# Vertically aligned carbon nanotubes - study of effective electric permittivity

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**Abstract**

In this paper we aim to assign effective electric permittivity values to vertically aligned arrays of carbon nanotubes fabricated by the state-of-the-art manufacturing techniques. The effective constitutive parameters of this artificial medium depend on the density of the carbon nanotubes. The overview of the densities of the grown aligned carbon nanotubes reported in the literature is given in the paper. The effective parameters are modelled by Maxwell-Garnett homogenization formulas. Carbon nanotube forests form artificial lossy dielectrics with the real part of the effective electric permittivity between $1$ and $2$ in the optical and near-infrared range.

## 1. Introduction

During recent years, carbon nanotubes (CNT) have evolved into one of the most intensively studied type of materials and are currently at the center of the nanotechnology research [1]. As artificially structured media with interesting properties such as high mechanical strength, light weight, good heat conductance and high aspect ratio, carbon nanotubes can be classified as metamaterial structures.

The vertically aligned carbon nanotubes (VA-CNTs) are one of the forms of CNTs synthesized perpendicular to the substrate and referred to as CNTs forests or CNTs carpets. Recently, an ideal black material formed by a low-density array of VA-CNTs and characterized by extremely low index of refraction ($n = 1.01 - 1.10$) has been reported [2]. The aim of this paper is to identify the range of effective electric permittivity values that can be synthesized with VA-CNT forests. For this purpose effective medium theory and homogenization techniques are applied and values of achievable CNT densities are overviewed.

## 2. CNT modelling

Constitutive parameters of CNTs are typically described by the dielectric function of graphite, tabulated e.g. in [3]. In transferring the dielectric constants to cylindrical multishells, it can be assumed that CNTs are locally identical to graphite [4]. CNTs are modelled as solid cylinders, as it is shown in Fig. 1a [5]. The electromagnetic properties of the nanotubes are characterized by a diagonalized dielectric[1] tensor with the relative permittivity components given in Cartesian coordinates by [5, 6]:

$$\varepsilon_x = \varepsilon_y = \sqrt{\varepsilon_o \varepsilon_e} \qquad\qquad \varepsilon_z = \varepsilon_o \tag{1}$$

where $\varepsilon_o$ and $\varepsilon_e$ characterize dielectric properties of the bulk graphite in the cleavege plane and along the $c$-axis, respectively [3]. The graphite properties adopted from [7, 8] are shown in Fig. 1b.

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[1] The CNT structure is non-magnetic, i.e. $\mu_r = 1$.

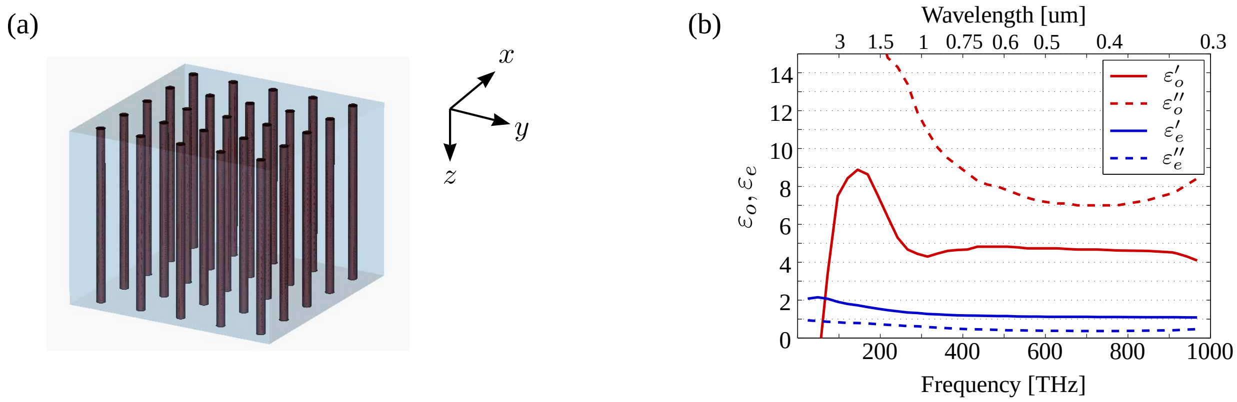

Fig. 1: (a) VA-CNT array. (b) Electric permittivity of graphite.

Effective electric permittivity of the VA-CNT forest is approximated by homogenization formula based on Maxwell-Garnett theory. As VA-CNTs are anisotropic and aligned along a particular ($z$) direction, the effective representation of the forest is anisotropic. The components of the homogenized permittivity tensor of a VA-CNTs array characterized by volume fraction $f$ are given by [5]:

$$\varepsilon_{\mathrm{eff},x} = \varepsilon_{\mathrm{eff},y} = 1 + \frac{f(\varepsilon_x - 1)}{1 + \frac{1}{2}(\varepsilon_x - 1)(1 - f)} \qquad \varepsilon_{\mathrm{eff},z} = f\varepsilon_z + (1 - f) \tag{2}$$

The volume fraction is related to the density of the grown VA-CNT forest and the nanotubes' diameter. The overview of the realized density values is shown in Fig. 2. For the parameters denoted by (a)-(e) effective electric permittivity is shown in Fig. 3.

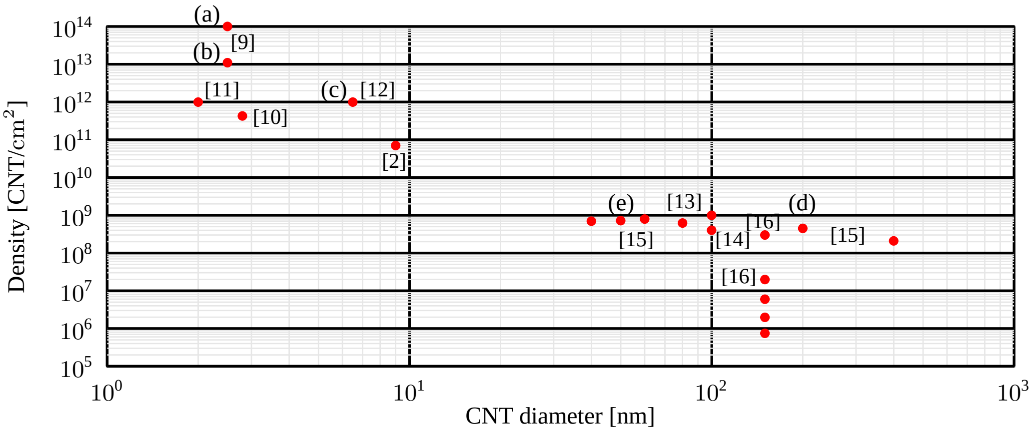

Fig. 2: Density of the reported VA-CNTs arrays vs nanotube diameter with the corresponding references.

For near-normal wave incidence ($z$-direction) the homogenized results indicate that the effective electric permittivity of the forest achieves values $1 < \varepsilon_{\mathrm{eff},x}, \varepsilon_{\mathrm{eff},y} < 2$ in the optical and near-IR regime (Fig. 3a). The CNT arrays of higher density are characterized by higher losses (significant values of $\varepsilon''_{\mathrm{eff}}$). These losses are even more pronounced for the permittivity component parallel to the nanotubes (Fig. 3b).

There are few approximations in the presented modelling method. First of all, hollow nanotubes are represented by solid cylinders. This approach is more appropriate for multi-walled than single-walled CNTs. Generally, the optical properties of single-walled CNTs (SWCNTs) and multi-walled CNTs (MWCNTs) should be considered separately [5]. The optical properties of SWCNTs with diameters less than 1 nm depend on the detailed atomic structure (chirality). On the other hand, MWCNTs, due to their larger diameter (larger than ca. 3 nm) have more regular and uniform optical properties [5].

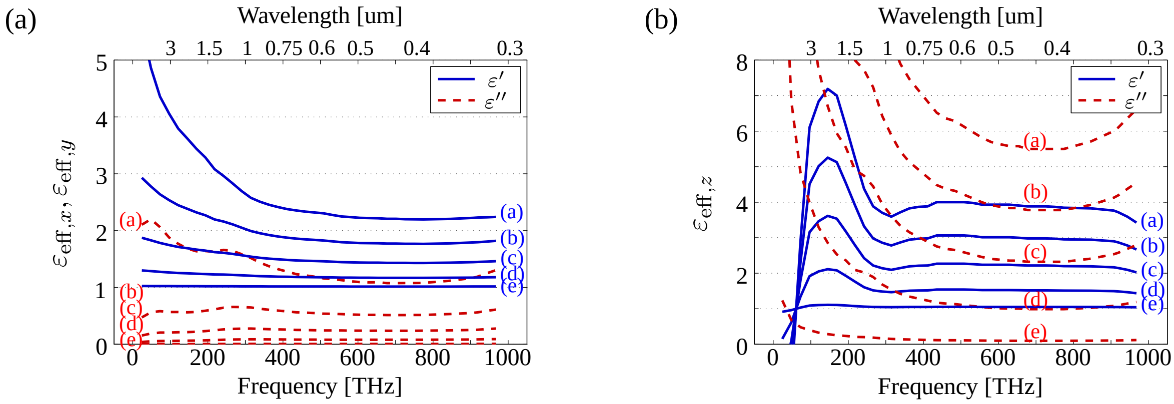

Fig. 3: Effective electric permittivity of homogenized VA-CNT arrays ($\varepsilon'$ - solid line, $\varepsilon''$ - dashed line). The curves described by (a)-(e) correspond to the CNT densities indicated in Fig. 2.

## 4. Conclusion

Effective electric properties of vertically aligned CNT arrays are modelled with Maxwell-Garnett homogenization approach. For near-normal wave incidence, VA-CNTs forests are equivalent to lossy artificial dielectrics with effective electric permittivity values between $\varepsilon'_{\mathrm{eff}} = 1$ and $\varepsilon'_{\mathrm{eff}} = 2$.

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