

A General Technique for THz Modeling of Vertically Aligned CNT Arrays

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Abstract-In this paper a general technique for the simulation of the single- and multi-wall carbon nanotubes is proposed based on a multi-conductor transmission line (MTL) model. The analytical form of the 2-port S-parameter is calculated from the 2n-port transfer matrix of the CNT array, which takes the mutual couplings of CNTs into consideration. The result is compared with that of previously used models. The simulated input impedance and absorption provides information of CNTs for potential THz applications.

I. INTRODUCTION

Carbon nanotube (CNT) is a seamless hollow cylinder with the wall thickness of only one single carbon atom. Since its discovery, it has attracted an increasing research interest due to its extraordinary electronic and mechanical properties. The vertically aligned CNT arrays can easily be synthesized with chemical vaporation deposition (CVD) and has potential applications as THz antennas, absorbers and VLSI interconnects. To explore its applications requires the study of modeling techniques, which have since been worked on by many researchers. Luttinger liquid theory was first used as a model of the CNTs' electrical properties in GHz and an RF transmission line (TL) model was derived from the theoretical analysis that predicts the wave velocity and characteristic impedance of a metallic single wall CNT [1]. Also, from 1-D electron fluid model a similar TL model was derived [2]. To reduce the high DC resistance of an isolated CNT, bundles of parallel CNTs have also been studied and an effective single conductor (ESC) TL model of both a stand-alone multi-wall CNT (MWCNT) and a single-wall CNT (SWCNT) array was derived in [3] and [4]. Finally, a diameter dependent circuit model was proposed in [5].

In the aforementioned ESC models however the magnetic inductance between CNTs are usually neglected, resulting in a simplification of the mutual coupling in the array. There have been studies that suggests when the CNT bundle becomes large, such simplification may not be valid and drew the conclusion that inductances should not be neglected [6]. In this paper we propose a full MTL model analysis and calculate the 2n-port transfer matrix of a CNT array. By incorporating with the terminal conditions the 2-port input impedance, S-parameters and absorption can be solved analytically with all the mutual coupling taken into calculation. Finally, the results of this technique and that of previous studies are compared and the potential application at THz is discussed.

II. MODELING TECHNIQUES FOR CNT ARRAYS

The geometry of the cross section of CNT array above a sufficiently large, perfect conducting ground plane is shown in Fig. 1.

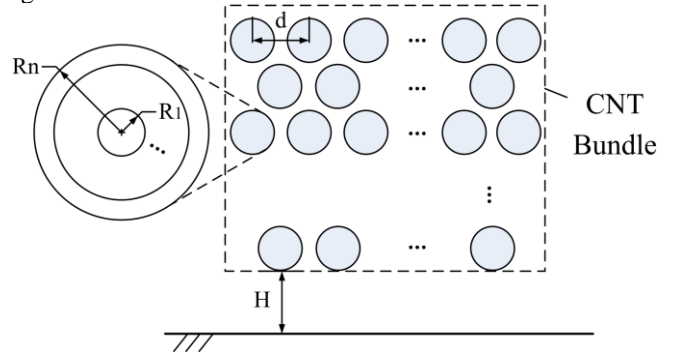


Figure 1. Configuration of MWCNT array above ground

The CNT inside the array can be either single wall or multi wall. In general, a CNT has n concentric shells, with the innermost shell radius R_1 and the outermost shell radius R_n . The distance between neighboring shells is set to be 0.34nm, as determined by the Van de Waals gap and the distance between the outermost shell of the CNT at the bottom of the array and the ground plane is H . If $n=1$, the CNT becomes a SWCNT, which can be modeled as several 1-D parallel channels connected in parallel. According to different chirality, SWCNTs can be categorized as armchair, zigzag or chiral, whose number of conducting channels N_c depends on the chirality, radius and temperature. Thus, a SWCNT can be either metallic or semiconducting. Armchair SWCNTs are always metallic with $N_c=2$ and for zigzag and chiral SWCNTs the average number of conducting channels n in an array follows [4].

$$N_c = \begin{cases} k_1 \cdot T \cdot r + k_2 & r > 650/T \\ 2/3 & \text{other} \end{cases}, \quad (1)$$

where $k_1 = 7.74 \times 10^{-4}$, $k_2 = 0.2$ and T is temperature. In this paper, room temperature (300K) is assumed in all simulations.

The difference from the TL model of CNTs and conventional TL is that apart from the electrostatic inductance

and capacitance, the kinetic inductance and quantum capacitance are also present due to the quantum band structure and 1-D electron movement. The per unit length RLC parameters of each shell can be described as [4]

$$R_i = \frac{h}{4n_i e^2 v_F \tau}, L_{k_i} = \frac{h}{4n_i e^2 v_F}, C_{q_i} = \frac{4n_i e^2}{h v_F}, \quad (2)$$

where τ is the diffusion time defined as the division of the mean free path (MFP) l_{eff} and the Fermi velocity v_F .

The mutual coupling between shells of MWCNT and neighboring SWCNTs in an array can be modeled with the well-defined electrostatic equations. From the MTL analysis [7] the matrix formed telegrapher's equation can be solved and thus the transfer matrix $[\Gamma]_{2n \times 2n}$ of the $2n$ -port network can be obtained and the transfer matrix $[\Phi]_{2n \times 2n}$ with quantum resistance R_s and contact resistance R_c at the terminal can be calculated using by cascading the terminal resistance matrix and Γ .

With the transfer matrix $[\Phi]$, it is possible to calculate the 2-port S-parameter of the CNT array, under the common mode excitation, i.e. all the CNTs in the array is connected in parallel at the two ports and excited with a same voltage $\vec{V}_s = [V_s \ V_s \ \dots \ V_s]^T$, the KCL and KVL equation can be easily written. Then, by further exploiting the common mode excitation conditions, the original KCL and KVL equations that contain $2n$ unknowns, i.e. the current flowing into and out of each CNT in the array, can be turned into a new set of equations with only 2 unknowns, namely the total current flowing into and out of the entire CNT array, which is sufficient to calculate the S-parameters of the CNT array.

$$\begin{cases} \sum \vec{I}(0) = \frac{\sum \sum ([\Phi_{22}] \cdot [\Phi_{12}]^{-1}) + P}{1 + z_0 \sum \sum ([\Phi_{22}] \cdot [\Phi_{12}]^{-1}) + z_0 \cdot P} \cdot V_s \\ \sum \vec{I}(l) = \frac{\sum \sum [\Phi_{12}]^{-1} \cdot [V_s - z_0 \sum I(0)]}{1 + z_0 \sum \sum ([\Phi_{12}]^{-1} \cdot [\Phi_{11}])} \end{cases} \quad (3)$$

where z_0 is the reference impedance at the source and load and

$$P = \frac{z_0 \left[\sum \sum [\Phi_{21}] - \sum \sum ([\Phi_{22}] \cdot [\Phi_{12}]^{-1} \cdot [\Phi_{11}]) \right] \sum \sum [\Phi_{12}]^{-1}}{1 + z_0 \sum \sum ([\Phi_{12}]^{-1} \cdot [\Phi_{11}])}$$

Note that in this process only terminal conditions and matrix transformation techniques are used and no simplification of the mutual coupling is made. Thus the result keeps the full cross-talk information inside the array.

Once the total port currents are solved, the input impedance, S-parameters and absorption for the CNT array can be easily calculated from (3).

III. RESULTS AND DISCUSSION

A. a stand-alone MWCNT

First of all, four stand-alone MWCNTs are simulated using the proposed model and the ESC model. The MWCNTs have a distance of 1um above ground and a length of 10um. The inner: outer radii are 2:4, 5:10, 10:20 and 8:24 respectively. As the estimated input impedance of CNTs is very high at several kilo Ohms, the reference impedance z_0 is set to the quantum diffusion resistance of the metallic SWCNT (6.5k Ω) and neglect the contact resistance which appears in reality where the connector touches the CNTs. Thus, a rough matching is achieved to make the S-parameter more visible. The simulation frequency is from 0.1 to 2 THz.

The simulated S11 and S21 results of the above four MWCNTs using MTL (solid) and ESC (dashed) model is shown in Fig. 2 (a) and (b). Clearly, the CNT with larger outer: inner radius ratio tends to give slightly more errors. Nevertheless the two models give almost identical results, indicating that neglecting the mutual coupling in a stand-alone MWCNT does not affect much the simulation results. This is expected because the walls in a MWCNT behave like conductors that shield the cross-talk between the inner and outer walls and restrict it only between directly neighboring walls [10]. Thus the influence of the mutual coupling is largely reduced and can be neglected.

The simulated input impedance Z_{in} is shown in Fig. 2 (c). The real and imaginary part both changes periodically across the frequency, showing the Fabry-Perot resonance due to the mismatching at terminals. Within each period, the imaginary part $[\text{Im}]Z_{in}$ cross the zero point twice, where the real part is the

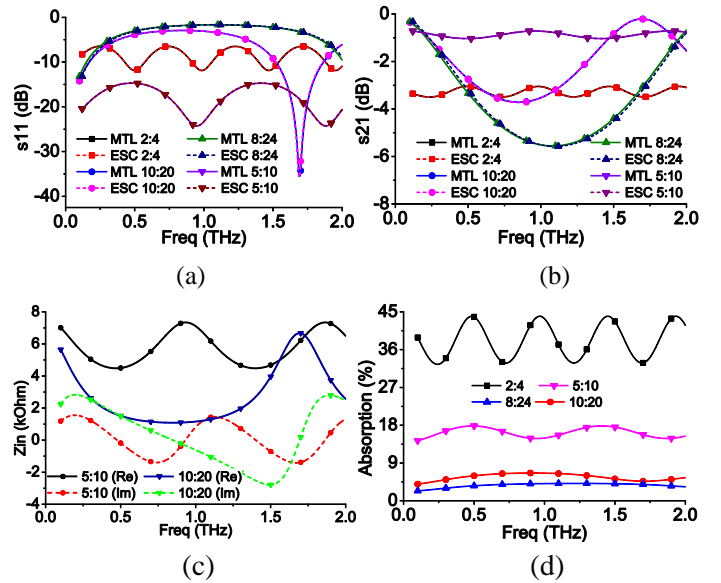


Figure 2. The simulated (a) S11 and (b) S21 results of four MWCNTs with different radius using proposed MTL model and ESC model.

minimum and maximum point, respectively. Also, for these two points, the S11 and S21 in Fig. 2 (a) and (b) reaches either maximum or minimum at the same time, according to the value of the reference impedance z_0 chosen. This is very interesting because while the minimum point of $[\text{Re}]Z_{in}$ can be used as the working frequency for antennas, the maximum point of $[\text{Re}]Z_{in}$ is potentially suitable to be used with THz photomixers, as they generally have a very high and real output impedance.

The absorption in Fig. 2 (d) shows that CNTs have very good absorbing capabilities, due to the large intrinsic impedance of the quantum wire. The smaller the radius of a CNT, the better absorber it is, as the conducting channels are connected parallel, the increase in their number reduces the overall resistance in the transmission. The maximum and minimum of the absorption of each CNT also appears at the two zeros points of the input impedance, where the minimum of $[\text{Re}]Z_{in}$ corresponds to the absorption peak and the minimum to the absorption valley, suggesting that the application with photomixers would have a higher efficiency than with antennas.

B. SWCNT arrays

Next, four SWCNT arrays are simulated using the proposed model and ESC model. The length of the arrays and distances above the ground remains the same as the MWCNT case, and the radius of the SWCNTs inside the array is 10nm. The array sizes are 2×2, 5×5, 10×10 and 20×20, respectively.

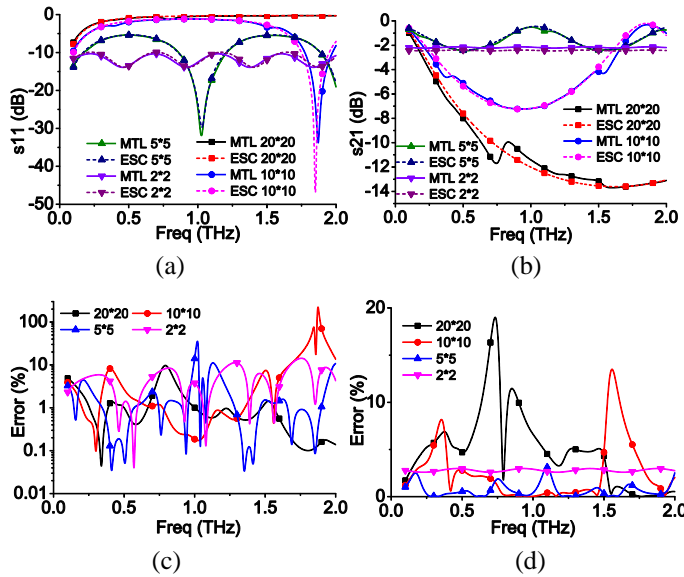


Figure 3. The simulated (a) S11 and (b) S21 results and the relative error of (c) S11 and (d) S21 between the proposed MTL model and ESC model for four different SWCNT arrays.

The simulated S-parameters are shown in Fig. 3 (a) and (b). Compared to the results of the stand-alone MWCNT, the SWCNT array shows more errors, due to the non-shielded coupling between every two CNTs inside the array. Several resonant points are present across the frequency, where the difference between two models is the largest. The relative errors are more explicitly shown in Fig. 3 (c) and (d). As seen, the maximum error for S11 occurs at the resonant frequency,

where the magnitude of the input impedance gets closest to the reference impedance z_0 while the error for S21 is mainly because of the lacking of consideration of mutual coupling when the wave propagates along the CNT array. The maximum error of S11 increases with the increase of the array size and for a 10×10 array it can reach more than 100%. As the simulated frequency is not high enough for the first resonant point to appear in a 20×20 array, the maximum is not shown, but it can be expected to be even higher than the 10×10 array. Similarly, the error of S21 in the 20×20 array, which is 19.08%, is also the highest in all four arrays simulated. So the conclusion for SWCNT arrays is that the ESC model is not suitable as the large mutual coupling between CNTs is no longer negligible in THz. This conclusion is supported by [6].

IV. CONCLUSION

In this paper a general approach of S-parameter analysis for an arbitrary MWCNT bundle has been proposed based on the MTL modeling techniques. A comparison with previously used ESC model shows that for large CNT arrays the ESC model introduce large errors. The S-parameters analysis shows that there are several resonant points periodically distributed across the frequency band. Due to large input impedance, in terms of interconnection application, the size of the CNT and bundle must be such that the input impedance can achieve a matching to the reference impedance in the desired frequency band. The input impedance simulation provides potential THz application with high output impedance devices. Finally, the absorption analysis shows that for small bundles, one of the potential applications is wideband nano-absorbers that can be more effective than traditional absorbers while still being much more compact in size.

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