Extraordinary Optical Transmission in Copper and Carbon Nanotube Devices at Terahertz Frequencies

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Abstract: While light is poorly transmitted through an aperture in a conductive thin film, in the phenomenon known as extraordinary optical transmission (EOT), it is transmitted when incident on an array of sub-wavelength periodic apertures at a resonant frequency determined by the geometry of the aperture array and the metal-dielectric interface. Using the COMSOL Multiphysics® software RF Module, a polarized electromagnetic plane wave at terahertz (THz) frequencies propagating through a hypothetical air-filled waveguide is simulated. Unit-cells of copper-based and carbon nanotube (CNT) based EOT devices are modeled in order to verify theoretical calculations of the resonant frequency response using S-parameter calculations. Both devices show good agreement with the experiments and a slight shift from the calculated resonance. Woods anomalies are seen in the simulated CNT-based EOT.

Keywords: Terahertz, EOT, CNT, COMSOL, SPPs

1. Introduction

The terahertz gap of the electromagnetic spectrum lies between 100 GHz and 30 THz [1] and has been drawn significant attention in photonic research due to its capabilities associated with the characterization of materials properties. The extensive progress of THz applications has stimulated research seeking more understanding of the behavior of materials in this regime and other fields such as plasmonics and quantum cascade lasers [1]. Extraordinary optical transmission (EOT) in metallic subwavelength apertures has been observed in the THz region, although at such a low frequency, the transmitted wave through one aperture is significantly low and inversely proportional to the fourth power of the wavelength [2]. The reason behind this transmission through an array of apertures is attributed to the propagation of a surface wave on the metal at a resonant frequency determined by the periodicity length of the array and both metal and dielectric relative permittivities [3]. After surface plasmon polaritons (SPPs) are initiated at the apertures' edges when light is incident on the metal surface, they propagate along the surface of the metal and then decouple into free space and recouple at the apertures' edges [4]. Although such a transmission has been observed 1998 [2], there is no unified theory that fully explains the enhancement of the transmitted low frequency light through two-dimensional aperture arrays [4]. According to the time-of-flight qualitative model, the polarization direction and the geometry of the thin film apertures such as the dimensions, shape and area notably contribute to the resonance of the transmitted wave [4]. The geometry of the most enhanced transmission reported for a copper thin film that had asymmetric apertures [4] was further used to show the transmission with a carbon nanotube (CNT) based EOT on a silicon substrate [5]. However, the transmission for the case of a free standing CNT-based EOT was shown to have a more enhanced transmission through symmetric apertures [6] and was broadband with symmetric apertures on a silicon substrate [7]. The facility of simulating EOT devices as a function of various geometries of the apertures array as well as the material properties could lead to better understanding of the EOT devices. Additionally, the thin-film's electromagnetic properties can be characterized using extraordinary optical transmission as a method leading to effective characterization of novel thin film materials. In this work, copper-based and free standing CNT-based EOT devices are simulated using the COMSOL Multiphysics®, RF modules.

2. COMSOL Modeling

In order to study both copper and CNT EOT devices, a polarized THz wave is excited in a hypothetical air waveguide by defining one port

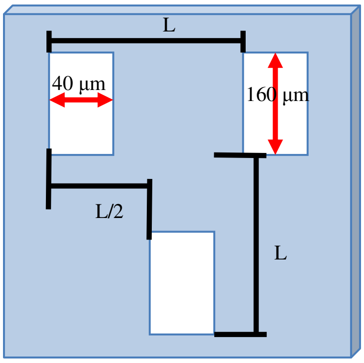

Figure 1. The aperture dimensions and lattice arrangement of the copper-based EOT device.

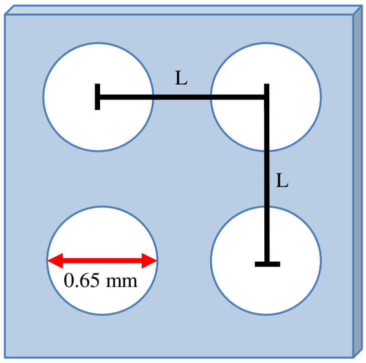

Figure 2. The aperture dimensions and lattice arrangement of the CNT-based EOT device.

in front of the sample while the other port is defined behind the sample to verify the resonance of the transmitted wave using S-21 parameter calculations. The modeling methodology is divided into 3 sections describing the geometry, materials, and boundary conditions.

2.1 Geometry

The geometry of the array of the EOT device plays an important role to determine the resonant frequency that can be determined from [3]

$$\lambda_{peak} = L\sqrt{\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}}$$

where ϵ_m and ϵ_d are the dielectric constants of the metal and dielectric interface respectively and L is the periodicity length of the array. Based on the time-of-flight model, the geometry of the copper-based EOT device has a 50 μm thickness and was selected so as to yield enhanced transmission at 0.96 THz. The geometry of the CNT thin film [7] is used to simulate the CNT-based EOT and has a 25 μm thickness that has a calculated resonance at ≈0.25 THz. The geometry of both samples can be seen from Figure 1 and 2.

2.2 Materials

For the copper-based EOT, the material is defined as copper using COMSOL's built-in library while the electrical properties of the CNT thin film were extracted from experimental data from Wang et. al [7]. The CNT thin film is consisted of multilayer of multi-walled carbon nanotube synthesized by catalytic chemical vapor position. The holes are milled using an excimer laser [7]. In our model, the dielectric constant is defined as a function of the frequency dependent refractive index results

$$\epsilon = (n^2 - k^2) + i(2nk)$$

where n and k are the real and imaginary refractive indices respectively. For simplicity, the conductivity is described by the Drude model as given by [8]

$$\sigma = \frac{\omega}{4\pi i}(\epsilon - 1)$$

where ω is the angular frequency of the incident light.

2.3 Boundary Conditions

The THz wave propagates in a hypothetical air-filled waveguide that is set with perfect electric conductors (PEC) on the sides normal to the polarization direction while the other sides are set as perfect magnetic conductors (PMC). This particular configuration allows one to excite an infinite plane wave in these directions and model an infinite periodic array (Figure 3). Because of the low penetration of the THz wave in copper and CNT materials (values calculated from the skin depth of both devices), the outer faces of the EOT device are set with the impedance boundary condition (IBC). The boundaries at the end of the air waveguide along the propagation direction are defined as perfectly

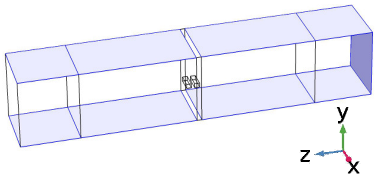

Figure 3. The PEC boundaries are chosen to be normal to the electric field polarization direction (along y) while the other sides are defined to be PMC's. This configuration yields an infinite plane wave and infinite thin film.

matched layers (PML) in order to minimize the undesired reflections. Meshing of both devices is defined to be physics controlled mesh with maximum element size equal to $\frac{\lambda}{6}$ where λ is the wavelength of the incident wave. The maximum element size of the IBC boundaries is defined to be less than the skin depth of both materials. The mesh of the copper device model is shown in figure 4.

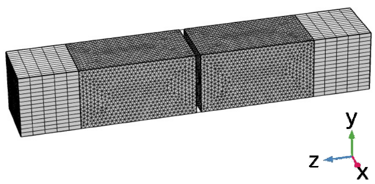

Figure 4. Meshing of both devices is defined by a physics controlled mesh with maximum element size equal to $\frac{\lambda}{6}$. The maximum element size of the IBC boundaries is defined to be less than the skin depth of both materials.

3. Results

The copper-based EOT device exhibits a red-shifted resonant transmission frequency at 0.86 THz (figure 5) that is red-shifted experimentally as well for a copper-based EOT device which has similar dimensions of its apertures. The transmitted wave at 0.6 THz and at the resonant frequency is shown in figure 6 (a) and (c). Woods anomalies of the destructive interferences is seen experimentally and at 1 THz

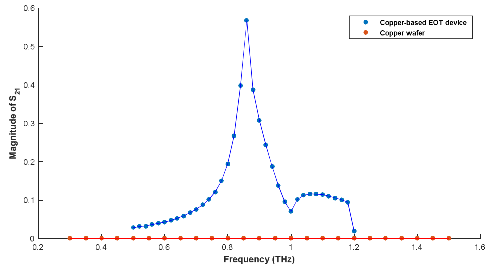

Figure 5. The magnitude of the S21-parameter of the copper-based EOT device exhibits a resonant frequency at 0.86 THz. The red line shows the low transmission through a copper wafer.

in the model as well. The surface wave that confirms the EOT is seen on the surface of the copper device as in figure 7 (a) and (c).

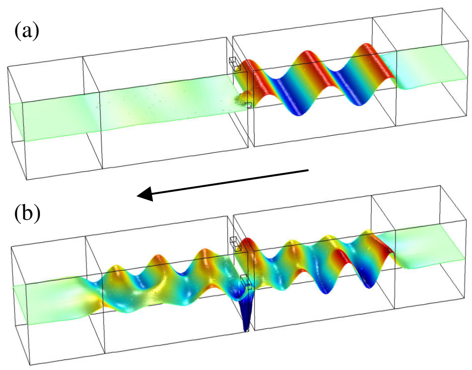

Figure 6. The transmitted wave through the copper-based EOT device at (a) 0.6THz (b) the resonant frequency 0.86 THz. The wave is propagating from right to left.

The S-21 parameter calculations of CNT-based EOT device (figure 8) shows a very sharp resonance at 0.235 THz followed by a dip at 0.25 THz that corresponds to Wood anomalies and it starts increasing again until 0.35 THz followed by another dip. According to the designed CNT-based device, the resonant frequency is in good agreement with the experiment where both of them are slightly shifted from the calculated resonance although Wood's anomalies are seen in our model only. The coupling and decoupling of the z- component of the electric field on the surface of CNT device are seen as in figure 7 (b) and (c). In order to verify whether we have mesh dependent mode, finer mesh has been tested and showed no difference.

4. Conclusions

Modeling both copper-based EOT and CNT based EOT shows good agreement with the experimental data although the CNT-based EOT didn't show Woods anomalies dip as seen in the simulation results. In addition, the surface wave is seen on the thin film surfaces which confirms the propagation of the SPPs that has been considered as the main reason behind the EOT. The extracted experimental data of the CNT can be fitted to a Drude-Lorentz model for more validation. The promising agreement between the simulation and the experiments opens an opportunity to study the EOT devices as a function of the material's properties, aperture's geometry and the polarization direction.

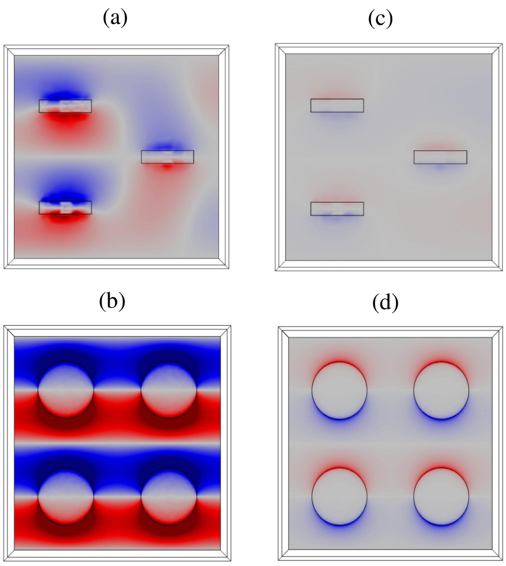

Figure 7. The z-component of the electric field on the surface (xy plane) of the copper-based EOT device at (a) 0.86 THz (b) 0.235 THz shows the coupling and propagating of the wave on the surface. The propagation of the surface wave cannot be seen at a lower frequency (a) 0.60 (b) THz 0.1. THz The intensity scale is the same for both images.

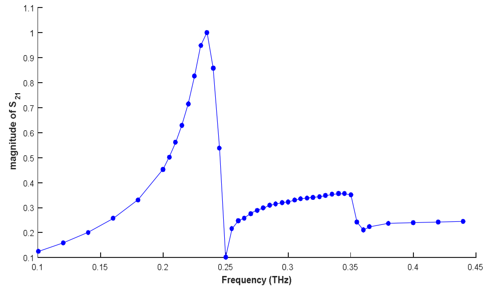

Figure 8. The magnitude of the S21-parameter of the CNT-based EOT device exhibits a resonant frequency at 0.235 THz.

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