Impact of functionalization patterns on the performance of CNTFETs

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INTRODUCTION

Covalent functionalization of carbon nanotubes (CNTs) might be an option to optimize the behavior of CNT field effect transistors (FETs) [1] (despite all related technological problems). In principle, the atoms or molecules used for functionalizing are placed randomly along the CNT or they are high-ordered in decoration patterns. Here, only high-ordered functionalization patterns are studied (*i*) to convert metallic CNTs into semiconducting CNTs and (*ii*) to reduce or to increase the ambipolarity of a semiconducting CNT.

Different numerical quantum-based device simulation methods at different abstraction levels ranging from ab-initio studies over tight-binding (TB) simulation methods to the solution of the effective-mass (EFM) Schrödinger equation are available for the simulation of functionalized CNTFETs. Here we discuss a path towards a multi-scale simulation approach for the functionalization of CNTFETs. Band structure calculations are performed using a simple orthogonal TB representation [2]. In a next step, the TB band structures are employed for calibrating the EFM simulator as used in [3] (which allows for an energy-dependent effective-mass) to study the ballistic transport behavior of covalently functionalized tubes.

Two chiralities are investigated: a seminconducting (14,0)-tube ($E_{\mathrm{g,clean}} \approx 0.8\,\mathrm{eV}$) and a metallic (10,10)-tube ($E_{\mathrm{g,clean}} = 0\,\mathrm{eV}$). The tubes are embedded into a three-dimensional CNTFET structure which is very close to the experimental device structure published in [4]. Only the $9\,\mathrm{nm}$ long CNT channel region is assumed to be functionalized. For both tubes, several functionalization patterns are studied where n (fn) C-atoms of a unit cell are arbitrarily chosen to be covalently functionalized. In general, covalent functionalization converts sp2-bonds to sp3-bonds and results in a reorganization of the remaining π-electron system and, hence, in a change of the electronic band structure including a change of the band gap and band curvature. The properties of the contact regions are left unchanged.

RESULTS

The transfer characteristic of the (10,10)-tube is shown in Fig. 1 for different functionalization patterns. It is obvious that the band gap (see inset of Fig. 1), which varies between $0\,\mathrm{eV}$ and $0.8\,\mathrm{eV}$ significantly impacts the $I_{\mathrm{on}}/I_{\mathrm{off}}$-ratio. The smaller the band gap the larger is the contribution of the band-to-band tunneling on the total current. Fig. 2 shows the output characteristic. Obviously, the larger the band gap, the smaller is the contribution of the band-to-band tunneling on the total current, and, thus, the stronger is the current saturation. For a reasonable saturation, a band gap of about $0.5\,\mathrm{eV}$ is required.

The transfer characteristics and the band structures for the functionalized (14,0) CNTFETs are shown in Fig. 3. The different current behavior for positive voltages can mainly be attributed to the different band gaps associated with the different functionalization patterns.

For comparison, experimental results [4] are shown in the same figure. The contact parameters are chosen such that the simulation results for the non-functionalized tube match the experimental results (see [3] for more information). From the simulation results one could conclude that some decoration patterns might be helpful to change the device ambipolarity and the associated $I_{\mathrm{on}}/I_{\mathrm{off}}$-ratio for a given tube chirality and contact formation.

The intrinsic transit frequency $f_{\mathrm{T,i}}$ for the (14,0)-tube is shown in Fig. 4. The different band gaps lead to more or less pronounced near-contact barriers (inset of Fig. 4) which significantly impact the peak of $f_{\mathrm{T,i}}$.

ACKNOWLEDGMENT

The authors acknowledge the Cfaed and the DFG project CL384/2-1 for financial support.

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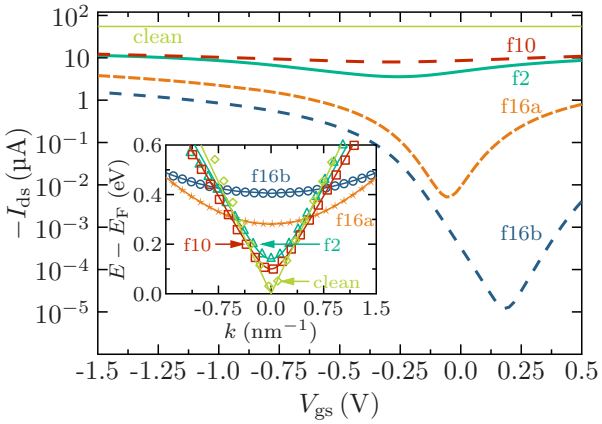

Fig. 1: Transfer characteristic of a 9 nm long (10,10)-tube with different functionalization patterns ($V_{ds} = -0.4$ V). The inset shows the related electronic band structures (symbols - TB results, lines - fit for EFM).

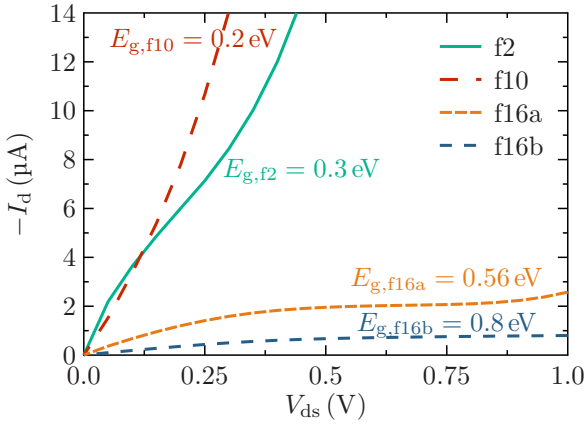

Fig. 2: Output characteristic of a 9 nm long (10,10)-tube for different functionalization patterns ($V_{gs} = -0.5$ V).

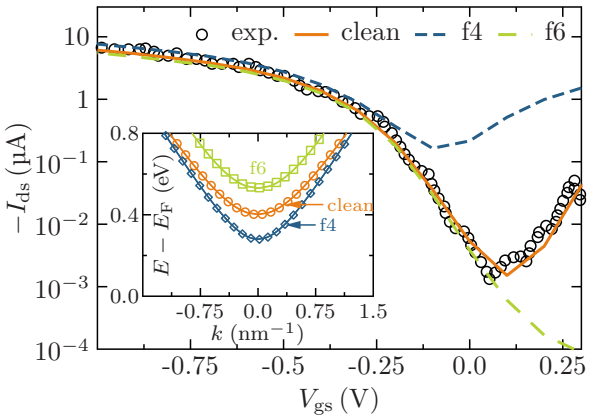

Fig. 3: Transfer characteristic for $V_{ds} = -0.4$ V for a 9 nm long (14,0)-tube for different functionalization patterns. The inset shows a comparison between the TB DOS (circles) and the band structure (solid lines) used in the EFM approach. The related band gaps are $E_{g,clean} = 0.8$ eV, $E_{g,f4} = 0.56$ eV and $E_{g,f6} = 1.1$ eV.

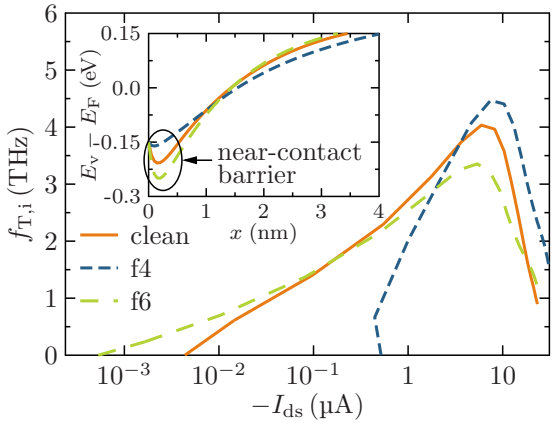

Fig. 4: Intrinsic transit frequency $f_{T,i}$ ($V_{ds} = -0.4$ V) for a 9 nm long (14,0)-tube for different functionalization patterns. The inset shows the valence band near the source contact at peak $f_{T,i}$.