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# Improved understanding of metal–graphene contacts

F. Driussi<sup>1\*</sup>, S. Venica<sup>1</sup>, A. Gahoi<sup>2</sup>, A. Gambi<sup>1</sup>, P. Giannozzi<sup>1</sup>, S. Kataria<sup>2</sup>, M.C. Lemme<sup>2,3</sup>,  
P. Palestri<sup>1</sup>, D. Esseni<sup>1</sup>

<sup>1</sup>DPIA, Università degli Studi di Udine, via delle Scienze 206, Udine 33100, Italy;

<sup>2</sup>RWTH Aachen University, Aachen, Germany;

<sup>3</sup>AMO GmbH, Advanced Microelectronic Center, Aachen, Germany

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## Abstract

Metal–graphene (M–G) contact resistance ( $R_C$ ) is studied through extensive experimental characterization, Monte–Carlo transport simulations and Density Functional Theory (DFT) analysis. We show that the back–gate voltage dependence of  $R_C$  cannot be explained only in terms of the resistance of the junction at the edge between contact and channel region. Experiments and DFT calculations indicate a consistent picture where both Ni and Au contacts have a M–G distance larger than the minimum energy distance, and where the M–G distance is crucial in determining the  $R_C$  value.

**Keywords:** graphene, contacts, modeling, Monte-Carlo, DFT

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## 1. Introduction

The excellent physical properties of graphene, such as high electron velocity and tunable optical absorption [1], make it suitable for many applications such as RF transistors [2], fast photodetectors [3], NEMS/MEMS and sensors [4], terahertz modulators [5], supercapacitors [6] and displays [7].

However, metal–graphene (M–G) contacts still exhibit large resistance ( $R_C$ ), which is a major hindrance for graphene transistors as, for instance, it degrades severely the output conductance and the maximum oscillation frequency of graphene–FETs (GFETs) [2]. An improvement of  $R_C$  is thus mandatory to boost graphene technology [8].

The physical understanding is a prerequisite for the engineering of M–G contacts, but it is still partly lacking. Advanced modelling techniques [9] and first principle simulations [10], combined with a dependable experimental characterization [11] are the best options to understand and then improve the large  $R_C$  values of M–G contacts.

This work presents a comprehensive analysis of  $R_C$  for different M–G contacts that starts from experimental characterization based on the Transfer Length Method (TLM), and then leverages on Density Functional Theory (DFT) and semi–classical Monte–Carlo (MC) simulations. For the first time to our knowledge, a consistent picture is identified where the short (Ni contact) or long range nature (Au contact) of the M–G interaction and the actual M–G distance have a substantial influence on the  $R_C$  value.

## 2. Devices and experiments

Transfer Length Method structures (series of back–gated GFETs) with monolayer CVD graphene (G) and Ni, Cu and Au contacts were fabricated via photolithography. The complete fabrication description can be found in [12]. DC characterization was carried out at 300 K in ultra–high vacuum conditions ( $<10^{-6}$  mbar) to avoid air induced Dirac Point (DP) shifts and  $R_C$  extraction errors [13].

The total resistance  $R_T$  of GFETs was calculated from current ( $I_{DS}$ ) versus back–gate voltage ( $V_{BG}$ ) curves at fixed drain–source voltage ( $V_{DS}$ ) as  $R_T = V_{DS}/I_{DS}$ .  $R_T$  consists of the channel sheet resistance ( $R_{SH}$ ) and  $R_C$ :

$$R_T = R_{SH}L_{CH}/W + 2R_C$$

where  $W$  is the channel width and  $L_{CH}$  is the contact spacing. We extracted  $R_{SH}$  and  $R_C$  by linear fitting of  $R_T$  vs.  $L_{CH}$  experiments [11]. The average  $R_{SH}$  vs.  $V_{BG}$  curves (Fig. 1a) show that the graphene quality is similar and independent of the metal contacts. Data for the best device (lower  $R_{SH}$ , Au contact) are also reported. Instead,  $R_C$  depends on the metal (Fig. 1b), with larger values observed for Ni than for Au. Figure 1c shows that the G quality and  $R_C$  are correlated.

Typically,  $R_C$  consists of: a) the specific contact resistivity  $\rho_C$ , b) the  $R_{SK}$  of graphene underneath the contact, c) the  $R_{JUN}$  of the junction at the edge of the contact due to different G charge densities in the

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\* Corresponding author. *e.mail:* francesco.driussi@uniud.it



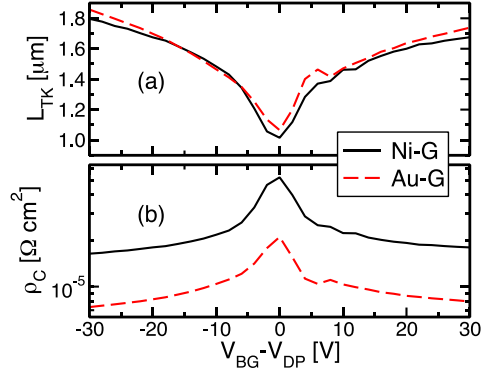


Fig.5.  $L_{TK}$  (a) and  $\rho_C$  (b) extracted from experiments for the Ni-G and Au-G contacts.

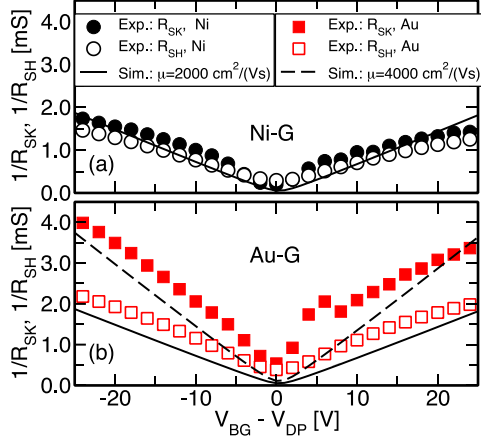


Fig.6.  $R_{SH}$  and  $R_{SK}$  (symbols) measured for Ni-G (a) and Au-G (b) and  $R_{SH}=[\mu q(n+p)]^{-1}$  calculated for the G/oxide/back-gate system (lines).  $q$  is the elementary charge,  $n$  and  $p$  are electron and hole density,  $\mu$  is the mobility.

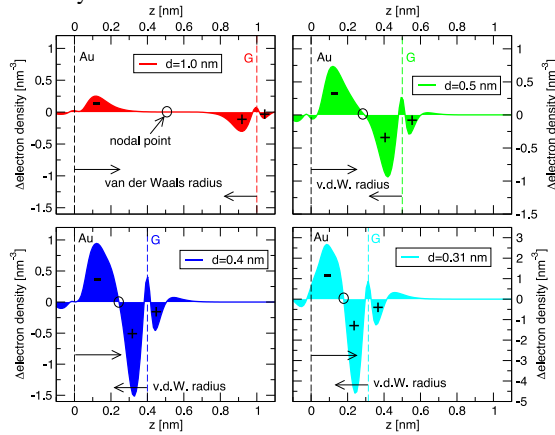


Fig.7. Induced net charge along  $z$  (perpendicular to graphene) for different Au-G distances. Dashed lines are the positions of atoms, while arrows are the van der Waals atomic radii.

### 3. DFT simulations of Au-G and Ni-G contacts

We performed DFT simulations of Ni-G and Au-G stacks by using Quantum ESPRESSO [16]. The 111 surface of Ni and Au crystals (3 layers) was matched to the G lattice [10]. For Ni-G, we considered a 1x1 graphene cell with a lattice constant of  $a=0.246$  nm. For Au-G we matched the Au lattice with a 2x2 G

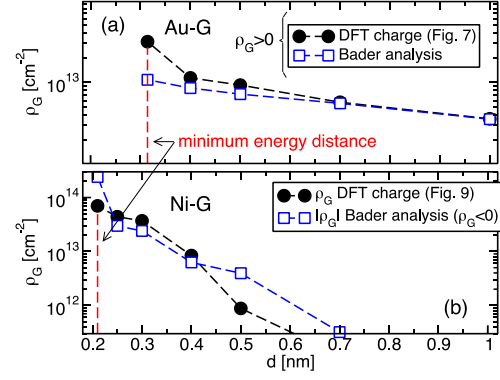


Fig.8.  $\rho_G$  vs.  $d$  in Au-G (a) and Ni-G (b), calculated by integrating the charges (circles) in Figs. 7 and 9 or via Bader analysis (squares). For Au-G the  $\rho_G$  extraction techniques agree.  $\rho_G$  extraction is more complex in Ni-G, showing also a shorter-range interaction than Au-G.

supercell [10]. Local-spin density approximation, plane-wave basis sets and gradient-corrected exchange-correlation functional (PBE) were used for Ni, Au and C atoms. Van der Waals interactions and dipole correction were considered [16]. In the simulations, we varied the M-G distance  $d$  and the minimum energy distance for Au-G ( $d=0.31$  nm) and Ni-G ( $d=0.21$  nm) are obtained by force minimization.

#### 3.1. The Au-G contact

To analyze the graphene doping due to the Au contact, we calculated the difference between the valence electron density of the Au-G stack and the isolated Au and G layers [17]. Figure 7 shows the results averaged over the graphene plane: by lowering  $d$ , positive charge accumulates near the graphene, while negative charge builds up near Au. To evaluate the graphene doping ( $\rho_G$ ), we integrated these dipoles along  $z$  (perpendicular to graphene) up to the nodal points (circles, Fig. 7).

To exclude possible contributions by the charge redistribution due to Pauli repulsion [17], we also calculated the charge variation of each C atom induced by the Au proximity via Bader analysis [18]. Bader charges (Fig. 8a, squares) agree well with the dipole integration (circles), except at  $d=0.31$  nm; in this case  $d$  is shorter than the sum of the Au and C atomic radii (Fig. 7), so Au and C charges are largely overlapping at a given  $z$ , precluding a meaningful determination of  $\rho_G$  via dipole integration. Fig. 8a shows that graphene is  $p$ -doped by Au for distances up to 1 nm, revealing a long-range interaction.

#### 3.2. The Ni-G contact

We repeated the analysis also for the Ni-G stack. Figure 9 shows a more complex Ni-G interaction (several dipoles along  $z$ ); thus, it is difficult to discriminate between Ni and G charges. The integration of the charge up to the nodal point closest to graphene (circles, Fig. 9) leads to a  $p$ -doping of

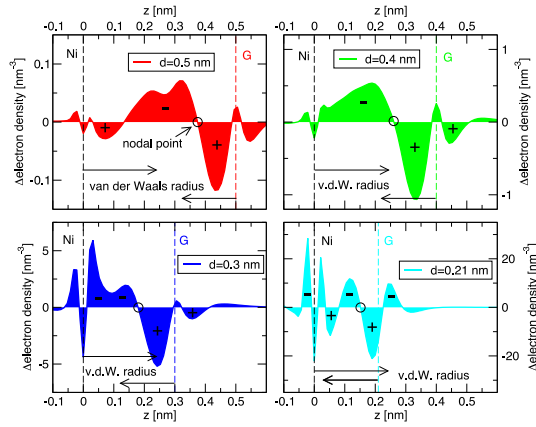


Fig.9. Induced net charge along  $z$  (perpendicular to graphene) for different Au–G distances. Dashed lines are the positions of atoms, while arrows are the van der Waals atomic radii.

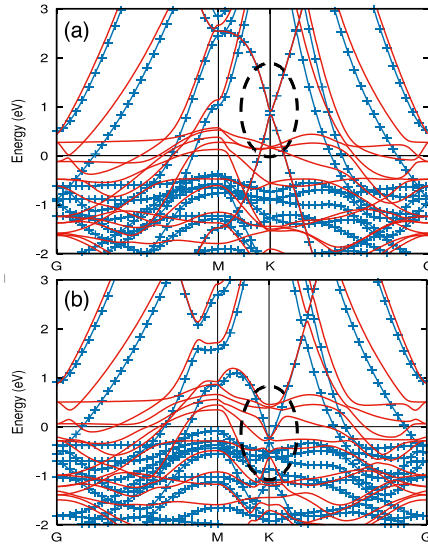


Fig.10. (a)  $d=0.5$  nm: energy bands of Ni–G stack are the superimposition of Ni and G bands: Dirac cone is visible at the  $K$  point. (b)  $d=0.3$  nm: Ni induces gaps in graphene and Dirac cone vanishes. Blue lines are for spin up, red lines are for spin down.

graphene ( $\rho_G > 0$ , Fig. 8b, circles). Bader charges reveal, instead, a  $n$ -doping ( $\rho_G < 0$ , squares).

Concerning this discrepancy, in Fig. 9, van der Waals radii of Ni and C largely overlap for  $d < 0.4$  nm, which makes the dipole analysis inadequate to determine  $\rho_G$  for the Ni–G stack. In this respect, the energy band diagrams of Ni–G in Fig. 10 support this picture. For  $d=0.5$  nm, the bands of the Ni–G system still resemble the bands of Ni and graphene alone (Fig. 10a) and, in particular, the Dirac cone of graphene can be recognized at the  $K$  point. Instead, when  $d$  is reduced to 0.3 nm (b), the Dirac cone disappears, opening of an energy gap [10], so it is difficult to interpret the Ni–G stack in terms of a Ni and a G sub-systems.

However, the Ni–G interaction vanishes for  $d > 0.5$  nm (Fig. 8b), leading to  $|\rho_G| < 10^{12} \text{ cm}^{-2}$  and suggesting a shorter-range interaction compared to Au–G. This

explains the experiments in Fig. 6: Ni fails to dope graphene ( $R_{SK} \approx R_{SH}$ ), probably because of an ineffective Ni–G distance (e.g.  $d > 0.5$  nm), whereas Au does improve  $R_{SK}$  compared to  $R_{SH}$  (Fig. 6b), most likely because the longer-range interactions enable a G doping despite a possible not optimal Au–G distance.

#### 4. Conclusions

Ni has a strong chemical interaction with graphene at the minimum energy distance, which however vanishes for Ni–G distances larger than 0.5 nm. Experiments show a large and strongly  $V_{BG}$  dependent  $R_C$ , suggesting that Ni fails to effectively dope graphene and a Ni–G distance larger than 0.5 nm.

For Au–G contacts, a longer-range interaction and significant G doping are predicted for distances up to 1 nm, which explains the lower experimental  $R_C$  compared to the Ni–G contact.

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