A physics-based model of gate-tunable metal–graphene contact resistance benchmarked against experimental data

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Abstract
Metal–graphene contact resistance is a technological bottleneck in the realization of viable graphene-based electronics. We report a model that is useful for finding the gate-tunable components of this resistance, determined by the tunneling of carriers between the 3D metal and 2D graphene underneath, followed by Klein tunneling to the graphene in the channel. This model quantifies the intrinsic factors that control that resistance, including the effect of unintended chemical doping. Our results agree with experimental results for several metals.

1. Introduction
While graphene has emerged as a promising material for future electronic devices thanks to its unique electronic properties, the metal–graphene contact resistance ($R_c$) remains a limiting factor for graphene-based electronic devices [1]. In particular, for high frequency electronics it is an issue very much influencing figures of merit like the maximum frequency of oscillation, the cutoff frequency, and the intrinsic gain [2]. Therefore it is necessary to understand the intrinsic and extrinsic factors determining $R_c$, which displays a strong variation depending on the metal contact and fabrication procedure details [3–5]. To gain understanding of these factors to render a better control of the contact’s technology feasible, a comprehensive physics-based model of $R_c$ is an absolute requirement. One relevant model has already been proposed by Xia et al [6] for describing the transport in metal–graphene junctions, as tunneling processes from the metal to graphene over an effective transfer length ($L_T$), followed by injection to the graphene channel (see figure 1(a)). However, there is an important ingredient determining $R_c$, namely, the transmission from a 3D system (metal) to a 2D system (graphene), that has so far not been taken into account properly, on a physics basis. Evidence of the current crowding effect over $L_T$ has been reported by Sundaram et al using photocurrent spectroscopy [7].

In order to improve on the current understanding, we have considered the issue of the carrier transmission between materials of different dimensionality. Specifically, we have developed a physics-based model where the first process is responsible for the resistance between the metal and the graphene underneath ($R_{mg}$), and the second process includes the resistance due to a potential step across the junction formed between the graphene under the metal and the graphene channel ($R_{gg}$). The total contact resistance is then the series combination of the two contributions, $R_c = R_{mg} + R_{gg}$, accounting for any current crowding effect near the contact edge. The calculations of $R_{mg}$ and $R_{gg}$ are based on the Bardeen transfer Hamiltonian (BTH) method [8, 9] and on the Landauer approach [10], respectively. The BTH method allows us to get information about the matrix elements for the transition between 3D metal and 2D graphene states and, combined with Fermi’s golden rule, yields a compact expression for the specific contact resistivity $\rho_c$. On the other hand, the Landauer approach allows us to get the conductance of carriers across the potential step between the graphene under the metal and the
graphene in the channel, where the angular dependence of the transmission of Dirac fermions and the effective length of the potential have been taken into account. To model $R_c$, we have considered it as a building block of an FET device, so its value will strongly depend on the gate voltage applied.

2. Methods

2.1. Electrostatics

In this paper we start with the graphene electrostatics. We considered a three-terminal graphene FET (GFET) device controlled by a global back-gate voltage ($V_g$), as sketched in figure 1(a), although it could easily be adapted to a device with both top and back gates as we will show later on. We split the electrostatic problem up by considering two 1D heterostructures, namely, the metal/graphene/oxide/semiconductor (MGOS) and graphene/oxide/semiconductor (GOS) heterostructures in the contact and channel regions, respectively. In figure 1(b) the corresponding band diagram of the MGOS heterostructure is shown. For each of these regions, we model the gate voltage dependence of the graphene Fermi level relative to its Dirac energy, namely $\Delta E_m$ and $\Delta E_g$ for the graphene under the metal and the graphene in the channel, respectively. The energy potential loops at the interfaces encircled in figure 1(b), together with Gauss’s law, are considered, resulting in equations (1a)–(c).

Because of the charge transfer between the metal and graphene, a dipole layer of size $d_1$ inside the equilibrium separation distance $d_{eq}$ is set up [11]. Also a difference, $eV$, between the metal and the graphene Fermi level in the contact region, supplied by the drain terminal, has been assumed. The workfunctions of the metal and graphene are $W_m$ and $W_g$, respectively:

$$W_m = \phi_d + \Delta d + \Delta E_m - eV, \quad (1a)$$

$$W_g + \Delta E_m = \phi_d + W_c - e(\phi_s + V_g - V). \quad (1b)$$

In equation (1a), the term $\Delta d$ is the potential drop in the dipole layer which can be expressed as $\Delta d = \Delta d_c + \Delta d_h = -Q_m/C_d + \Delta ch$, where $\Delta d_c$ corresponds to the charge transfer and $\Delta d_h$ to the chemical potential interaction, describing the short range interaction from the overlap of the metal and graphene wavefunctions [11, 12]. In equation (1b), the back-gate voltage $V_g$ is referred to the source metal electrode potential, $W_c = \phi_s + eV - \phi_d$ is the semiconductor workfunction and $\phi_s$ is the semiconductor surface potential. In equation (1c), $Q_m = -C_d \Delta d_c$, describes the charge per unit area induced in the surface metal, $Q_0 \approx 2(e/\pi \hbar^2 V_F^2) |\Delta E_m| + Q_0$ is the net charge sheet density within the graphene layer [13] plus the charge density due to possible chemical doping [14] ($Q_0$), and $Q_c = C_{ox} \Delta d_{ox}$ describes the charge per unit area induced in the semiconductor. Here, $C_d = \epsilon_d/d_1$ and $C_{ox} = \epsilon_0/T_{ox}$ describe the capacitive coupling to the metal and back gate, respectively. The value of $d_1$ can differ from the equilibrium distance $d_{eq}$ (∼0.3 nm) due to the spatial extension of the carbon p$_z$ and metal d orbitals. The value of $\Delta d_h$ strongly depends on the separation distance $d_{eq}$ and it becomes negligible for $d_{eq} \gtrsim 4$ nm [11]. Combining equations (1) and assuming that $\phi_s$ saturates at strong inversion and accumulation, we get a simple quadratic equation for $\Delta E_m$:

$$\Delta E_m \left[\Delta E_m + \left(C_{ox} + C_d\right) \Delta E_m\right] + eC_{ox} \left(V_g - V_D\right) = 0, \quad (2)$$

where $a = e^2/\pi \hbar^2 V_F^2$, with $V_F$ (∼1 × 10^6 cm s$^{-1}$) the Fermi velocity, and

$$V_D = \frac{C_d}{C_{ox}} \left(W_m - W_g + eV - e\Delta d_h\right) + \left(\phi_s + eV - \phi_d - \frac{Q_0}{C_{ox}}\right). \quad (3)$$

represents the Dirac gate voltage required to achieve $\Delta E_m = 0$ and defines the back-gate voltage value for $Q_c + Q_m + Q_g = 0$. \quad (1c)
which \( \rho_c \) and the resistance \( R_{mg} \) become maximum, as we will see later.

Because the dipole layer has been modeled as an insulator, the channel region electrostatics under the influence of both top and back gates can be described in way similar to that presented in equation (1), so the Fermi level shift in the channel (\( \Delta E_g \)) can be obtained from

\[
\Delta E_g = \left[ \Delta E_g \right] + \left( C_b + C_i \right) \Delta E_g + eC_b \left( V_b - V_g \right) = 0, \quad (4)
\]

with

\[
eV_{g0} = \frac{C_i}{C_b} \left( W_m - W_g - eV_t \right) + \left[ \chi + e\phi - W_g - \frac{Q_0}{C_b} \right]. \quad (5)
\]

In the last equations, \( C_b \) and \( V_b \) are the back (top) capacitance and gate voltage, respectively. The new Dirac voltage \( V_{g0} \) must be understood as the back-gate voltage needed to achieve \( \Delta E_g = 0 \) at a fixed top-gate voltage \( V_t \). When there is only a back gate, like in our experimental devices, we can get \( \Delta E_g \) for the GOS structure simply by setting \( C_i \to 0 \).

With the electrostatic model given by the above equations, the key quantities \( \Delta E_m \) and \( \Delta E_g \) can be determined, and in turn are needed for calculating the contact resistance; figure 2 shows both \( \Delta E_m \) and \( \Delta E_g \) at equilibrium (\( V \to 0 \)), each as a function of the back-gate bias, using palladium (Pd) as the metal electrode and SiO\(_2\) as the oxide, with thickness \( T_{ox} = 90 \) nm. These results can be obtained by solving either equation (1) or the simplified form 2, with there being very little difference between them. Different kinds of junctions may build up depending on the back-gate bias, namely pp-type, pn-type, and nn-type junctions. Here, we have assumed that \( Q_0 \) is only affecting the graphene channel, and not the graphene under the metal. The impact of \( Q_0 \) in determining the crossing of \( \Delta E_g \) with zero can be seen in the figure. To capture the transition between the pp-type and pn-type junctions, which was observed at \( V_b = V_{g0} \sim 23 \) V [6], the parameter \( Q_0/e \) was set to \(-5.4 \times 10^{12} \text{cm}^{-2}\). Next, the transition produced between the pn-type and nn-type junctions was captured by our model at \( V_b = V_{g0} \sim 46 \) V, in accordance with the experiment of Xia et al. The electrical parameters that we have assumed for all of the simulations presented in this work are shown in table 1. Because of the charge transfer between the graphene under the metal and the graphene in the channel, a potential step of effective length \( \lambda \) arises at the contact edge. A sketch of that potential step is shown in figure 2. Once we get the electrostatic model, we are ready to discuss how to model the contact resistance.

2.2. The resistance \( R_{mg} \) and the resistivity

The procedure for modeling \( R_{mg} \) is based on the transmission line method [15–17], which in turn requires determination of \( \rho_c \), namely,

\[
R_{mg} \left( \Delta E_m \right) = \sqrt{\rho \frac{R_{sh}^2}{W}} \coth \left( L_c/L_T \right)/W, \quad (6)
\]

where \( \rho \left( \Delta E_m \right) = (dI/dV)^{-1} \mid_{V=0} \) represents the specific contact resistivity, \( R_{sh}^2 \) (250 \( \Omega \)\text{cm}^{-1} in this work) is the graphene sheet resistance under the metal, \( L_T = \sqrt{R/R_{sh}} \) is the characteristic length over which current injection occurs between the metal and the graphene layer (transfer length), and \( L_c/W \) is the length (width) of the contact. Here, \( \rho_c \) is calculated by means of the BTH method, which allows us to split the metal–graphene system into separate metal and graphene subsystems with known Hamiltonians. In the framework of the BTH method, the probability of elastic tunneling is calculated using Fermi’s golden rule. This gives a quantitative estimate of the coupling between the metal and graphene states, so it is possible to get an analytical formula with key parameters for \( \rho_c \) as a function of \( \Delta E_{mg} \). In the supplementary data, we show how to calculate \( \rho_c \) from the tunneling current density \( J \) using the BTH approach. The resulting compact analytical expression for \( \rho_c \) as a function of

![Graphene Fermi level shifts with respect to the Dirac point for different values of \( Q_0 \), using Pd as the metallic contact. Solid lines: numerical solution of equations (1); symbols: solution of equation (2). The inset shows the potential step between the graphene under the metal and the graphene in the channel, with effective length \( \lambda \).](image)

**Table 1.** Electrical parameters for selected metal electrodes. They were extracted from previous reports [6, 11], except the quantities marked with asterisks, which were considered as fitting parameters for matching the experimental results.

| Metal | \( W_{mg} \) (eV) | \( d_{mg} \) (Å) | \( \Delta_{mg} \) (eV) |
|-------|-----------------|----------------|-----------------|
| Ni    | 5.47            | 2.05           | 0.8             |
| Ti    | 4.65            | 2.10           | 0.9             |
| Pd    | 5.67            | 3.00           | 0.90            |
| Cu    | 5.22            | 3.26           | 0.99            |
| Pt    | 6.13            | 3.30           | 0.93            |
| Au    | 5.54            | 3.31           | 0.93            |
| Ag    | 4.92            | 3.33           | 0.88            |
| Al    | 4.22            | 3.41           | 0.77            |

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$\Delta E_m$ under the metal at $V = 0$, for a given temperature $T$, can be written as

$$\rho_{c}(\Delta E_m) = \frac{\pi e^2 \hbar}{16\gamma} \exp\left(2\kappa d_{eq}\right)$$

$$\times \left(\frac{E_{\|} - \Delta E_m + \frac{1}{2} \gamma^2 E_{\perp}}{\sqrt{E_{\perp}^2 - (E_{\|} - \Delta E_m)^2}}\right)$$

$$\times \frac{1}{2kT \ln \left(\exp \left(\frac{\Delta E_m}{kT}\right) + 1\right) - \Delta E_m},$$

(7)

where $\gamma = m/m_0$, with $m$ and $m_0$ the effective electron masses in the metal and the dipole layer, respectively. The factor $\kappa$ is the electron decay constant in the dipole layer and has the form $\sqrt{2m\phi/\hbar^2 + k_0^2}$ [13], where $\phi \sim W_\alpha$ has been taken as the barrier height and $k_0$ is the parallel momentum at the K or K' points (i.e., $4\pi/3a$). For a typical metal the workfunction is $W_\perp \sim 5$ eV, so $\kappa \sim 20$ nm$^{-1}$. As a consequence, $E_\perp = \hbar^2 k_0^2/2m \sim 11$ eV and $E_\parallel = \hbar^2 k_0^2/2m \sim 16$ eV.

From equation (7), we can infer that the maximum value of $\rho_c$ depends exponentially on the equilibrium separation distance $d_{eq}$ and that the maximum resistivity is located at $V_{\phi} (\Delta E_m = 0)$. Figure 3 shows $\rho_c$ at $T = 300$ K as a function of the back-gate bias overdrive $(V_g - V_{\phi})$, considering different metals. After sorting the metals by peak contact resistivity, it appears that $d_{eq}$ is the main factor controlling it, the Ni contact being the best option, followed by Ti. Here we have assumed SiO$_2$ as the insulator, with $T_{\text{ox}} = 90$ nm, and equal effective masses for all metals. According to table 1, the Ni-graphene (Al-graphene) contact has the smallest (largest) equilibrium distance $d_{eq}$ among the metal contacts represented here, giving rise to the smallest (largest) value of $\rho_c$ at $V_{\phi}$. The values of $\rho_c$ predicted from equation (7) are consistent with experimental results reported by Nagashio and Berdebes [18, 19] for Ni, Ti and Pd. Although the Ni happens to be the best option for getting the lowest $R_c$, other effects that contribute to the lateral resistance must be considered. As a matter of fact, $R_c$ for Ni can become comparable to that of Pd, as we will show later. Our model predicts how $\rho_c$ depends on factors like the workfunction difference, the equilibrium distance, the chemical interaction potential, the gate capacitance and the temperature.

2.3. The resistance $R_{gg}$

Next, we model the lateral contact resistance $R_{gg}$ across a potential step with effective length $\lambda$ (see the inset of figure 2), relying on the Landauer approach. The potential along the transport direction $x$ can be described via a simple space-dependent Fermi level shift [10]:

$$\Delta E(x) = \Delta E_m + \Delta E_g \exp(-x/\lambda) + 1,$$

(8)

where we have considered that the metal electrode covers the left half-plane ($x < 0$). The type (n or p) and density of carriers in both the left and the right half-planes are tuned via the back gate. The important quantity to be determined is the probability of reflection of Dirac fermions across the potential step, which has been derived by Cayssol et al [10], namely,

$$R_{\text{step}} = \frac{\sinh\left(\frac{\pi\Delta k^+}{\lambda}\right) \sinh\left(\frac{\pi\Delta k^-}{\lambda}\right)}{\sinh\left(\pi\Delta k^+\right) \sinh\left(\pi\Delta k^-\right)},$$

(9)

where the momenta are given by $k^{\rho\sigma} = \left(\Delta E_g - \Delta E_m\right)/\hbar v_F + \rho \kappa^{\rho\sigma} + \sigma \kappa^{\rho\sigma}$, with $\rho, \sigma = \pm 1$. The longitudinal momentum $k_x$ is related to the transverse momentum $k_y$ by the Pythagorean relationship

$$k_x^{(i)} = \frac{\text{sgn}(\Delta E_i)}{\sqrt{\left(\Delta E_i/\hbar v_F\right)^2 - k_y^{(i)^2}}},

i = m, g,$$

(10)

where the positive (negative) sign indicates that the doping is of p (n) type.

By means of the Landauer formula, the conductance can be obtained from

$$R^{-1}_{gg} (\Delta E_m, \Delta E_g) = \frac{2e^2}{h} W \int_{-k_F}^{k_F} T_{\text{step}} \text{dk}_y,$$

(11)

where $T_{\text{step}} = 1 - R_{\text{step}}$ is the transmission probability and $k_F = \text{min} \left(\frac{\Delta E_m}{\hbar v_F}, \frac{\Delta E_g}{\hbar v_F}\right)$. Figure 4(a) shows the probability of transmission of the Dirac fermions across the potential step as a function of $V_g$ for different incidence angles, assuming Pd as the metal. In particular, it indicates the absence of backscattering at normal incidence ($k^{(m,g)}_x = k^{(m,g)}_F$ or $\theta = 0$)—because of the orthogonality of incoming and reflected spinor states. In contrast, the transmission of the bipolar contacts (case pn) tends toward zero for incident carriers when $\theta \to \pi/2$.

So far we have not considered the effect of the drain bias ($V_d$) in defining the contact resistance on the drain side ($R_{cd}$). However, for radio-frequency (RF) applications, $V_d$ is usually placed in the
saturation region, so its value could be high compared with $V_g$. In such a case, the drain and source contact resistances can be very different. Our model for $R_c$ is still valid and useful for determining $R_{cd}$ in this situation. For this purpose it would be necessary to evaluate $R_c$ at the effective gate voltage $V_{g,eff} = -V_{Vg}$, that is $R_c = R_{c}(V_{g,eff})$.

3. Results and discussion

Until now, in the description of our model, we have not taken into account any broadening of the graphene states in the $R_c$ model. To get a more realistic model, an effective broadening describing the coupling between the metal and the quasi-bound graphene states underneath and/or the spatial variations of the graphene–metal distance in the contact surface [11] must be taken into account. This effect can be considered upon application of a Gaussian function $G_1$ of width $t_1$, the broadening energy. In addition, we have included the random disorder potential in the graphene channel using a Gaussian function $G_2$ of width $\pi = \frac{\hbar}{\sqrt{2\pi n_0}}$, where $n_0$ is the minimum sheet carrier concentration. Then, the two components of $R_c$ have to be recalculated as shown in equations S16–17 of the supplementary data.

In figure 4(b) we show the effect of $t_1$ on $R_{gg}$ when it varies from 100 to 300 meV with $t_2 \sim 100$ meV ($n_0 = 5 \times 10^{11}$ cm$^{-2}$). $R_{gg}$ exhibits a main peak corresponding to the minimum DOS in the channel ($\Delta E_g = 0$ or equivalently $V_g - V_{Dg} = 0$) and another secondary peak corresponding to the minimum DOS in the graphene under the metal ($\Delta E_m = 0$ or equivalently $V_g - V_{Dm} \sim 23$ $V$). According to the experimental data reported by Xia et al [6] for Pd as the metal electrode, the latter peak does not appear in the $R_c$ curve, suggesting a large $t_1$ value (>300 meV), as reflected in figure 4(b).

As complementary information, the dependence of $R_{gg}$ on the effective length $\lambda$ of the potential step between the metal-doped graphene and the gate-controlled graphene channel is presented in figure 4(c). For unipolar junctions, $R_{gg}$ is almost independent of $\lambda$, while for the bipolar pn junction it moderately increases as $\lambda$ changes from 2 to 128 nm.

After presentation of the $R_c$ model, the next task is benchmarking it against experimental measurements on graphene FETs using the transfer length method (TLM) for metal electrodes such as palladium (Pd), nickel (Ni) and titanium (Ti), as shown below.

In figure 5, we have plotted the data reported by Xia et al considering Pd as the metal electrode. Here the graphene sheet was transferred to SiO$_2$ of 90 nm thickness. Our model reveals that $R_{gg}$ and $R_{cg}$ play similar roles. The absence of a peak in the experimental $R_c$ data at $V_g \sim 46$ $V$ suggests a large value of $t_1$, as has been discussed previously. To match the experimental data, we have assumed $Q_0/e = -5.4 \times 10^{13}$ cm$^{-2}$, $t_1 = 300$ meV, $t_2 = 100$ meV and $\lambda = 100$ nm. Interestingly, we capture the correct value of the Dirac voltage at $V_{Dg} \sim 23$ $V$ and the moderate asymmetry between the left and right branches: $R_c$ is lower for the left branch because of the much better carrier transmission of the unipolar pp junction as compared with the bipolar pn junction (see figure 4(a)).

Next, we compare with experimental data for GFETs with Ni as the metal electrode (figure 6). In this
case, the back-gated graphene transistors have been fabricated by photolithography on Si wafers covered with 300 nm of thermal oxide. Graphene grown by chemical vapor deposition (supplier: Bluestone Global Tech) was transferred by the standard PMMA method [20] to the substrate and patterned using oxygen plasma. Nickel contacts have been fabricated using sputter deposition and a lift-off technique. The distance between the source and drain contacts was 0.6, 0.9, 1.3, 1.7 and 2.7 μm for different devices on the chip, to allow extraction of $R_c$ by the TLM. The channel width was 10 μm. Finally, the devices were encapsulated using 85 nm of Al$_2$O$_3$, deposited by atomic layer deposition. After making some electrical measurements, we obtained, and report in figure 6(a), a comparison between the experimental data and the usual model of the source–drain resistance $R_T$ given by [21]:

$$R_T = \frac{R_{ch}^2}{W} L_{ch} + 2R_c.$$ (12)

Here, the channel sheet resistance $R_{ch}^2$ has been modeled as $R_{ch}^2 = \frac{\mu e \sqrt{n_0^2 + n(V_D)^2}}{1 + n(V_D)^2}$, with $\mu = 1793$ cm$^2$ V$^{-1}$ s$^{-1}$ and $n_0 = 5 \times 10^{11}$ cm$^{-2}$, which were extracted from the experiment, and $n \propto \Delta E_F^2$ is the charge sheet concentration in the graphene channel region. In this case we have assumed a possible doping concentration in the graphene channel of $Q_D/e = -2 \times 10^{10}$ cm$^{-2}$ in order to capture the position of the Dirac voltage. Details of the electrostatic behavior of the Ni–graphene contact can be found in the supplementary data. For the quasi-static measurements of the resistance shown in figure 6(a), hysteretic behavior is observed, which is typical for graphene FETs. This hysteretic behavior occurs mainly because of charge traps generated by adsorbates, typically O$_2$/H$_2$O redox couples, at the graphene/dielectric interface [22, 23]. This effect has not been considered in this model. Regarding the contact resistance (figure 6(b)), our model gives values between 150 and 350 Ω μm, which are consistent with the experimental values extracted by the TLM for the gate voltages $V_g = -20$, 0 and 20 V: $R_c \sim 220$, 400 and 220 Ω μm with correlation coefficients $R^2 = 0.9894$, 0.9740 and 0.9754, respectively. The values of $\lambda$ and $t_1$ were determined as around 4 nm and 300 meV, respectively, for getting $R_c$ values in that range. It is worth mentioning that $R_{bg}$ is the dominant part of $R_c$, which is in contrast with the Pd contact case analyzed before, where $R_{bg}$ and $R_{mg}$ played similar roles.

A third comparison was carried out for GFETs with Ti as the metal electrode with geometrical parameters $L_{ch} = 1$ μm, $W = 10$ μm and $T_{ox} = 360$ nm (SiO$_2$). Here graphene synthesized by photothermal CVD on copper was used to fabricate the GFETs [24, 25]. For the source–drain resistance, the experimental data are shown in figure 7(a), together with the model prediction for $R_T$. Like for the Ni case, we have considered the following electrical parameters: $\mu = 1805$ cm$^2$ V$^{-1}$ s$^{-1}$, $n_0 = 7 \times 10^{11}$ cm$^{-2}$, as extracted from the experimental data. A chemical doping $Q_D/e = -4.6 \times 10^{12}$ cm$^{-2}$ was fed into the model to get the position of the Dirac voltage $V_D$ at around 75 V in accordance with the observation. Details of the electrostatic behavior of the Ti–graphene contact can be found in the supplementary data. Using these together with the parameters given in table 1, our model results in the contact resistance shown in figure 7(b). The calculated $R_c$ agrees well with the values extracted from the TLM at gate voltages $V_g = -75$, 15, 45 and 75 V: $R_c \sim 500$, 500, 400 and 600 Ω μm with correlation coefficients $R^2 = 0.9932$, 0.9915, 0.9986 and 0.9997, respectively. The values of $\lambda$ and $t_1$ were determined as around 50 nm and 300 meV, respectively, for getting $R_c$ values in the range mentioned. Unlike Pd and Ni, $R_c$ in the Ti–graphene contact exhibits a huge asymmetry between left and right branches, with $R_c$ lower for the right branch. This asymmetry agrees qualitatively with measurements carried out for Ti and reported by Xia et al [6].
4. Conclusions

In summary, we have developed a model of gate-tunable metal–graphene contact resistance. First of all, we modeled the behavior of the Fermi level shift $\Delta E$ in both the graphene under the metal and the graphene in the channel. $\Delta E$ becomes zero under the metal at a gate voltage named as $V_D$ which is controlled by intrinsic electrical parameters like the workfunction, the capacitive coupling between the metal and the gate, and the value of the chemical interaction. In the channel region, $\Delta E$ is zero at gate voltage $V_{GD}$, which is strongly determined by the unintended chemical doping. Once we have obtained $\Delta E$ for each region, we use a combination of the BTH method and the Landauer formula to independently determine the contribution of each $R_c$ component: the BTH method to determine the resistance between the metal and the graphene underneath ($R_{mg}$), and the Landauer formula for the resistance between the graphene under the metal and the graphene in the channel ($R_{gg}$). Using the BTH method we have found a simple analytical expression for the specific contact resistivity $\rho_c$, which elucidates its dependence on the metal–graphene equilibrium distance. Specifically, among the metals considered here, Ni and Ti exhibit the smallest value of $\rho_c$ at their respective Dirac voltages $V_D$. However, given the voltage dependence of $\rho_c$ and the different $V_D$ values displayed by the metals, Cu or Pd could show a $\rho_c$ even smaller than those for Ni or Ti, depending on the applied gate voltage. The calculation of $\rho_c$ is key for getting $R_{mg}$ by means of the transmission line method. This resistance shows a peak at $V_g = V_D$. On the other hand, the lateral resistance or $R_{gg}$ in principle, exhibits two peaks, one of them at $V_{GD}$ and another at $V_D$. However, when a broadening of the graphene states under the metal ($t_1$ in this work) is considered, the latter peak could disappear. We have also found that $R_{gg}$ is sensitive to the effective length ($\lambda$) of the junction potential step, especially when a bipolar pn junction builds up. Depending on the metal electrode and the chemical doping of the graphene channel, the two components of $R_c$ could be either similar in magnitude or of very different orders. In particular, for Pd those two components compete, but for Ni and Ti, the lateral resistance is the dominant component.

Our model is in agreement with experimental data for several metals under test. In particular, we have benchmarked the model against experiments using Pd, Ti, and Ni. The proposed model unveils the interplay between different intrinsic and extrinsic factors in determining the contact resistance of graphene-based electronic devices, which should be useful for its optimization.

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References

[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 Science 306 666–9
[2] Schwierz F 2013 Proc. IEEE 2013 101 1567–84
[3] Huard B, Stander N, Sulpizio J A and Goldhaber-Gordon D 2008 Phys. Rev. B 78 121402 R
[4] Nagashio K, Nishimura T, Kita K and Toriumi A 2009 IEEE International Electron Devices Mtg 5424297
[5] Russo S, Craciun M F, Yamamoto M, Morpurgo A F and Tarucha S 2010 Physica E 42 677–9
[6] Xia F, Perebeinos V, Lin Y-m, Wu Y and Avouris P 2011 Nat. Nanotechnol. 6 179–84
[7] Sundaram R S, Steiner M, Chiu H-Y, Engel M, Bol A A, Krupke R, Burghard M, Kern K and Avouris P 2011 Nano Lett. 11 3833–7
[8] Bardeen J 1961 Phys. Rev. Lett. 6 57–9
[9] Tersoff J and Hamann D R 1985 Phys. Rev. B 31 805
[10] Cayssol J, Huard B and Goldhaber-Gordon D 2009 Phys. Rev. B 79 075428
[11] Khomyakov P A, Giovannetti G, Rusu P C, Brocks G, van den Brink J and Kelly P J 2009 Phys. Rev. B 79 195425
[12] Chaves F A, Jiménez D, Cummings A W and Roche S 2014 J. Appl. Phys. 115 164513
[13] Feenstra R M, Jenk D and Gu G 2012 J. Appl. Phys. 111 043711
[14] Ni Z H, Wang H M, Luo Z Q, Wang Y Y, Yu T, Wu Y H and Shen Z X 2010 J. Raman Spectrosc. 41 479–83
[15] Schroder D K 2006 Semiconductor Material and Device Characterization 3rd edn (Hoboken, NJ: Wiley–IEEE Press)
[16] Léonard F and Talin A A 2011 Nat. Nanotechnol. 6 773
[17] Reeves G K and Harrison H B 1982 IEEE Electron Device Lett. 3 111–3
[18] Nagashio K, Nishimura T, Kita K and Toriumi A 2010 Appl. Phys. Lett. 97 143514
[19] Berdebes D, Low T, Sui Y, Appenzeller J and Lundstrom M 2011 IEEE Trans. Electron Devices 58 3925–32
[20] Li X et al 2009 Science 324 1312–4
[21] Kim S, Nah J, Jo I, Shahrijerdi D, Colombo L, Yao Z, Tutuc E and Banerjee S K 2009 Appl. Phys. Lett. 94 062107
[22] Xu H, Chen Y, Zhang J and Zhang H 2012 Small 8 2833–40
[23] Lee Y G, Kang C G, Cho C, Kim Y, Hwang H J and Lee B H 2013 Carbon 60 453–60
[24] Riikonen J, Kim W, Li C, Svenski O, Arpiainen S and Lipsanen H 2013 Carbon 62 43–50
[25] Kim W, Riikonen J, Li C and Lipsanen H 2013 Nanotechnology 24 395202