# Terahertz Metasurface Sensor Based on Multi-Walled Carbon Nanotube Aggregates for Protein Detection

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## PURPOSE OF THE STUDY

**The main tasks:** optimization of the carbon nanotubes (CNT) content in the composite to achieve maximum sensitivity. Tuning the resonant frequency of the metasurface to a frequency range where characteristic signs of the HSA solution permittivity dispersion are observed. Assessment of the potential of using CNTs as resonant elements to create electromagnetic field "hot spots". The EM field distributions were analyzed to explain the sensing behavior.

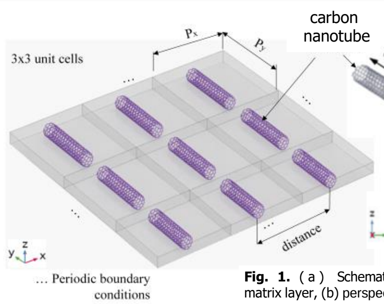
## MODELLING

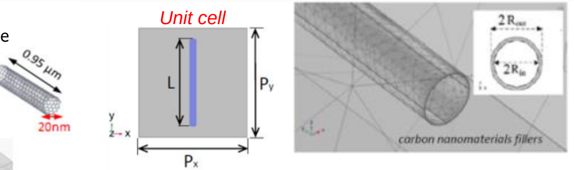
**Unit cell:** periodic array with periods Px=1 μm and Py=0.1÷1 μm. Resonant element: CNT with diameter D=45 nm and length L=0.95 μm. Substrate: Dielectric layer with thickness td=1÷0.125 μm in which the CNTs are embedded. The analyte layer is 0.01 μm.

**Analyte:** water solutions of HSA.

**Method:** numerical simulations were performed using Comsol Multiphysics software and the dielectric property dispersion of HSA solutions on concentration, where the real and imaginary parts of the dielectric permittivity vary from 1.31 to 1.42 and from 0.62 to 0.71 depending on the HSA concentration [1].

## STRUCTURE AND PARAMETERS



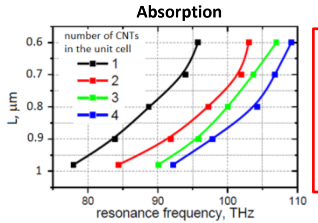





| Px, μm | Py, μm | L, μm | d, μm | td, μm | $R_{in}$, nm | $R_{out}$, nm |
|---|---|---|---|---|---|---|
| 1 | 1–0.1 | 0.95–0.6 | 0.125 | 1-0.125 | 35 | 45 |

**Fig. 1.** ( a ) Schematic view of 3 x 3 unit cells of the metasurface containing one MWCNT in a dielectric matrix layer, (b) perspective and top view (c) of the metasurface unit cell with containing 4 MWCNTs per unit cell

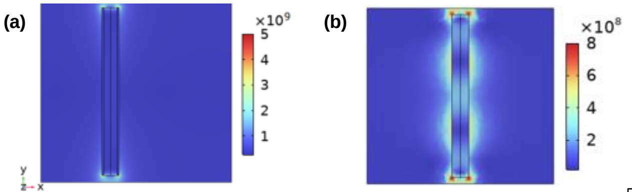
## ENHANCED SHIELDING IN PTFE COMPOSITES VIA CARBON RODS AND NANOTUBES




**Resonance response:**

The metasurface resonances were tuned to a frequency in the region of maximum field localization at the ends of the nanotubes.

**Top view of the E- field distributions in MWCNT/PTFE unit cell for dipole (a) and lattice (b) resonances**




[1] Shiraga K, Hydrogen Bond Network of Water around Protein Invest. with THz and Infrared Spectroscopy. Biophys J. 2016, 111(12):2629-2641

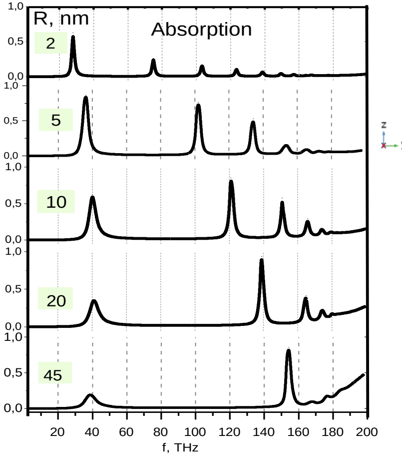



**Fig. 2.** Absorption spectra of the metasurface for changing of the nanotube radius R= 1÷45 nm, Py=1μm, Px=0.1μm, td=0.125μm

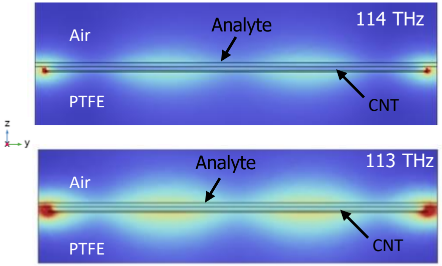



**Fig. 3.** E- field distributions in MWCNT/PTFE unit cell of the metasurface at resonance frequency 113 THz and near resonance frequency 114 THz with HSA solutions on top of the metasurface sensor

**Field enhancement:** The use of the metasurface with CNTs leads to the formation of electromagnetic "hot spots", which significantly enhances absorption and interaction with the biological layer, the main component of which is water.

**Sensitivity:** When the HSA concentration changes from 0 to 150 mg/mL the resonance frequency shifts from 113.02 THz to 112.63 THz. The sensitivity of the proposed metasurface is 3.58 THz/RIU.

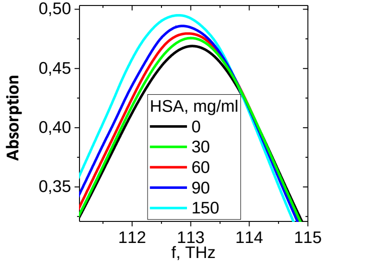



**Fig.4.** Absorption in MWCNT/PTFE metasurface containing one MWCNT in unit cell depending on the HSA concentration in water solution