Multiscale modeling of graphene-metal contacts

T. Cusati, G. Fiori, A. Fortunelli*, **G. Iannaccone**
Dipartimento di Ingegneria dell'Informazione Università di Pisa, Via Caruso 16, 56122 Pisa, Italy
*CNR Institute for Chemical and Physical Processes, Via G. Moruzzi, 1 - 56124 Pisa, Italy
e-mail: g.iannaccone@unipi.it

ABSTRACT

The quality of contacts between metals and two-dimensional materials is a critical aspect for the performance of transistors based on two-dimensional materials. In this talk we focus on an approach to multiscale modeling of graphene-metal contacts, considering both chemisorbed and physisorbed materials. We show that it is possible to use density functional simulations of contacts to extract a set of physical properties that enable accurate device-level simulations at a higher level of abstraction. We also show that – properly evaluated - the *intrinsic* conductance of graphene-metal contacts is higher than that predicted in previous studies.

INTRODUCTION

One of the most important challenges related to the use of two-dimensional materials in electronic and optoelectronic devices is to understand and control the contact between metal and 2D materials. For example, a low contact resistance between graphene and metal electrodes is required for obtaining high performance in graphene devices, as it directly impacts the f_{MAX} for analog applications and the propagation delays of digital gates. The transport properties of the graphene-metal interface have experimentally been investigated through transfer length and four-probe methods, in order to measure the contact resistance (R_c) between graphene and different metals (i.e. Cr, Ti, Cu, Au, Ni, Pd and Pt). Unfortunately, graphene contact fabrication technology is not mature and fully reproducible, and therefore a broad range of experimental values of R_c is obtained even for the same metal [1-5]. Indeed, the contact resistance is highly dependent on several factors including metal work function, number of graphene layers, deposition temperature, process. A systematic study of the electrical characteristics of metal-graphene contacts is highly desirable. From this perspective, a theoretical study of the achievable R_c would provide physical insights on the metal-graphene interface.

APPROACH

We have performed ab-initio calculations with Quantum Espresso of the structures shown in Fig. 1, using a plane wave basis set and a gradient-corrected exchange-correlation functional (Perdew-Burke-Ernzerhof (PBE)). We have considered four different metals (Ni, Cu, Pt, Pd) divided in two categories, based on the binding energy and the metal-graphene distance: chemisorbed metals (Ni and Pd), with stronger bonds and physisorbed metals (Cu and Pt), that lead to weaker bonding (Fig. 2).

We have then computed the transmission coefficient via the solution of the scattering problem considering incoming and outgoing Bloch states as implemented in the PWCOND module of Quantum Espresso (Fig. 3). Finally, we have extracted for each contact the interface transmission coefficient and the relative position of the Dirac point at the interface with respect to the electrochemical potential. This information can be used to accurately describe the contact at a higher level of abstraction (Fig. 4). At the device level, using the Landauer-Buttiker linear response formalism, we have computed the contact conductance *G* at room temperature.

CONCLUSIONS

We have developed a multiscale procedure for taking into account the essential physics of graphene-metal contacts in device simulation. We show that according to our model the intrinsic conductance of contacts is higher than that extracted with previous measurements and simulations (compare table 1), because the latter typically include also the effect of surrounding partially depleted graphene, which can be optimized with doping or contacts. Further investigation on Pd-graphene is needed.

ISBN 978-0-692-50554-0

ACKNOWLEDGMENT

Authors would like to acknowledge support from the EC 7FP through the Projects GRADE (Contract 317839), GONEXTs (Contract 309201), Graphene Flagship (Contract 614391), and from Quantavis s.r.l.

REFERENCES

[1] Z. Chen, J. Appenzeller, VLSI Symp. Tech. Dig. 13, 128 (2009).
[2] E.J.Lee et al., Nat. Nanotechnology, 3, 486 (2008)
[3] W. S. Leong et al., Nano Lett. 8, 994 (2014)
[4] J. Maassen et al., Appl. Phys. Lett. 97, 142105, (2010).
[5] K. Stokbro, et al, Phys. Rev. B, 85, 165442 (2012)
[6] X. Ji et al., Phys. Chem. Chem. Phys. 15, 17883, (2013).
[7] E. Watanabe et al., Diamonds & Related Materials. 24, 171, (2012).

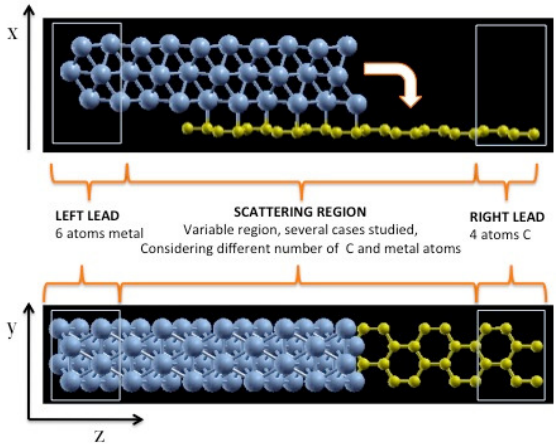

Fig. 1. Simulated structure. Three regions are highlighted: the left and the right leads and the so-called scattering region (central part). Left and right leads are ideally connected to semi-infinite bulk metal leads (left side) and graphene monolayer (right side). Since we want to directly compute transport from metal to graphene, we need to ensure that the right lead contains only the metal and the left one only graphene.

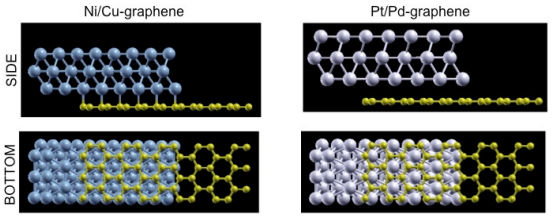

Fig. 2. Side and bottom views of the scattering region considered for the DFT and transmission calculations, for the Ni-, Cu-, Pt- and Pd-graphene contacts.

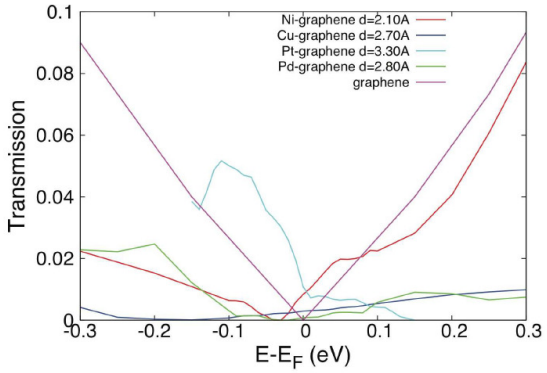

Fig. 3. Transmission for metal-graphene systems obtained with PWCOND for different metals (Cu,Ni,Pd,Pt) compared with the transmission of the ideal graphene monolayer.

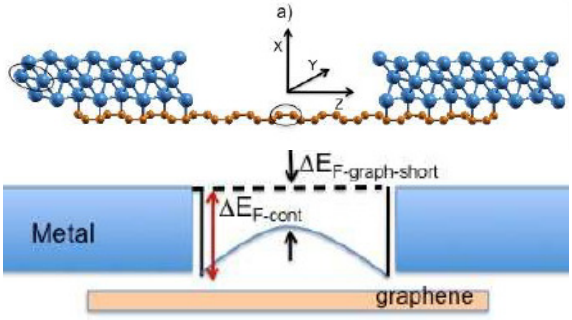

Fig. 4. Power conversion efficiency of the investigated OSC with graphene transparent electrode for different materials as active layer.

Materials	Intrinsic Resistance (Ω•μm)	Data from the literature - Resistance (Ω•μm)
Ni	80	300 [3] 600 [6]
Cu	350	44 [4] – 627 [7]
Pd	4500	403 [6], 600 [7]
Pt	10	764 [6]

Table 1: Comparison between the intrinsic resistance of metal-graphene contacts and results obtained from the literature. Resistances from the literature are usually higher because they typically include the effect of the partially depleted graphene region surrounding the contact, which is not strictly part of the "intrinsic" graphene-metal contact, and can therefore be optimized with electrostatics and/or doping.