Effect of Metal Coupling on Schottky Barrier Height Extraction

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***Abstract* — This paper investigates the impact of metal contact coupling strength and Fermi energy on temperature-dependent currents and the extraction of Schottky barrier height. As the scaling of contact length becomes increasingly important, understanding the role of metal coupling in establishing good contacts with low-dimensional materials is crucial. A coupled mode-space NEGF approach with Schottky contacts that accounts for the coupling strength between metal and carbon atoms is utilized to simulate the temperature-dependent currents in CNT devices. For weakly coupled contacts, the effective Schottky barrier height at the on-state is comparable to the flat band value, while for strongly coupled contacts, it can be reduced to the point of becoming negative, implying distinct degrees of dominance between thermal-assisted and direct tunneling. These findings may guide experimental measurements and inform strategies to achieve high-quality contacts with low-dimensional materials for scaled devices.**

Keywords- Low dimensional material, Contact resistance, Schottky barrier extraction, metal coupling, NEGF

I. INTRODUCTION

Increasing transistor density through continuous scaling of lateral dimensions is a key direction for meeting the demands of data-intensive computing applications [1]. The challenges of scaling Si technology has stimulated interests in low dimensional materials (LDMs), such as two-dimensional (2D) transition metal dichalcogenides (TMDs) and 1D carbon nanotubes (CNTs) [2, 3]. One of the most significant challenges associated with LDMs is their contact with metals. The alignment between the metal Fermi energy E_F and the semiconductor conduction/valence band edge E_C/E_V is a critical factor that determines contact resistance R_C. To determine the barrier height, temperature-dependent measurements are typically used to differentiate the mechanisms of current injection [4]. However, unlike contact to bulk material, the LDM underneath the contact is atomically thin. The Schottky barrier model, commonly used in bulk materials, is inadequate for explaining the injection of carriers across metal and LDMs due to the lack of well-defined band dispersion in the out-of-plane direction. Additionally, the interaction between the contact metal and LDMs further complicates the situation [5].

Therefore, in this paper, we aim to examine how the coupling strength between the contact and LDMs influences temperature-dependent currents and the extraction of Schottky barrier height. This work focuses on CNT channels, where the impact of metal coupling can be more significant compared to the diffusive-limited “current crowding” effect and is crucial for R_C when aiming to reduce the contact length L_C, due to their long mean free paths [5, 6].

II. METHODOLOGY

To simulate device performance at various temperatures (T), we employ a coupled mode-space Non-Equilibrium Green's Function (NEGF) approach, utilizing a k.p electronic Hamiltonian [7] and incorporating phonon scattering in the self-energy term [8]. The carrier flow between the extension leads and the source/drain (S/D) electrodes is described by Schottky contacts formed at the metal-CNT interfaces, where the alignment between the metal Fermi energy (E_F) and the semiconductor conduction/valence band edge (E_C/E_V) is defined. In the case of side-bonded contacts, a diagonal term, $-i\Delta$, representing the coupling strength (Δ) between the metal and carbon atoms, is included in the CNT Hamiltonian (fig. 1a) [10, 11]. While Δ can be determined from *ab initio* calculations [10, 12], it has been observed experimentally that contact properties can exhibit significant variability even with the same contact metal [13]. This variability could be attributed to different metal wetting on the CNT surface during fabrication [10, 14]. In our study, we focus on zigzag (13, 0) CNTs with a diameter of approximately 1 nm, as they offer a good compromise between on-state current (I_{ON}) and off-state current (I_{OFF}) [3, 5]. The device structure and a representative wrap-around contact are shown in fig. 1. The results obtained are also applicable to different contact geometries and channel materials.

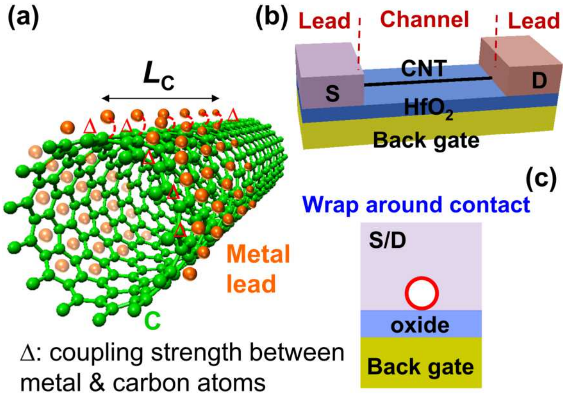

Fig. 1 Schematic representation of (a) the coupling strength Δ between metal and carbon atoms of the CNT, (b) CNT Schottky barrier FET structure with 5 nm HfO_2 based on the experiment [13], and (c) cross section of wrap-around contact geometry employed in simulations.

III. RESULT & DISCUSSION

The significance of metal coupling strength Δ and Fermi energy E_F in establishing good contacts for scaled L_C is highlighted in fig. 2, where a comparison of theory and experimental data for I_D-V_{GS} and R_C-L_C is presented [5]. For low $|V_{GS}|$ in fig. 2a, contacts with weaker coupling strength (Δ=3.5 and 10 meV) exhibit higher current I_D and transconductance G_m compared to contacts with stronger coupling (Δ=0.3 eV). However, as $|V_{GS}|$ increases, I_D saturates while G_m decreases for weakly coupled contacts. This observation suggests that a strongly coupled contact requires high extension doping N to improve R_C in a CNT MOSFET (CNFET), whereas improving R_C through high N for weakly coupled contacts is less efficient.

Understanding the relationship between R_C and L_C is crucial for scaling assessment, as depicted in fig. 2b with a comparison to experimental data [5]. Stronger coupling contacts show a lower change in R_C with L_C, enabling the possibility of extreme contact length scaling. In contrast, the R_C of weakly coupled contacts increase exponentially for short L_C. This behavior is attributed to the physics of Breit–Wigner resonances at balanced coupling [11]. For small Δ, the coupling between metal lead and CNT becomes excessively weak for short L_C, involving only a few bonding atoms. Consequently, strong enough coupling contacts with high extension doping and a low energy difference between E_F and E_V/E_C are desirable for scaled CNFETs.

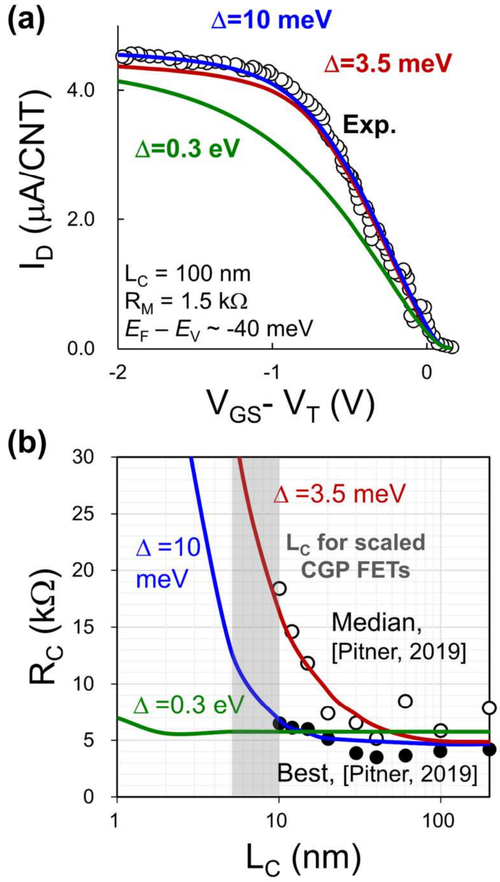

Fig. 2 Redraw from Ref. [5]. (a) I_D versus V_{GS}-V_T for different coupling strength Δ=0.3 eV (green), 10 meV (blue), and 3.5 meV (red). Contact length L_C is 100nm and V_{DS}= -0.05 V. E_F is ~40 meV lower than valence band edge E_V of CNT. Metal wire resistance R_M=1.5 kΩ is included for comparing with experimental data (symbol) [13]. (b) R_C as a function of L_C for theory with different coupling strengths (lines) and experimental data (open symbol: median; filled symbol: best from [13])

To establish a connection between E_F, Δ, and measurable electrical quantities, we conduct simulations to investigate the temperature dependence of I_D and determine the effective Schottky barrier height (SBH) at the contacts. Devices with weak and strong coupling contacts exhibit contrasting temperature dependencies at high $|V_{GS}|$, as depicted in fig. 3. Specifically, the I_D of weak coupling contacts increases with increasing temperature, while the I_D of strong coupling contacts decreases. By analyzing the Arrhenius plot, we extract the SBH, which aligns with the energy difference between E_F and E_V at the flat band. However, in the case where $E_F < E_V$ for pFETs, there is still a slight positive SBH present at the flat band. It is important to note that the extracted SBH corresponds to the energy difference between the CNT within the metal contact and the channel in the transport direction even for side-bonded contacts. It should be acknowledged that there is no well-defined band dispersion on the side of the CNT in these contacts. Consequently, it is inappropriate to define a "SBH" between the metal and CNT for side-bonded contacts. Instead, the transmission between the metal and carbon atoms is described by the coupling strength Δ, which is assumed to be temperature independent. This assumption is reasonable considering that carrier injection across the van der Waals gap between the metal and low-dimensional materials (LDMs) should occur through direct tunneling, which is temperature insensitive from an atomistic perspective.

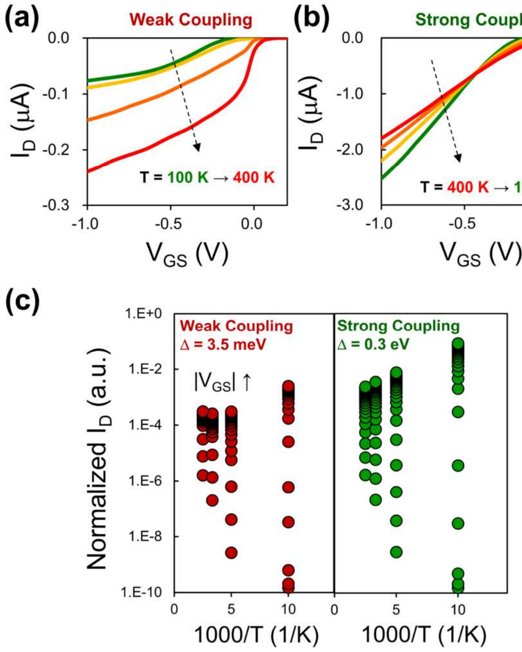

Fig. 3 I_D-V_{GS} for weak coupling Δ=3.5 meV **(a)** and strong coupling Δ=0.3 eV **(b)** at different temperatures T with E_F-E_V = 130 meV. **(c)** Corresponding Arrhenius plot: Normalized I_D by a factor $T^{\frac{N+1}{2}}[\exp\left(\frac{qV_{DS}}{k_BT}\right)-1]$ with N=1, V_{DS}= -0.05V versus 1000/T for different V_{GS}.

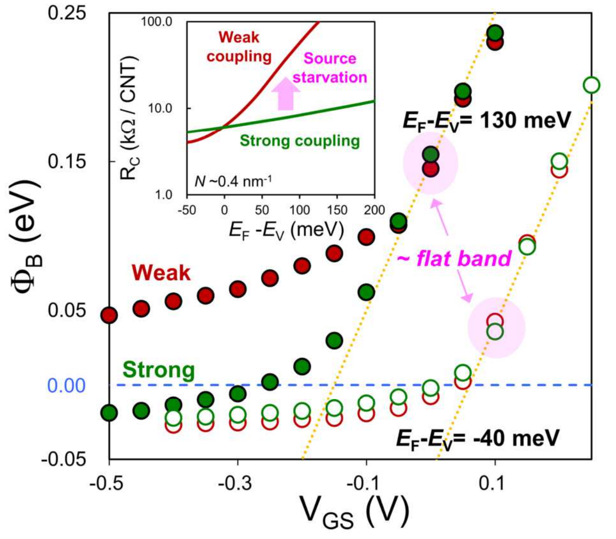

Fig. 4 Extracted barrier height Φ_B versus V_{GS} for weak (red Δ=3.5 meV) and strong (green Δ=0.3 eV) coupling contacts with long L_C 100 nm. Filled symbol: E_F-E_V = 130 meV; open symbol: E_F-E_V = -40 meV. Inset shows the impact of E_F on R_C for strong (green) and weak coupling (red) contacts with 100 nm L_C and ~0.4 nm^{-1} carrier density N.

Apart from extracting the SBH at the flat band, it is also possible to uncover the metal coupling strength, which has not been previously detected through temperature-dependent measurements, by analyzing the bias-dependent SBH. In the case of strongly coupled contacts, the SBH at high $|V_{GS}|$ (on-state) can be significantly lower than its value at the flat band, and it may even become negative, indicating dominant tunneling processes associated with the small tunneling effective mass in CNTs as discussed in Ref. [4]. On the other hand, for weakly coupled contacts, the difference in SBH between the flat band and the on-state is relatively small, suggesting the presence of non-negligible thermal-assisted tunneling even at high $|V_{GS}|$.

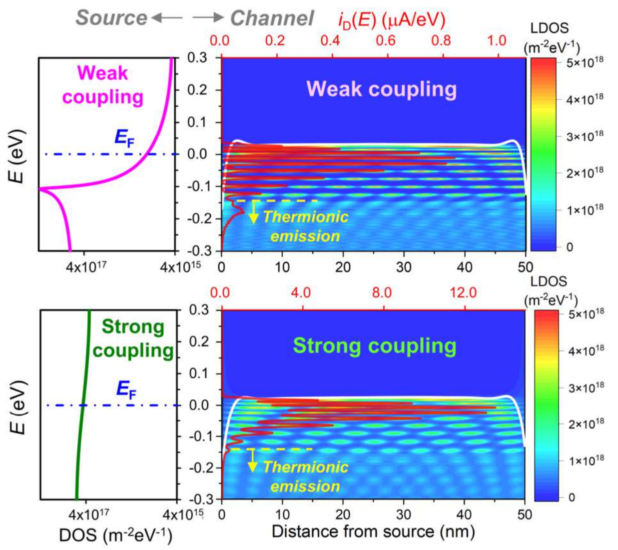

Fig. 5 (Left) density of states DOS of CNT at the source; (Right) Local density of states LDOS (colormap), valence band edge (white line) and energy resolved current $i_D(E)$ (red line, top x-axis) in the channel for weak Δ=3.5 meV (up panel) and strong Δ=0.3 eV (bottom panel) coupling strength contacts at V_{GS}= -0.5 V and 300 K corresponding to the case of E_F-E_V=130 meV of fig. 3 and 4.

The explanation for these observations lies in the density of states (DOS) of the CNT at the source and the energy-resolved current, $i_D(E)$, as depicted in fig. 5. In the case of weakly coupled contacts, the limited presence of metal-induced gap states (MIGS) around E_F inhibits the formation of tunneling states in the channel, leading to a reduction in tunneling current at the on-state. By comparing the energy distribution of the local density of states (LDOS) and the current spectrum in the channel between weakly and strongly coupled contacts, it becomes evident that there are distinct degrees of dominance of tunneling current (see fig. 5). Due to strong tunneling in strongly coupled contacts, the effective SBH at the on-state exhibits insensitivity to the E_F. Conversely, weakly coupled contacts display high sensitivity of the effective SBH to E_F. As a result, the R_C of weakly coupled contacts is more sensitive to E_F than that of strongly coupled contacts, even when the extension doping is high (~0.4 nm^{-1}) for CNFETs, as illustrated in the inset of fig. 4.

IV. CONCLUSION

We find that in addition to metal Fermi energy E_F and effective mass of semiconductor, the coupling strength of contact metal affects the dependence of effective SBH on gate bias. As $|V_{GS}|$ increases, the effective SBH decreases and can become negative for strongly coupled contacts, indicating dominant tunneling. Conversely, the effective SBH in the on-state is closer to the flat band value for weakly coupled contacts, implying that direct tunneling is less important due to limited MIGS. By examining the difference in effective SBH between the flat band and on-state, one can use temperature-resolved electrical measurements to gain insight into the coupling strengths of different metals, or even the same metal subjected to different fabrications.

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