Extended Abstracts of the 2018 International Conference on Solid State Devices and Materials, Tokyo, 2018, pp715-716

Contact Resistivities at Graphene/MoS_2 Lateral Heterojunctions

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Abstract

The ballistic transport properties of 2D graphene/MoS_2 lateral heterojunctions are theoretically investigated, using first-principles simulations based on density functional theory. The computed contact resistivities are shown to be correlated to the interface barrier heights, which are sensitive to the presence of dipole layers (e.g. polar C-Mo bonds) or interface defects (like sulfur dangling bonds) at the interface. The contact resistivities of ideal (defect-free) graphene/MoS_2 interfaces are predicted to lie in the range 2-5x10^{-9} Ω cm^2. Such low contact resistivities are promising for performant 2D-based field effect devices.

1. Introduction

Two dimensional materials like graphene and transition metal dichalcogenides are currently triggering a lot of interest, due to their promising applications in future nanoelectronic applications, like logic, photonic, and spintronic devices [1-3]. However, one important issue for these applications is the high contact resistance at metal/2D semiconductor interfaces [4], typically in the range of 10^3-10^5 Ω μm.

Lateral graphene/MoS_2 interfaces have been fabricated recently [5-7] and also studied theoretically [8,9]. These interfaces provide a promising platform for realizing low contact resistance between 2D metal (graphene) and 2D semiconductors (like 2H-MoS_2), being of potential interest for 2D-based devices.

In this work, we have theoretically studied the contact resistivity ρ_c of graphene/MoS_2 (2H) lateral heterostructures, using density functional theory (DFT). Different interface models have been considered, based on the type of edge contact (armchair or zigzag). Low contact resistivities, in the range of few 10^{-9} Ω cm^2, are predicted at ideal (defect-free) graphene/MoS_2 interfaces. The presence of sulfur dangling bonds at the interface results in an increase of the interface barrier height (due to the Fermi level pinning), leading to an increase of ρ_c by about two orders of magnitudes.

2. Computational details

The ballistic current-voltage characteristics of lateral graphene/MoS_2 interfaces are computed using the non-equilibrium Green's function method, as implemented in the TranSiesta DFT simulation package [10]. The generalized gradient approximation [11] is used for the exchange-correlation functional. The valence electrons are described by single-zeta basis sets, and the core electrons are described by norm-conserving pseudopotentials [12].

Four different graphene/MoS_2 lateral heterostructures are considered. Large supercells are employed (containing about 250 atoms), in order to minimize the strain in the graphene and MoS_2 layers, as a result of their lattice mismatch; the residual strain is typically below 1.5% in both layers.

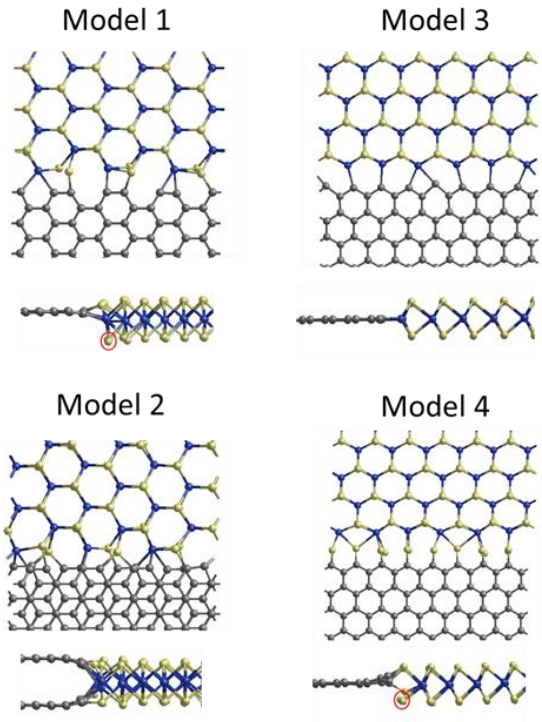

Fig.1. Relaxed lateral graphene/MoS_2 heterostructures considered in this work. The S dangling bonds present in model 1 and model 4 are encircled in red.

3. Results and discussion

The relaxed graphene/MoS_2 interface models are shown in Fig.1. Model 1 is based on an armchair-edge contact, with a single graphene layer. Both C-Mo and C-S bonds are

formed at the interface, and S dangling bonds (from the bottom sulfur layer) are also present. In model 2, a graphene bilayer is used, which enables to saturate all the S dangling bonds of the armchair edge MoS_2 layer, by forming C-S bonds. Model 3 is based on a zigzag-edge contact, terminated by Mo atoms. After relaxation, only C-Mo bonds are formed, and the interface is "defect free". Model 4 is based on a S-terminated zigzag edge contact. In this case, only C-S bonds are formed, but S dangling bonds are present in the bottom S layer.

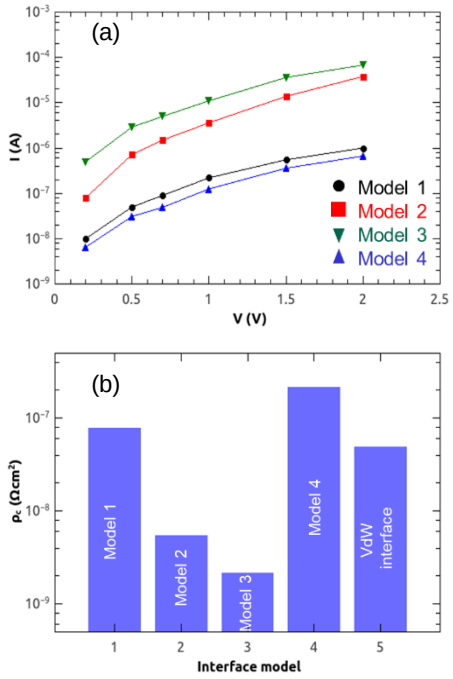

Fig.2. (a) Computed ballistic current-voltage characteristics of the four interface models presented in Fig. 1. (b) Contact resistivities at 0.5 V, extracted from the I-V curves shown in (a). The contact resistivity of a van der Waals graphene/MoS_2 interface is also shown for comparison.

The computed ballistic current-voltage characteristics of the different interface models are compared in Fig.2 (a), and the corresponding contact resistivities ρ_c, extracted at 0.5 V, are shown in Fig. 2(b). The contact resistivity for the "defect-free" interface models (model 2 and 3) are typically lying between 2 and $5x10^{-9}$ Ω cm^2, corresponding to a contact resistance of about 200-500 Ω μm, being close to target values for nanoscale MOSFETs (about 100 Ω μm) [4]. On the other hand, the contact resistivity is about 2 orders of magnitude larger at graphene/MoS_2 interfaces with S dangling bonds.

The contact resistance is correlated to the barrier height Φ_B at the graphene/MoS_2 interface, as shown in Fig.3; the barrier heights were computed from the electrostatic potential profiles along the graphene/MoS_2 slab models. In the case of model 2 and model 3, these barriers are typically 0.1-0.2 eV, and are close to the difference between the graphene work-function (4.4 eV) and the MoS_2 electron affinity (4.2 eV); it is slightly smaller at the Mo-terminated zigzag interface, due to the presence of a large density of polar C-Mo bonds, forming a dipole layer at the interface. On the other hand, Φ_B is increased by about 0.2 to 0.3 eV when S dangling bonds are present at the interface. In this case, the Fermi level is pinned at the charge neutrality level of these defects, which lies at about 0.5 eV below the MoS_2 conduction band edge. The presence of these defects is thus detrimental for the contact resistivity of lateral heterostructures.

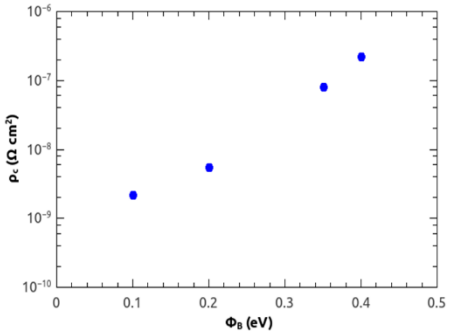

Fig.3. Contact resistivity as a function of the barrier height at lateral graphene/MoS_2 interfaces.

4. Conclusions

The ballistic transport properties and contact resistivities of several graphene/MoS_2 lateral heterostructures have been computed from first-principles simulations. Defect-free interfaces, as obtained from armchair edge bilayer graphene/MoS_2 contacts or Mo-terminated zigzag contacts, are predicted to have low contact resistivities, in the range of few 10^{-9} Ω cm^2. Such contact resistivities are promising for performant 2D-based field-effect devices. However, defects like S dangling bonds, present at armchair single layer graphene/MoS_2 contacts or S terminated zigzag edge contacts, have a detrimental impact on the contact resistivity, which is increased by about two orders of magnitudes at these interfaces.

Acknowledgements

Part of this work has been financially supported by the 2DFun project, an ERA-NET project in the framework of the Graphene Flagship, as well as by the KU Leuven Research Funds, project C14/17/080.

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