Atomic-scale model for the contact resistance of a nickel-graphene interface

Anders Blom, Kurt Stokbro, Mads Engelund

QuantumWise A/S, Lersø Parkallé 107, 2100 Copenhagen, Denmark
anders.blom@quantumwise.com

A question of great importance for the possible use of graphene in integrated circuits is the magnitude of the contact resistance between graphene and metal electrodes, since a high contact resistance would limit the performance of field-effect transistors [1]. Several experimental studies have investigated the topic, but there is no clear consensus on the value or the dependence of the contact resistance on contact area, temperature and applied gate potential. There is therefore a need for complementary theoretical studies which can give insight about the physical mechanisms at play at the metal-graphene interface.

Earlier first-principles calculations have focused on charge transfer between the metal and the graphene [2–5], but in this paper we aim to add new knowledge to the understanding of the graphene-metal contact by investigating the effect of covalent bond formation on the contact resistance. Graphene forms a strong covalent bond with nickel [2] which is similar to the bond formation between graphene and cobalt, palladium and titanium, thus, the theoretical predictions will also be relevant for these systems.

We will present quantum transport calculations of electron transfer from a free suspended graphene sheet to a nickel contact through different metal-graphene contact geometries, where we vary the orientation of the graphene and the contact area. We find that the contact resistance is independent of the orientation of the graphene, as well as of the contact area to the metal, in qualitative agreement with recent experimental observations [6].

Our calculations [7] show that indeed the low-field contact resistance is independent of the contact area, as well as of the direction of the graphene sheet. The edge contact resistance is about 30 Ωμm, corresponding to twice the ideal quantum contact resistance of pure graphene. We predict that this observation is generic for strongly bonded graphene, since we also see the same resistance when using a model contact between graphene and a hydrogen crystal or two overlapping graphene sheets.

We suggest that our obtained contact resistance is the theoretical limit for an ideal bond between nickel and graphene. This value is still rather far from experimentally observed values, which indicates that the experiments do not deal with ideal contacts – impurities and defects are in all likelihood important factors to consider. But our calculations do suggest that, however formidable the problems in forming a good contact are, the challenge is still practical rather than fundamental.

References

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Figures

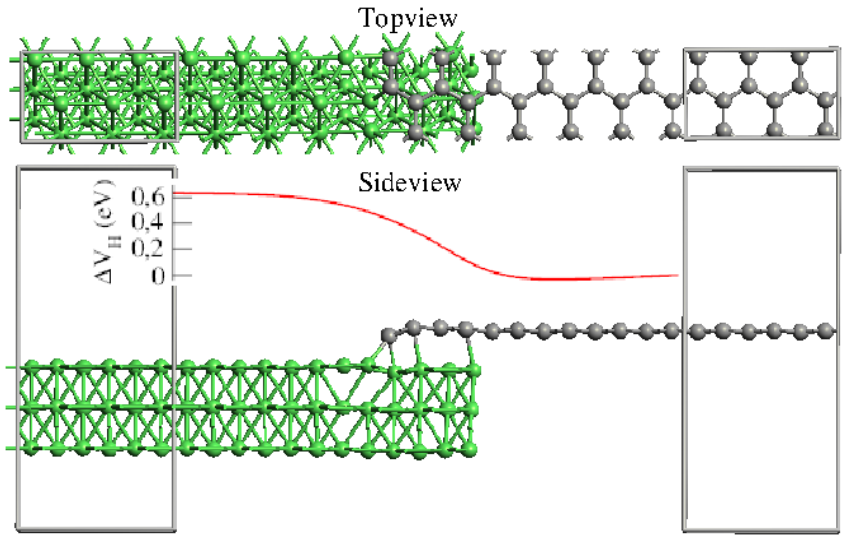

Fig 1. Top view (B-C plane) and side view (A-A-C plane) of one the systems investigated in this paper, viz. a zigzag edge graphene on top of a Ni(100) surface with 4 Å binding overlap. The transport direction is along the C direction. The red curve shows the average electrostatic potential in the vacuum region.

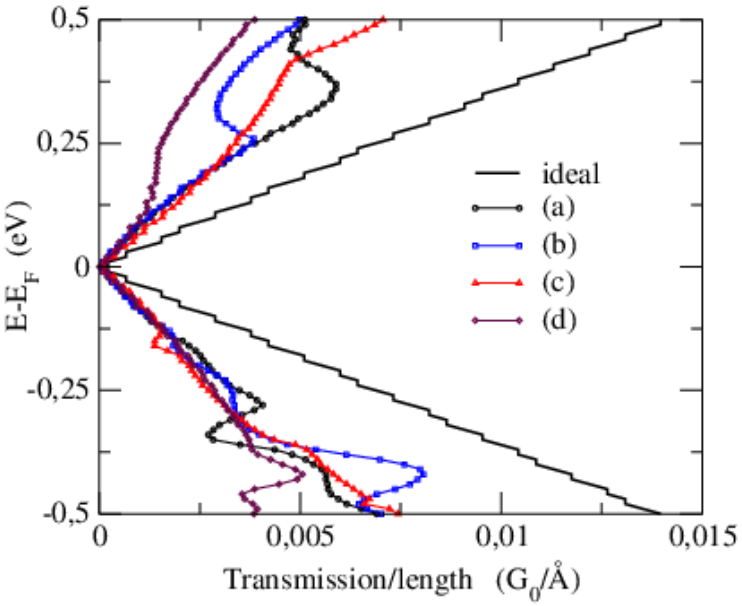

Fig 2. Transmission coefficient per transverse line segment at zero bias for the four different systems studied (the geometry of Fig. 1 is (a) here). Also shown is the transmission coefficient of an ideal graphene sheet.