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Aleksei S. Kadochkin, Igor O. Zolotovskii, Sergey G. Moiseev, Andrei A. Fotiadi, "Plasmon excitation in array of double-walled carbon nanotubes by free-electron beam," Proc. SPIE 12131, Nanophotonics IX, 121310X (24 May 2022); doi: 10.1117/12.2621584



Event: SPIE Photonics Europe, 2022, Strasbourg, France

Plasmon excitation in array of double-walled carbon nanotubes by free-electron beam

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ABSTRACT

A carbon nanotube (CNT) can be considered as a plasmonic waveguide enabling propagation of ultraslow (with the effective refractive index >100) surface electromagnetic waves in the THz range. In this work, we theoretically study excitation of SPPs in array of double-walled CNTs by electron beam. The most interesting specific features of the double-walled CNT modes are associated with the presence of interlayer modes enabling a strong confinement of the electromagnetic field between the nanowalls of CNT and thus providing a high deceleration coefficient at a relatively low absorption coefficient at the frequencies up to 40–50 THz. Due to the strong SPP confinement between nanowalls the neighboring CNTs have almost no effect on each other. Array of double-walled CNTs ensuring an effective conversion of the external pump energy into the SPP energy can be employed for design of slow-wave plasmonic nanostructures.

Keywords: carbon nanotube, surface plasmon polariton

1. INTRODUCTION

Carbon nanotubes (CNTs) can be considered as a plasmonic waveguide enabling propagation of an ultraslow surface electromagnetic wave (with the effective refractive index > 100) in the THz range [1,2]. Such ultraslow modes cannot be excited in CNT by an external electromagnetic wave using standard optical schemes due to a high effective refractive index of ultraslow waves propagating in CNTs. However, they could be generated and amplified through the injection of electron beams propagating along the parallel CNTs [3].

This work explores the plasmonic properties of parallel double-walled carbon nanotube (DWCNT) arrays. It is shown that nonrelativistic electron beams with the velocity less than 10^6 m/s can be used to excite SPPs in arrays of double-walled carbon nanotubes. For the SPP modes excited by an electron beam, the frequency range of SPP waves and electron beam velocities corresponding to the phase matching within a wide frequency range are determined. It opens the way to design slow-wave structures based on the dense arrays of multiwalled carbon nanotubes employing an efficient energy transfer from the pump to the SPPs.

2. DOUBLE-WALLED CNT CONDUCTIVITY MODEL

Various models taking into account an effect of the CNT structural properties on their conductivity have been proposed to describe CNT optical conductivity in the literature [1],[4],[5]. It has been shown that the plasmonic properties of doped CNT are determined mainly by the concentration of free carriers and by some definite doping level are almost independent of CNT chirality [6],[7]. To simulate the plasmonic properties of doped CNTs with a large diameter (more than several nm) the conductivity calculated for graphene can be used [8-10]:

Nanophotonics IX, edited by David L. Andrews, Angus J. Bain, Jean-Michel Nunzi, Proc. of SPIE Vol. 12131, 121310X · © 2022 SPIE · 0277-786X · doi: 10.1117/12.2621584

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$$\sigma^{(\omega)} = \sigma^{inter}(\omega) + \sigma^{intra}(\omega),$$

$$\sigma^{intra}(\omega) = \frac{2ie^2k_BT}{\pi\hbar^2(\omega + i\tau^{-1})} \ln\left[2\cosh\left(\frac{\mu}{2k_BT}\right)\right],$$

$$\sigma^{inter}(\omega) = \frac{e^2}{4\pi\hbar} \left[\frac{\pi}{2} + \arctan\left(\frac{\hbar\omega - 2\mu}{2k_BT}\right) - \frac{i}{2}\ln\frac{(\hbar\omega + 2\mu)^2}{(\hbar\omega - 2\mu)^2 + (2k_BT)^2}\right].$$
(1)

In Eq. (1), σ^{inter} and σ^{intra} are the contribution of inter- and intraband transitions, *e* is the electron charge, \hbar is the Planck constant, k_B is the Boltzmann constant, *T* is the temperature, μ is the graphene chemical potential, τ is the average lifetime of carriers. For numerical calculations, the following parameters are taken: T = 300 K, $\mu = 0.2$ eV, and $2\pi\hbar/\tau = 0.1$ meV [11]. The used value of chemical potential of doped graphene corresponds to the surface concentration of carriers $n = 1.2 \cdot 10^{13}$ cm⁻² [8] and corresponds to one extra charge carrier per thousand carbon atoms.

At the frequencies of some tens of THz, the intraband term σ^{intra} dominates in Eq. (1). At low temperatures, when $\mu \gg kT$ (it is the case for the used μ and T), Eq. (1) is reduced to the well-known Drude-like formula widely used for characterization of CNT conductivity in THz range [12]:

$$\sigma^{intra} \approx \frac{ie^2 |\mu|}{\pi \hbar^2 \left(\omega + i\tau^{-1}\right)} \,. \tag{2}$$

In this paper, to study the plasmonic properties of doped DWCNT we assume a CNT as a set of infinitesimally thin graphene sheets placed one into another with the conductivity determined by Eqs. (1) and (2).

3. SPP DISPERSION DEPENDENCES IN DOUBLE-WALLED CARBON NANOTUBES

The dispersion dependences of SPPs in DWCNT arrays (Figure 1) have been studied using the conductivity model described by Eq. (1). Using this model one can solve the eigenvalue problem for the given geometry and boundary conditions, i.e. to find the complex mode propagation constant $\beta = \beta' - i\beta''$ (here, β' is the SPP propagation constant, β'' is the attenuation constant) for a given frequency ω . To perform modal analysis we use 2D model with periodic boundary conditions in *x* and *y* directions, implemented using COMSOL Multiphysics software.



Figure 1. Schematic of double-walled CNT array: nanotubes in the array are irradiated by an electron beam. CNT parameters: outer diameter d = 10 nm, interlayer distance = 0.34 nm, array constant = 3d. The refractive index of a substrate is equal to one in numerical calculations. Electron beam should be periodically repeated due to periodic boundary conditions in *xy*-plane but is schematically shown only at one carbon nanotube of the array.

Figure 2 shows the real and imaginary parts of the SPP complex propagation constant as the functions of frequency. Negative value of β'' corresponds to the SPP attenuation during the propagation along the DWCNT axis. DWCNT arrays are modeled using the periodic boundary conditions for each unit cell as shown in Figure 1.



Figure 2. Dispersion curves for SPPs propagating in double-walled CNTs.

The cross-sections of plasmon modes in the array of double-walled CNTs are given in Figure 3. In a single-walled CNT (SWCNT) the mode field is concentrated near the surface exhibiting an exponential decrease with the distance from its wall in radial direction [2,13]. DWCNT supports propagation of the similar modes with the field concentrated near the outer layer and mainly outside the layer. Such SWCNT-like modes can provide the SPP effective refractive index (deceleration coefficient) of about 100 and a high attenuation coefficient of about 10⁸ 1/m in a wide frequency range. The observed high attenuation coefficient in such modes is due to effective interaction of wide exponential mode "tails" with the conducting walls of neighboring CNTs in the array. As a result, the SPP attenuation coefficient in the array of DWCNTs is one or two orders of magnitude higher in absolute value than in a single DWCNT. For a such SPP modes the Q-factor determined as

$$Q = \left| \frac{\beta'}{\beta''} \right| \tag{3}$$

is as small as 1. These features make such modes unsuitable for applications in slow-wave systems.



Figure 3. The absolute value of electric field strength (in a.u.) of the SPP modes. The numbers from 1 to 6 correspond to the numbers of the dispersion curves in Figure 2.

The most interesting specific features of DWCNT modes are associated with the presence of SPP modes enabling a strong confinement of the field between the layers and thus providing a high deceleration coefficient at a relatively low absorption coefficient ($|\beta''| \sim 10^6$ 1/m) at the frequencies up to 40–50 THz. Besides, due to the strong SPP confinement between layers in such modes the neighboring DWCNTs have almost no effect on each other. Thus, dense DWCNT arrays ensuring an effective conversion of the external pump energy into the SPP energy could be employed for design of slow-wave structures.

The devices based on the interaction between the SPP and drift current [2,13–16] exploit the electric field longitudinal component inherent to the interlayer modes. The parameter characterizing domination of the longitudinal field component [2]

$$\eta = \frac{|E_z|^2}{|E_x|^2 + |E_y|^2 + |E_z|^2} \tag{4}$$

ranges for interlayer modes from 0.85 to 0.65 within the frequency range of 20–60 THz allowing interaction of the SPP longitudinal field component with both a drift current in the configuration proposed elsewhere [2,13] and an electron beam [17].



Figure 4. a) Group velocity (solid line) and phase velocity (dashed line) of SPP propagating in the DWCNT array. b) Q-factor of interlayer mode in DWCNT.

The group and phase velocities corresponding to the fundamental mode are shown in Figure 4a. Within the frequency range of 0–78 THz, the group velocity is a positive function of the frequency. Importantly, in the frequency range from 10 to 75 THz phase velocity is almost linear and changes from 7×10^5 m/s to 4×10^5 m/s thus providing an effective

refractive index (the deceleration coefficient) lying within the range of 430–750. Such deceleration enables effective interaction of the SPP with the drift current running with the velocity of $0.5-1\times10^6$ m/s through the CNT [18,19], i.e., the phase matching can be achieved. In this case, an azimuthally symmetric mode with low losses can be excited in the DWCNT, the peak height is determined by the high Q-factor (about 100 at low frequencies, see Figure 4b).

Thus, DWCNTs are promising for application in devices employing an interaction between the SPP and drift current. The theoretical formalism elaborated elsewhere [16] and our previous studies [2,13] can be used for this purpose.

4. CONCLUSION

A simple model describing a DWCNT array has been proposed. It is shown that the high Q-factor highly confined SPP modes can exist in such arrays. Excitation of the surface plasmon modes by an electron beam has been investigated. The spectral density of electron beam energy transferred to the DWCNT modes is obtained by numerical calculations. We have determined the frequency range of SPP and electron beam velocities enabling the phase matching and efficient energy transfer within a wide frequency range. All this contributes to elaboration of the slow-wave structures based on the dense arrays of double-walled CNTs enabling efficient conversion of the pump energy into the SPP energy. Phase-matching simultaneously satisfied for a large array of parallel CNTs could be used for design of the IR- and THz generators based on the same operation principle as a traveling wave tube or the so-called O-type generators directly pumped by the injected or drift currents.

5. ACKNOWLEDGEMENTS

This work was supported by the Russian Foundation for Basic Research (grant #19-42-730010) and by the Ministry of Higher Education and Science of the Russian Federation (projects #0004-2022-0004, #0830-2020-0009, #075-15-2021-581).

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