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Mapping the resonance wavelengths of MWCNT as an optical nanoantenna

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Abstract We investigated the surface plasmon resonances of multi-wall carbon nanotube (MWCNT) for applications as the optical antenna. We calculated the near-field and far-field response of MWCNT using finite integral technique. In addition, the effect of shape and dimensions on the optical response of MWCNT was studied. Also, the dielectric properties of MWCNT obtained from the experimental results in the literature were fitted with a Drude–Lorentz model. Finally, a full mapping of the geometry (length and radius) dependence for MWCNT was presented and discussed.

Keywords Optical antenna · Multi-wall carbon nanotube · Surface plasmon resonances · Dielectric properties

1 Introduction

Optical nanoantennas have attracted great research interest due to their ability to localize surface plasmon (SP) resonance and redirect optical energy radiation (Liu et al. 2008). Optical nanoantennas have potential applications in bio-sensing, high resolution microscopy, and molecular communication, optical inter-connections, and communication between nano-electronic devices (Thammawongsa et al. 2012). Also, optical antennas hold great promise for increasing the efficiency of photovoltaics and LEDs (Pillai and Green 2010; Gao et al. 2010). There are some differences between radio and optical antennas, mostly given by the

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dielectric permittivity of metals. At optical frequencies, metals no longer behave as perfect conductors. The optical response of metal is described by a complex frequency dependent dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + \imath\varepsilon_2(\omega)$, which in turn affects the relation between the electric field $E(\omega)$ and the induced polarization density $P(\omega) = \varepsilon_0[\varepsilon(\omega) - 1]E(\omega)$; hence the associated skin-depth is comparable to the size of the nanoantennas. Thus a different wavelength scaling is required for the optical analogue of a $\lambda/2$ antenna (Bharadwaj et al. (2009)). Consequently, apart from the dielectric constants the same electromagnetic tools can be used for radio and optical antennas. For many years, nanoantennas development is slow because of technological difficulty in accessing nanoscale accuracy, but now the impressive improvements in nanotechnology have removed this main limit and opened up the possibility to build antennas operating in the visible and infrared spectral ranges (Simon and Gonzales 2011). For example, novel nanostructures such as carbon nanotube (CNT) can be used as optical antenna.

Generally, Au, Ag, Al and Cu have been used so far as the materials for metallic optical antennas. In terms of spectral properties, gold and copper are excellent candidates to build antennas for the red and near-IR spectral region while silver and aluminum are preferred for the blue–green part of the visible spectrum. Another factor which should be taken into account is the chemical stability of antenna materials. Cu and Ag are known to quickly corrode under ambient conditions, while Al is known to form a thin passivation layer of Al_2O_3. Au combines a favorable dielectric function in the red and near IR with excellent chemical stability and hence, it is the material that is extensively used in the experiments (Biagioni et al. 2012). Carbon nanotubes have been shown to exhibit light antenna behavior, such as polarization and length dependence, and enhancement of incident electromagnetic radiation at resonance (Wang et al 2004). Also, it had been shown that a single multi-wall carbon nanotube (MWCNT) acts as an optical antenna whose response is fully consistent with conventional radio antenna theory (Kempa et al. 2007).

The design of an optical nanoantenna requires great care since the conventional radio-frequency and microwave design rules that describe antenna parameters as a function of the operating wavelength are no longer valid (Dattoma et al. 2011). To the best of our knowledge, the dependence of resonant wavelength of MWCNT, as an optical antenna, on its geometry has not been reported in the literature. In this paper, we discuss this aspect feature for metallic MWCNT, considering an important step in design. Also, the spectral region where MWCNT can be applied is presented.

2 Modeling and simulation setup for MWCNT nanoantennas

2.1 MWCNT construction and optical properties

Carbon nanotubes were first discovered by Iijima (1991). CNT can be considered as a rolled graphene sheet and classified to single wall (SWCNT) or multi-wall (MWCNT) according to the number of rolls. The way the graphene sheet is rolled to form a nanotube cylinder affects the band gap of SWNT and hence its electrical conductivity. MWCNTs are mostly metallic and are able to carry high current densities. Also, MWCNTs have more regular and uniform optical properties due to their large size (Abdullah et al. 2013). MWCNT consists of concentric cylinders, having a hemispherical cap at tube ends. The normal concentric cap and tube spacing's are very close to the graphite half-cell spacing of 3.4Å (0.34 nm) (Murr 2008). Then the final shape of MWCNT is the same as nanorod antenna.

It has been reported that the general optical features observed in MWCNTs are very similar to those of bulk graphite and hence their dielectric properties are anisotropic, with different dielectric response functions $\varepsilon_{\perp}(\omega)$ and $\varepsilon_{||}(\omega)$ depending on the electric field being polarized along or perpendicular its c-axis, which is a symmetry axis perpendicular to the basal plane of the graphite layers (Butt1 et al. 2012; Lidorikis and Ferrari 2009). For electric field polarized parallel to the CNT axis $\varepsilon_{\perp}$ is only needed while for perpendicular we need consider both $\varepsilon_{\perp}$ and $\varepsilon_{||}$. The experimental results for $\varepsilon_{\perp}$ proposed by Djurisic and Li (1999) had been fitted with a Drude–Lorentz model:

$$\varepsilon_{\perp}(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} + \sum_{m=1}^{M} \frac{\sigma_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m} \tag{1}$$

where ω_p and τ are free electron plasma frequency and relaxation time, $\hbar\omega_m$, σ_m and γ_m are transition energy, oscillator strength, and decay rate for the Lorentz terms. Lidorikis and Ferrari (2009) presented an excellent fit between the experimentally measured graphite dielectric function and the calculated model while using $M = 7$. According previous experimental work which showed that the polarizing effect revealed an enhancement of the scattering of light polarized parallel to the nanotubes (Wang et al 2004), we will focus on the formula of parallel permittivity and assume that the field is parallel to the tube axis.

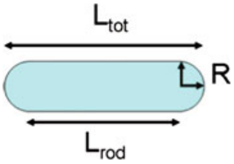
2.2 Excitation source

A plane wave incidence is usually employed for exciting nanoantenna. We have applied the magnitude of the incident plane wave as 1 V/m. During the simulation process, it is convenient to consider multiple frequencies and wide band calculations for determining the resonance wavelength. The incident plane wave is polarized along the MWCNT length.

2.3 Procedure for resonance wavelength mapping

In this work, MICROWAVE STUDIO (MWS) developed based on the finite integral technique (FIT) is used in the modeling process because it exhibits useful functions especially suitable for simulating nanoantennas in 3D. Also, it has the advantage of directly importing the given data to customize the dielectric constant curve as a function of frequency. Assuming MWCNT as a nonorod with hemispherical ends; a nanorod consists of a cylindrical rod, radius R and length L_{rod}, hemispherical ends, radius R, such that the total length $L_{\text{total}} = L_{\text{rod}} + 2R$ as shown in Fig. 1. We used a Matlab program to calculate the values for the dielectric constant as a function of frequency using Eq. (1) and the fitting data reported in Lidorikis and Ferrari (2009). The far field and the near field are determined as a function of wavelength. The peak in the response at the longest wavelength defines the first resonance.

Fig. 1 Schematic and dimensions of the simulated MCNT



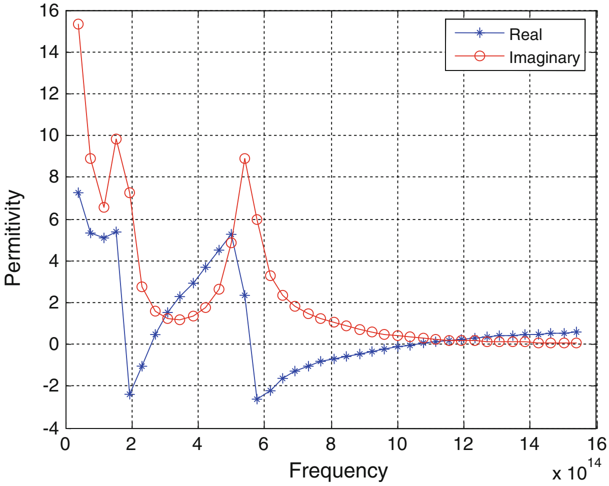


Fig. 2 Dielectric function $\varepsilon_{\perp}(\omega)$ of MWCNT for plane wave polarized along the nanotube using the Drude–Lorentz model used in reference Lidorikis and Ferrari (2009)

3 Results and discussions

Figure 2 shows the variation of both real and imaginary parts of MWCNT permittivity against the frequency as obtained from Eq. (1) and the data reported in Lidorikis and Ferrari (2009) for fitting.

The peak wavelength for the MWCNT resonance extracted from the normalized near field as a function of total rod length is shown in Fig. 3 for $R = 20$, 50, and 100 nm, respectively. Clearly, for the carbon nanotube of 20 nm in diameter the resonance wavelength increases, approximately, in a linear manner with increasing length of the nanotube up to 300 nm and nearly constant for the higher lengths. However, the variation of the resonance wavelength increases linearly up to 800 and 900 nm for the cases of applying nanotube with diameters 50 and 100 nm, respectively. Also, the resonance wavelength doesn't follow the traditional antenna design. In other words, the antenna no longer responds to the external wavelength but to a shorter effective wavelength.

With increasing the MWCNT length, additional, higher order, resonances appear at short wavelengths. Consequently, the MWCNT can resonate at lower wavelengths than gold. It is well known that gold nanoparticles resonate in the red part of the visible spectrum and resonance in the blue–green part as obtained through coupling of a number of nanoparticles (Biagioni et al. 2012).

The same data in Fig. 3 is used to highlight the R dependence. The variation in resonance wavelength as a function of MWCNT radius for fixed length is plotted as shown in Fig. 4. For the longer nanotube with length equal 500 nm the change in resonance wavelength for larger radii is very small while for smaller radii the dependence on the radius. On the other hand, the nanotube with short length from 250 nm up to 400 nm the resonances of MWCNT have very small variation, for small radii ($R < 20$ nm), while for large radii ($R > 20$ nm), it appears from Fig. 4 that resonances of MWCNT is relatively depend on both L and R. With a deep insight in spectral analysis for the near field we found that MWCNT provides an ultra wide band response in visible and near infrared. For example, MWCNT with a radius of 50 nm and a total length of 500 nm had been found to cover the band between

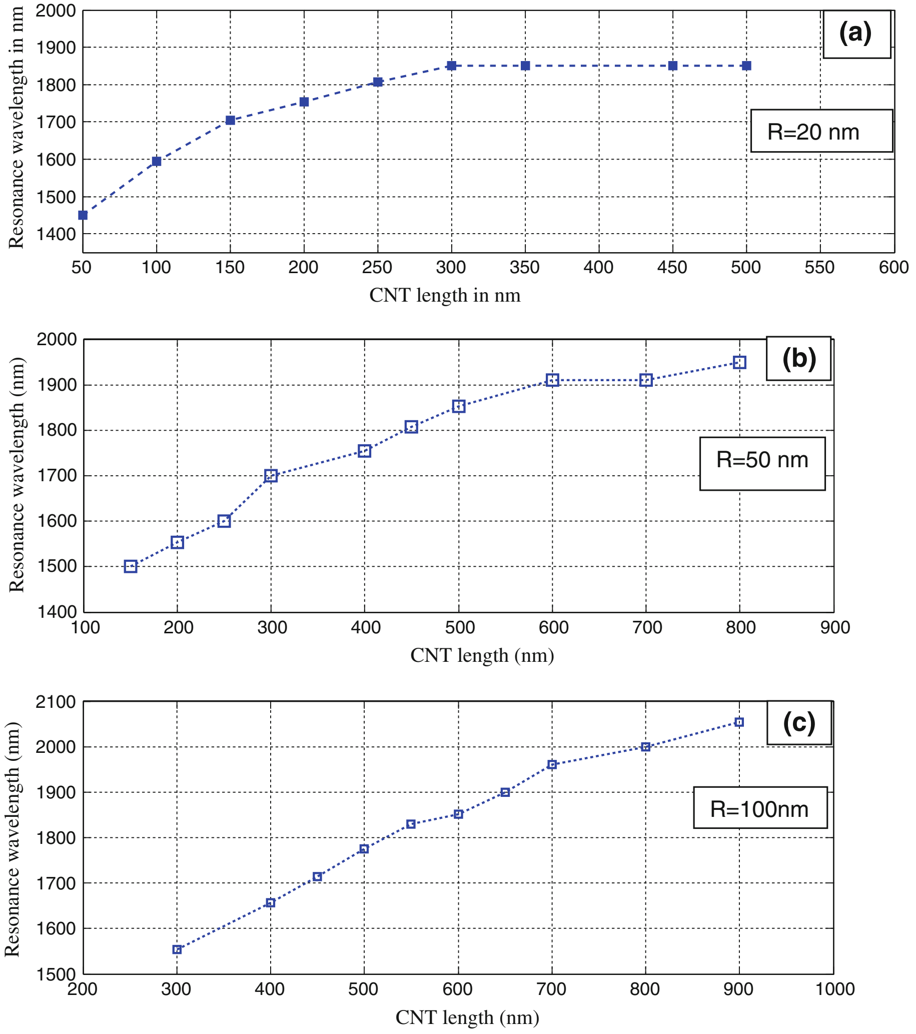


Fig. 3 Dependence of resonance wavelength on MWCNT total length for *R* of **a** 20, **b** 50 and **c** 100 nm (the resonance wavelengths extracted from the normalized near-field)

100 and 1000 THz with different field enhancement factors as shown in Fig. 5. Also, it appears from Fig. 5 that the first resonance of MWCNT occurs in NIR (near infrared) and depends on MWCNT dimensions, while the second resonance occurs in the visible band and has a little dependence on the tube dimensions as it resonates for red emission as shown in Fig. 5.

Many theoretical studies of nanorods followed the quasi-static model and considered only the dependence of resonances on the aspect ratio ($L_{\mathrm{total}}/2R$) (Pelton and Bryant 2013). Many of the theoretical studies of nanorods followed the quasi-static model and have considered only the dependence of resonances on the aspect ratio ($L_{\mathrm{total}}/2R$). In the quasi-static model, the resonance should be independent of the size and all curves should lie on a common universal curve (Pelton and Bryant 2013). In this work we have tested the validation of

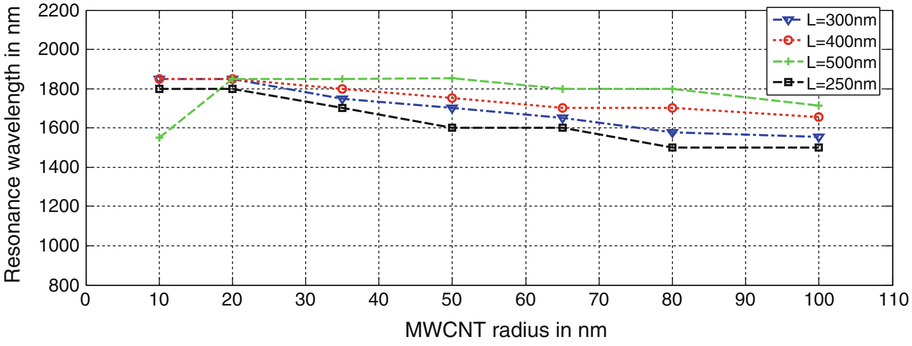


Fig. 4 Dependence of resonance wavelength on MWCNT radius for $L_{\text{total}} = 250$, 300, 400,and 500 nm

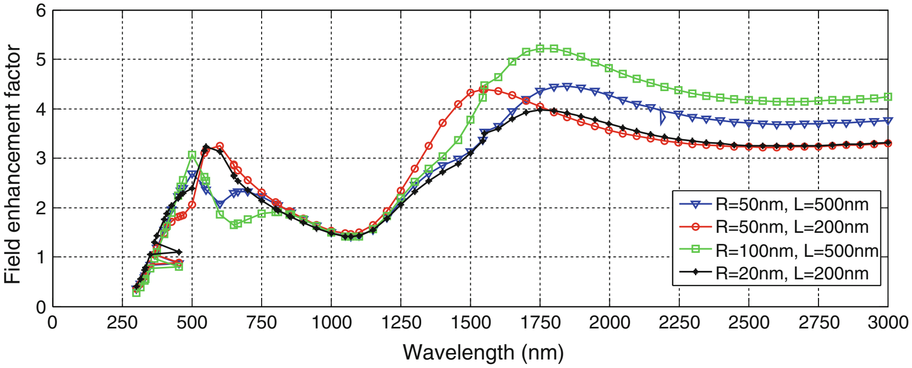


Fig. 5 Field enhancement factor at 1 nm from MWCNT end

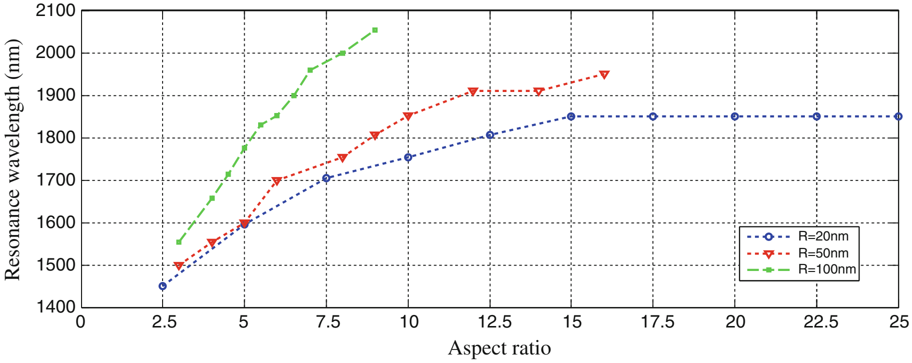


Fig. 6 Dependence of resonance wavelength of MWCNT on aspect ratio for different R

quasi-static model for MWCNT by plotting our results as a function of aspect ratio as shown in Fig. 6.

The results shown in Fig. 6 illustrate that MWCNT resonances don't follow the quasi-static limit. For example, the resonance red shifts by more than 600 nm in the range of R from 20 to 40 nm for an aspect ratio of 5. For larger difference in R and large aspect ratios, the red-shifts are even larger. We had investigated the far field response in the simulation range;

we found that far field resonances are far from near field resonances. Detailed investigations of the far field response of MWCNT are in progress and will be our future work.

We think that resonance wavelength mapping, presented in this paper, are of technological importance and provide useful information for locating plasmon resonances when designing nanoantennas based on MWCNT.

4 Conclusion

In this work, the FIT has been used to study the dependence of MWCNT plasmon resonances on its geometry (i.e. length and radius). The method is based on simulating MWCNT as a nanorod with dielectric constant obtained from the literature and fitted with a Drude–Lorentz model. Full map for variation of resonance in length and radius are presented. The results reveal that MWCNT antenna does not follow the quasi-static limit. MWCNT can be used as a nanoantenna for field enhancement at visible and infrared wavelengths. MWCNT near-field resonances are far from far-field resonances. The results presented in this paper provide an insight for designing nanoantennas based on MWCNT.

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