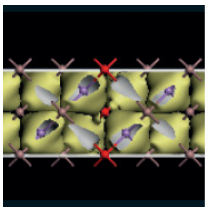

A hierarchical model for CNT and Cu-CNT composite interconnects: from density functional theory to circuit-level simulations

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Metallic carbon nanotubes (CNTs) and Cu- CNT composites have been regarded for years as one of the promising candidates for the future interconnects to replace Cu. Due to CNTs' small effective mass and 1-D structure, and strong C-C bonding, they have a very high ampacity, a large mean free path (λ), and excellent mechanical properties [1].

In this work, we have investigated the transport properties of CNT interconnects based on density functional theory (DFT) and compact model analysis. We also propose a hierarchical model to connect the DFT with circuit-level simulations.

We have used ATK [2] for DFT calculations involving the generalized gradient approximation (GGA). As the first step, a single-wall CNT (SWCNT) bundle as shown in Fig. 1 has been considered. In order to get optimal lattice constants, we have performed geometric optimization. All atoms are fully relaxed until the forces of any atom become less than 0.01 eV/Å. With the optimized atomistic structure, we have calculated the ballistic conductance (G_{bal}) at 300 K using the non-equilibrium Green's function (NEGF) formalism.

Fig. 2 shows G_{bal} of SWCNT bundles and stand-alone SWNCTs. The difference between them, caused by the interaction with the adjacent SWCNTs, decreases as the diameter of CNTs (D_{CNT}) increases.

Fig. 3 describes atomistic structures of iodine-doped SWCNT (24,0) and Cu- CNT(6,0) composite. In this work, the width (W) and height (H) of the local interconnect are assumed to be 8 and 16 nm, respectively, with reference to the ITRS node 2024 [3].

The resistance of the interconnect (Rw) made of SWCNT bundles, the doped SWCNT, bulk Cu, and the Cu-CNT composite is plotted in Fig. 4. For bulk Cu, we do not consider the surface and grain boundary scattering effects. To calculate the diffusive conductance ($Gdif$) from G_{bal}, we applied the mean free path approximation; $G_{dif} = G_{\mathrm{bal}}(1.0 + L/\lambda)^{-1}$, where $L$is the interconnect length. As can be seen in this figure, bulk Cu has smaller Rw for short interconnects. Due to the large λ of CNT, however, Rw of the SWCNT(6,0) becomes better as L increases. It is noticeable that Cu-CNT composite is characterized by combining the advantage of both Cu and CNT.

To calculate the propagation time delay ( ), we have considered a driverinterconnect-load system, as shown in Fig. 5. , , and C_L are assumed to be 35 kΩ, 7aF, and 14 aF, respectively [3]. The capacitance of the interconnect ( ) is defined by $C_W^{-1} = C_E^{-1} + C_Q^{-1}$, where C_E and C_Q are the classical electrostatic and quantum capacitances, respectively. CQ was extracted using the following relationship [4];

$$C_Q = \frac{e2}{4KT} \int D\,(E)\mathrm{sech}^2\frac{E}{2KT}\mathrm{dE}$$

where $D(E)$ is the density-of-states obtained from DFT-GGA calculations. The calculated CQ values are summarized in Table 1.

We have calculated t_d by using the Elmore formula; t_d = 0.69{(C_s +) + (R_wC_L +R_sC_w)+R_wC_w}. Fig. 6 shows the dependence of t_d on L and C_E. In this calculation, we assumed that C_E does not rely on the interconnect material. As expected, long interconnects have large t_d due to large R_w and C_w. When C_E = 10^{-3} pF/μm, the SWCNT(6,0) bundle has the smallest t_d because of its small Rw (See Fig. 4). As C_E increases (the feature size decreases), however, t_d of the SWCNT(24,0) bundle becomes smaller than that of the SWCNT(6,0) bundle because of the small C_Q of SWCNT(24,0).

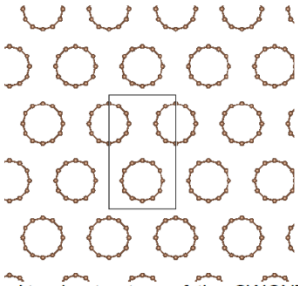

Fig 1. Atomic structure of the SWCNT(6,0) bundle. The black box indicates the primitive unit cell.

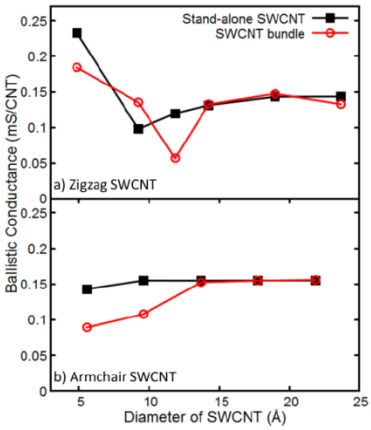

Fig 2. Dependence of G_{bal} on D_{CNT} of zigzag and armchair SWCNTs.

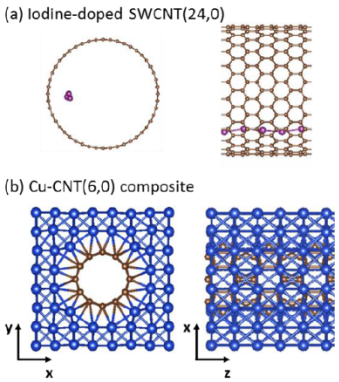

Fig. 3 Atomic structures of the iodine-doped SWCNT and the Cu-CNT composite.

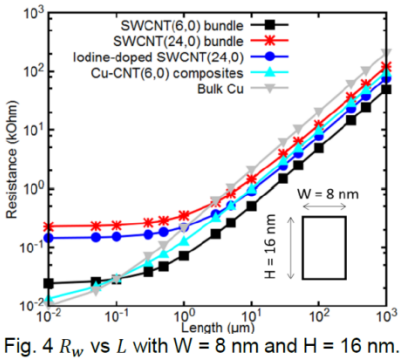

Fig. 4 R_w vs L with W = 8 nm and H = 16 nm.

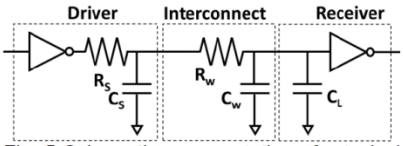

Fig. 5 Schematic representation of a typical interconnect.

Material	C_Q (pF/μm)
SWCNT(6,0) bundle	0.3227
SWCNT(24,0) bundle	0.0146
Iodine-doped SWCNT(24,0)	0.0321
Cu-CNT(6,0)	0.7370
Bulk Cu	0.7821

Table 1. C_Q of the interconnect with W = 8 nm and H = 16 nm at 300 K.

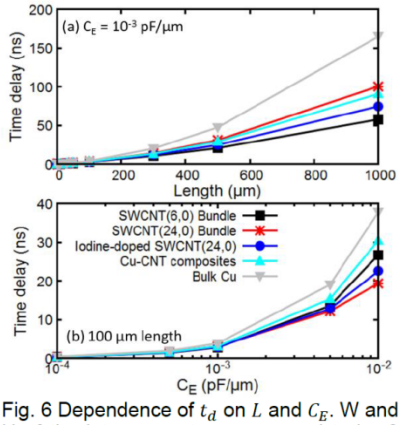

Fig. 6 Dependence of t_d on L and C_E. W and H of the interconnect are assumed to be 8 and 16 nm, respectively.

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