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Using a dedicated combination of the non-equilibrium Green function formalism and large-scale density functional theory calculations, we investigated how incomplete metal coverage influences two of the most important electrical properties of carbon nanotube (CNT)-based transistors: contact resistance and its scaling with contact length, and maximum current. These quantities have been derived from parameter-free simulations of atomic systems that are as close as possible to experimental geometries. Physical mechanisms that govern these dependences have been identified for various metals, representing different CNT-metal interaction strengths from chemisorption to physisorption. Our results pave the way for an application-oriented design of CNT-metal contacts.

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Carbon nanotube (CNT)-metal contacts play a crucial role in ensuring the success of CNT-based technologies—in particular, the technology of carbon nanotube field-effect transistors (CNTFETs). Minimization of the contact resistance and its scalability with respect to the contact length have been the subject of many recent experimental researches. Several materials and geometries have been investigated with the goal of optimizing the electrical CNT-metal contact properties.

The development of CNTFET technology would benefit from a better understanding of the physical mechanisms that determine the electrical properties of CNT-metal contacts (hereinafter, we restrict ourselves with side-contact geometries of metal/CNT contacts; end-contacts will be considered separately). The CNT-metal contact, however, is a new type of contact in electronics. Hence, it cannot be fully understood within the conventional paradigms, such as Schottky barriers or the transmission line model. Moreover, existing experimental data suggest that the charge carriers enter the metal-covered part of a tube gradually over distances up to 200 nm. Standard density functional theory (DFT)-based non-equilibrium Green function formalism (NEGF) methods become prohibitively expensive for simulating CNT-metal contacts limited to contact lengths/lengths, which is one to two orders smaller than the relevant dimensions. A new, dedicated combination of NEGF and DFT has been developed recently to treat this range of the contact lengths. In these publications, the ideal case of a fully covered tube resulting in the maximal achievable contact area was considered. In practice, however, fabrication typically leads to incomplete tube coverage. For example, a CNT can be placed on the dielectric substrate or on top of an electrode; “nanoislands” of the metal (Ti or Cr) can also lead to an imperfect CNT-metal interface.

So far, the impact of partial CNT coverage on the contact resistance, the on-state current flowing through a transistor, and the scalability of the contact resistance is not clear.

In this report, we study the impact of the degree of the metal coverage on the contact properties of CNT-metal contacts. To this end, we use a method based on the combination of DFT and NEGF, which is specially designed to treat contacts with gradually injected charge carriers (extended contacts). Here, we extended the method to treat the contacts of CNTs covered partially by the metal. We selected three technologically relevant cases: (1) the tube is fully embedded into the metal contact (Fig. 1(a)), (2) the tube is lying on top of a dielectric and is “top-covered” with a metal contact (Fig. 1(b)), and (3) the tube is lying on top of the metal (Fig. 1(c)). These three cases were modeled by an unfolded (16,0) CNT (which corresponds to the practically

![FIG. 1. The upper panel shows a cross-section of each of the contact geometries: (a) fully embedded CNT; (b) top-covered (partially embedded) CNT; and (c) on-top geometry. The lower panel shows the approximations used to represent each of the three geometries. We used unfolded CNT with a circular periodical boundary condition, and 100%, 50%, and 12.5% coverage rates to map each of the real contact geometries.](http://dx.doi.org/10.1063/1.4962439)

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relevant diameter of 1.25 nm) with cyclic periodic boundary conditions (CPBC). The CNTs are covered by the metal at 100%, 50%, and 12.5%, which maps each of the three geometries described above (Fig. 2 shows the central part of the simulated systems). These models are expected to describe the system of interest quite well. The system here consists of two CNT-metal contacts, separated by an uncovered CNT (Fig. 3). The distance between the left and right contacts (the channel length, \(L_{ch}\)) is \(\approx 9\) nm. We simulated these structures with different contact lengths \(L_c\), ranging from \(\approx 0.5\) nm to 400 nm. For comparison, we also simulated infinite contact lengths. In Ref. 19, it was shown that the metal contacts can be grouped with respect to the metal-CNT interaction strength into weakly (Pd, Sc, Pt, and Cr), intermediately (Rh, Au, Cu, and Al), and strongly interacting metals (Ni and Ti). All metals belonging to a specific group possess similar contact properties. Thus, we have simulated only one representative metal for each group—Pd, Rh, and Ti. This study can also be viewed from an alternative point of view: The degree of coverage can be thought of as a characteristic of an imperfection of an embedded contact. The coverage of 100% corresponds to the highest possible contact area, whereas the coverage rates of 50% and 12.5% correspond to low-quality contacts.

The initial information about the impact of the metal coverage rate on the contact resistance can be estimated already from the unbiased band diagram of our transistor-like structures. The band edges \((E_c, E_v)\)—derived from first-principle calculations, as described in Refs. 14 and 19—are shown in Fig. 4. For Rh and Pd contacts, the metal-induced doping of the embedded CNT part increases as the coverage rate increases. The channel remains slightly doped, and the transition region between these two regions resembles a \(p^+-p\) junction with different potential barriers for holes, depending on the coverage rate. In the case of a Ti-CNT contact, the CNT part covered by Ti is metalized in the sense that the projected density of states onto carbon orbitals has no band gap in contrast to the pristine (16,0) CNT. The electrostatic barriers between the covered and uncovered CNT regions for majority charge carriers (electrons for Ti-contacted CNTFETs) are of a Schottky-like type. Changes in the band profiles depending on the coverage rate are considerable only at the ends of the uncovered tube region (channel), which are weakly controllable by a gate electrode in real CNTFETs.

Quantitatively, the electrical quality of the contact can be characterized by a contact resistance \(R_c\), which is defined at a low drain-source voltage \(V_{ds}\) and sufficiently high over-drive voltage \(\pm(V_{gs} - V_{th})\), where \(V_{gs}\) and \(V_{th}\) are gate-source and threshold voltages, correspondingly; the signs “+” and “−” correspond to \(n\)- and \(p\)-type field-effect transistors (FETs), respectively. As far as (i) we do not intend to resemble the electrostatics of any particular device geometry and (ii) we are interested in very low drain-source voltages, we can readily include the influence of a gate electrode using the well-established approximation as follows. The potential felt by an electron in the tube due to the gate-source voltage is considered in accordance with Ref. 21

\[
V_{ch}(V_{ds}, V_{gs}) = -V_{gs}e^{-\frac{z_L}{z_c}} + V_{gs} + (V_{ds} - V_{gs})e^{\frac{z_L}{z_p}},
\]

where \(z_{L(R)}\) is a left (right) end of a channel.

The screening length \(\lambda\) characterizes the effectiveness of the gate control. It is related to the tube diameter and the oxide layer thickness via an empirical formula:22

\[
\lambda = \sqrt{\left(\varepsilon_{CNT}/\varepsilon_{ox}\right)d_{CNT}d_{ox}},
\]

where \(\varepsilon_{CNT}\) and \(\varepsilon_{ox}\) are the dielectric permittivity of the CNT and the oxide, respectively; \(d_{CNT}\) and \(d_{ox}\) are the CNT diameter and the oxide layer thickness. We have chosen: \(\varepsilon_{CNT} = 5\) (according to Ref. 23), \(\varepsilon_{ox} = 15\), \(d_{CNT} = 1.25\) nm, and \(d_{ox} = 5\) nm, yielding a screening length \(\lambda = 2.55\) nm. These parameters correspond to a (16,0) CNT with a planar 5-nm-thick HfO\(_2\) gate. This is similar to the geometry of the device fabricated in Ref. 7. The contact resistance has been calculated at \(\pm(V_{gs} - V_{th}) = 0.2\) V and \(V_{ds} = 0.025\) V as the total resistance divided by two. \(V_{th}\) is defined as \(V_{gs}\), which superposes \(E_c\) (for Ti) or \(E_v\) (for Pd and Rh) in the center of the channel with the Fermi level. This method for calculating \(R_c\) places all the metals and geometries in the same reference situation and allows for an unambiguous comparison with experimental results.

Fig. 5 shows the impact of the coverage rate on the contact resistance of the infinitely long contacts \(R_c^\infty \equiv R_c(L_c \rightarrow \infty)\) for three different metal types. As the coverage rate increases, \(R_c^\infty\) of the Pd-CNT contact decreases until the barrier height is shrunk to zero, which occurs for a half-covered CNT (Fig. 6(a)). \(R_c^\infty\) for the Ti-CNT contact is governed by two competing factors. First, the chemical bond formation destroys the original band structure of the CNT.19 As a result,
the transmission coefficient is reduced within the whole energy range. The higher the coverage rate, the stronger is this effect (Fig. 6(d)). Second, the height of the electrostatic barriers decreases as the coverage rate increases from 12.5% to 50% (Fig. 6(c)). This leads to an opposite effect. The two effects are almost equilibrated between 12.5% and 50% coverage rates; correspondingly, \( R_{\infty} \) increases only slightly. For coverage rates higher than 50%, the electrostatic barriers remain nearly unchanged. They do not contribute anymore to the contact resistance. Hence, \( R_{\infty} \) is defined exclusively by the first factor yielding an \( R_{\infty} \) increment by \( \approx 1/4 \) as the coverage rate increases from 50% to 100%. Rh-CNT contact is not sensitive to the coverage rate, because the electrostatic barrier is thin and low, down to a coverage rate of at least 12.5%.

Finally, from the calculated contact resistance \( R_c(L_c) \) (see supplementary material), we have identified the effective contact lengths \( L_{\text{eff}} \) for each of the contact metals and different coverage rates (see Fig. 7(a)). \( L_{\text{eff}} \) characterizes the length scaling of \( R_c \) and it is defined by the expression \( R_c(L_{\text{eff}}) = 1.5R_1 \). That is, it is the length at which the contact resistance has been increased by one half, compared to the infinitely long contact.

From the dependence of \( L_{\text{eff}} \) on the coverage rate, we can conclude that the effective length is governed by the metal type and it depends on the coverage rate. This means the scaling behavior of \( R_c(L) \) can be improved by not only by selecting the proper metal contact but also by increasing the coverage rate. This conclusion is common for all metal contacts. Underestimated values of \( L_{\text{eff}} \) obtained in Ref. 19, which considers 100%-covered CNT-metal contacts, can thus be attributed to the imperfection (i.e., reduced contact area) of the devices fabricated in Ref. 7.

Metal-induced doping of a tube by Rh and Pd defines the maximum on-state current of CNTFETs \( I_{\text{max}} \) for these metal contacts. To quantify this effect, we calculated \( I_{\text{max}} \) according to

\[
I_{\text{max}} = 1.5R_1
\]
This expression is derived from the Landauer formula, assuming that the tube has $n_m = 2$ open channels (which is the number of channels of a $[16,0]$ CNT near the valence band edge) within the voltage range $[E_F; E_v]$ and assuming zero temperature (in Eq. (2), $e$ is an elementary charge and $h$ is a Planck’s constant). Fig. 7(b) shows $I_{\text{max}}$ calculated for infinite Rh and Pd contacts depending on coverage rate. For a Ti contact, we cannot use these simple estimations of current, since electrons are injected from the gap-free composite CNT-metal system.

In conclusion, the metal coverage rate influences the electrical properties of CNTFET contacts differently depending on the strength of the CNT-metal interactions. For metals interacting weakly with a CNT (e.g., Pd), a larger coverage rate improves the electrical properties of a CNT-metal contacts in all regards: (i) $R_c$ of infinitely long contacts decreases due to lowering of the potential barrier between the metal-covered and uncovered tube parts; (ii) effective contact length $L_{\text{eff}}$ drops as the area of the contact increases; maximum current $I_{\text{max}}$ increases due to higher metal-induced doping. With respect to the contact resistance scaling and maximal on-state current of a transistor, the Rh-CNT contact (Rh is a metal that has an intermediate interacting strength with a CNT) closely resembles Pd-CNT contacts. However, the $R_c^{\infty}$ of the CNT-Rh contact is not sensitive to the coverage rate. This makes CNTFETs with long Rh contacts not sensitive to the possible variability of the contact coverage quality, which could be practically important. In contrast to Rh-CNT and Pd-CNT contacts, the $R_c^{\infty}$ of the Ti-CNT contact is governed by two competing factors, which makes the Ti-CNT contact with 12.5% coverage less ohmic than that of a full- or half-covered contact. Although the Ti-CNT contact possesses good scaling behavior for all considered coverage rates, it always remains high-ohmic.

See supplementary material for the technique of $L_{\text{eff}}$ extraction from the $R_c(L_c)$ dependences, details of the combined NEGF and DFT method, and the geometry of the atomistic systems.

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