Asymmetric Carbon Nanotube Dimers for Novel Sensing Applications

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***Abstract*—**In this work, we study the use of asymmetric carbon nanotube (CNT) dimers for the contactless detection of foreign nano-particles. Asymmetric CNT dimers create a unique field distribution, through the electromagnetic coupling, which in turn generates two distinct resonances representing the bonding and anti-bonding modes. The presence of a foreign nano-particle (NP) in the vicinity of the CNT dimer perturbs the dimer's field distribution and causes the bonding and anti-bonding resonances to shift by unequal amounts depending on the NP location. By studying the difference in the shift of the bonding and the anti-bonding resonances, we show that the NP relative location can be reconstructed. The computational experiments performed in this work show how asymmetric CNT dimers can be used for novel sensing applications.

***Index Terms*—**Anti-bonding modes, bonding modes, carbon nanotubes (CNTs), dimers, sensors.

I. INTRODUCTION

Carbon nanotubes (CNTs) are rolled versions of two-dimensional graphene sheets forming single-walled (SWCNT) or concentric multi-walled (MWCNT) tubes with high aspect ratios and exceptional mechanical, thermal and electrical properties [1]. Recent experimental and computational studies have demonstrated the existence of localized surface plasmon resonances (LSPR) in CNTs which vary depending on the CNT's length, shape, and environment [2]. This has paved the way for several potential applications of CNTs including nano-antennas, emitters, detectors, polarizers, and THz absorbers. [2]. In most of these applications, the CNTs are studied in bulk agglomerated form or in a large array [3]. A CNT pair, termed as CNT dimer, has recently received rising interest. If two CNTs of comparable dimensions are arranged in close proximity, they exhibit strong electromagnetic coupling and develop bonding and anti-bonding modes or resonances [4]. In the bonding resonance (BR), the currents of the two CNTs are in phase whereas in the anti-bonding resonance (ABR) the currents of the two CNTs are out of phase. This phenomenon exhibited by a CNT dimer is similar to the energy level splitting effect under optical illumination in plasmonic nano-particle assemblies [5].

We have re-investigated this dual-mode feature of CNT dimer and shown its potential in sensing applications. In order to get a strong expression from both the ABR and BR, we used length asymmetry in the CNT dimer assembly [4]. Each of these modes shows a unique near-field distribution that is sensitive to any external perturbations. Our analysis shows that the presence of an external nano-particle (NP) in the vicinity of the CNT dimer will perturb the near-field distribution and produce unequal shifts in the BR and ABR, depending on the particle location. The unequal shifts in the resonances can then be translated into a measure of the external NP's location.

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II. COMPUTATIONAL MODELLING

The far-field electromagnetic response of the CNT dimer assemblies was calculated using our in-house full-wave Method of Moment (MOM) algorithm for Arbitrary Thin Wires (ATW) [4], and the near-field response was calculated using commercial electromagnetic solver FEKO [6]. The schematic configuration of the CNT dimer along with a foreign NP (a 50 nm long perfectly conducting nano-wire) is shown in Fig. 1 (a). Both the CNTs and the foreign NP are positioned in the *xy*-plane and aligned parallel to the *x*-axis. The assembly in Fig. 1 (a) is excited with a normally incident plane wave with an *x*-polarized electric field. Both CNTs are single-walled, have an armchair (9, 9) chirality, and a radius $a = 0.61\ nm$. However, to create an asymmetric dimer, the CNTs are chosen of slightly different lengths, 96 nm and 86.4 nm separated by a constant gap of $20a = 12.2\ nm$. The position of the foreign NP is varied schematically over the five different locations as highlighted in Fig. 1 (b).

III. ISOLATED CNT VS ASYMMETRIC CNT DIMER

In Fig. 2 (a), we compare the absorbed power of an isolated 96 nm long CNT1, in the absence of CNT2, versus that of an asymmetric CNT dimer. The asymmetric dimer exhibits two resonances whereas the single CNT exhibits only a single resonance. Fig. 2 (b) shows the *x*-component of the near electric field generated by a single CNT. Fig. 2 (c) and Fig. 2 (d) show the *x*-component of the near electric field generated by the asymmetric CNT dimer at the ABR and BR, respectively. Apart from the differences in magnitude, the near-field pattern changes considerably from the isolated CNT to the dimer case as shown in Fig. 2 (b) to Fig. 2 (d). These differences in the near-field distribution help in sensing the relative location of the foreign NP.

IV. SENSITIVITY TO FOREIGN NP LOCATION

Keeping all the previous parameters constant, we varied the *y*-location of the foreign NP symmetrically about the dimer axis

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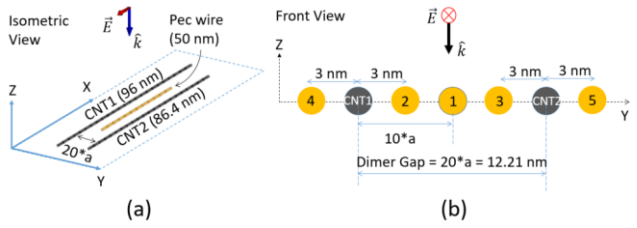

Fig. 1. (a) Asymmetric CNT dimer along with a PEC nano-wire placed at the center of the dimer gap excited with an *x*-polarized normally incident plane wave, and (b) schematic view of five different *y*-locations of the PEC nano-wire on the same plane as the CNT dimer.

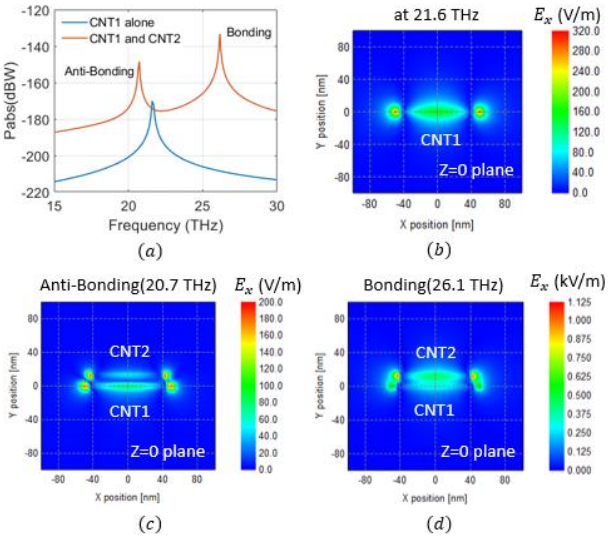

Fig. 2. (a) Absorbed power spectrums: CNT1 alone Vs CNT Dimer with 20a dimer gap (calculated by in-house algorithm). (b) Magnitude of E_x near-field component for CNT1 at 21.6 THz. (c) CNT-dimer at 20.7 THz (Anti-bonding mode). (d) CNT-dimer at 26.1 THz (Bonding mode). (Simulated in FEKO 3D MOM solver [6]).

as shown in Fig. 1 (b), and calculated the corresponding absorbed power spectrums as shown in Fig. 3. The percentage shifts in resonances relative to unperturbed dimer configuration have been tabulated in Table 1. When the foreign NP is placed in Position 1, it produces almost no shift in the ABR but a large shift in the BR. This is because, in the middle of the dimer, the anti-bonding mode has a vanishing near-field (Fig. 2 (c)) whereas the bonding mode has a strong near-field (Fig. 2 (d)). Moving the NP from Position 1 to Position 2, i.e., close to CNT1, where the anti-bonding near-field increases (Fig. 2 (c)) causes an increasing shift in ABR. The shift in BR remains the same since there is no relative change in the bonding mode near-field between Position 1 and 2 (Fig. 2 (d)). The opposite happens when we move NP from Position 1 to Position 3. If the NP is not in the dimer gap and is close to CNT1 (Position4) we see a comparatively bigger shift in ABR compared to BR. The opposite happens when we place NP at Position 5. Therefore, the main conclusion from Fig. 2., Fig. 3. and Table I is that the shifts in ABR and BR are proportional to their respective near-field intensity values at the location of the NP. However, due to the non-linear nature of the near-field variation (Figs. 2 (c)-(d)), the resonant frequency shifts will have a non-linear relationship with the NP position. There are many ways to control the near-field distribution of the dimer modes, such as by varying the CNT shape, orientation, conductivity, and dimer gap. The inclusion of these parameters can give extra degrees of freedom to the existing model.

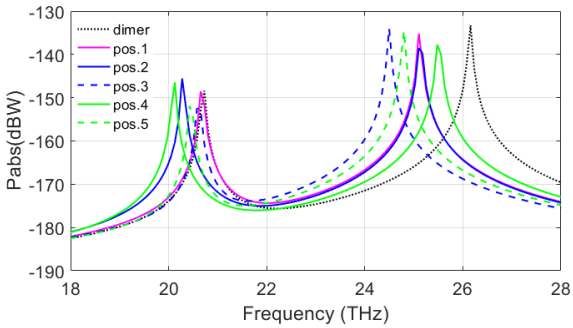

Fig. 3. Sensing foreign NP location by observing relative shifts in bonding and anti-bonding resonances of CNT dimer (calculated by in-house MOM algorithm). 1

Table 1: Shift in resoances compared to unperturbed dimer

Position of NP	Shift in Anti-bonding Resonance	Shift in Bonding Resonance
1	-0.38%	-4.05%
2	-2.17%	-4.05%
3	-0.38%	-6.34%
4	-2.89%	-2.6%
5	-1.45%	-5.2%

V. Conclusion and Future Work

The unique sensing abilities of asymmetric CNT dimers have been presented with several computational experiments. This study reveals that the location of a foreign NP can be traced by mapping the relative frequency shifts of dimer anti-bonding and bonding mode resonances. However, the sensitivity and reliability of this mechanism may have a dependency on the geometrical and material properties of CNTs as well as target NP. A more detailed analysis is required to set the allowable tolerance levels for this mechanism to work precisely.

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