graphene are ferromagnets (FMs), the junction works as a spin field effect transistor. Recently, a magnetoresistance effect has also been observed in a non-local measurement [4, 5].

So far we have calculated the conductance and magnetoresistance (MR) of grapheme junctions with ferromagnetic electrodes [6, 7]. In the former study, we have ignored effects of disorder on the conductance and MR. However, various types of disorder may exist in realistic functions. In order to clarify the role of disorder on the conductance and MR, it is necessary to perform real space simulations for finite size graphene junctions. We will report features of conductance and MR in graphene junctions 1) with a finite width of graphene, 2) with disorder effects in the graphene, and 3) with finite contact width between graphene and electrodes.

2. Model and method of calculation

We assume that the structure of electrodes is a square lattice, and that the graphene is connected to the electrodes at the zigzag edge as shown in figure 1. We use a tight-binding model including *s*-orbital for electrodes with the square lattice, *s*- and *p*-orbitals with the graphene nanoribbon. The conductance is calculated by using the linear response theory (Kubo formalism) and the recursive Green's function method. Values of the band parameters are taken from textbook [8]. The length of graphene sheet (L) is 1~1000 chains. The graphene sheet is in contact with the electrode at only the zigzag edge. Effects of disorder are included by adding δ-function type potentials v randomly on carbon sites. The values of $|v|$ are dependent on orbitals, and are taken to be 4.98 eV and 2.33 eV for *s* and *p* orbitals, respectively. In order to fix the position of the Fermi level, we introduce the same amount of impurities with positive and negative values of v, which may correspond to boron and nitrogen impurities, respectively.

3. Calculated results

We present in figure 2 the conductance calculated for graphene junctions with finite width W. Dashed curves are results without disorder for W = 100, 101 and 102, and results with standard deviation are those with disorder. The standard deviation has been determined by taking an average over finite number of samples with various distribution of the impurity potential. The conductance of a junction without disorder with W = 100 tends a constant value with increasing L, while those for W = 101 and 102 decrease rapidly with L. Generally, there exists a kind of three-fold periodicity.

We may interpret the results using the conductance calculated for junctions with infinite width including no disorder. In a graphene with infinite size, two Dirac points (K and K' points in the Brillouin zone) contribute to the electric current. Without disorder, the momentum $k_{||}$ parallel to the junction plane is conserved, and the conductance can be resolved in terms of $k_{||}$. In the $k_{||}$ resolved conductance $\Gamma(k_{||})$, $\Gamma(k_{||})$ is e^2/h only at K' point

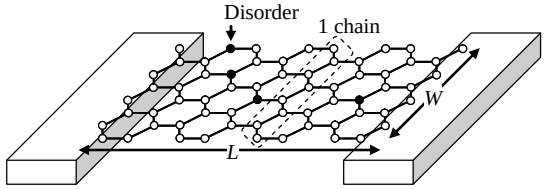

Fig. 1 Structure of graphene junction with the zigzag edge contacts.

and decreases exponentially with $k_{\|} - K'$. When the number of $k_{\|}$ is insufficient, K' point is not always included in $k_{\|}$ points. We find that a three-fold periodicity appears in the conductance with increasing number of $k_{\|}$ points N, that is, one out of three, the conduction channel hits the Dirac points, and the conductance becomes finite for large value of L. In other words, since $k_{\|} = 2\pi n/N$ and $K' = 2\pi/3$, one of many $k_{\|}$ points hits the K' point when $n = N/3$. Therefore, with increasing N, a $k_{\|}$ point hits the K' point when $N = 3\delta$, where δ is an integer number. The three-fold periodicity in graphene junctions with finite width may be interpreted in a similar way.

When a disorder is included in the graphene sheet by introducing impurities for example, the conductance becomes larger than that without disorder for $W = 100$ as shown in figure 2. This is attributed to a fact that the conservation of $k_{\|}$ needs not to be satisfied anymore, and as a result the number of the conduction channels increases effectively. The result is consistent with that reported before [2].

Because the electrical conduction in the junction without disorder is realized through states near the K' point, matching or mismatching of the conduction channel between the electrodes and the graphene is crucial for both the conductance and MR. On the other hand, in the junctions with disorder, the momentum $k_{\|}$ need not be conserved, and the matching of the conduction channel will be less important. Here we study the role of disorder on the conductance and MR for junctions with finite width using a simple model. These features can be understood from the electronic structure of the graphene ribbon. The details will be reported in the presentation.

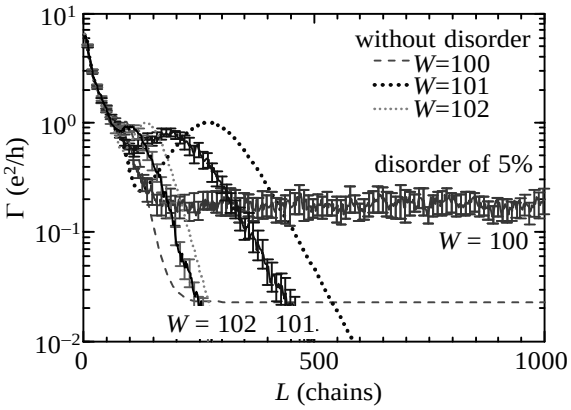

Fig. 2 Conductance for square lattice/graphene/ square lattice junctions.

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