

Analysis of Photonic crystals for biochemical sensing in the terahertz region using the finite-difference time-domain method with recursive convolution

Hamza Kurt, David S. Citrin

School of Electrical and Computer Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0250, U.S.A.

Photonic crystals (PC) are periodic dielectric structures that have attracted interest to control the flow of light.[1] Analytical approaches to analyze these structures are difficult. Therefore, numerical techniques are used for this purpose. The finite-difference time-domain (FDTD) method is one of the most commonly employed numerical techniques. It is based on the spatial discretization of Maxwell's equations in space and time.

We have shown, based on simulations, that PC's can be used for biochemical sensing in the terahertz region, modeling that absorption of the DNA molecule as a Lorentz medium.[2] The use of terahertz radiation for chem/bio sensing has not been investigated fully due in part to the lack of sources and detectors even though large biomolecules have fingerprint (vibrational and rotational modes) in this region of the spectrum. The effective path length over which the terahertz pulse interacts with the biological material should be very long. This can be achieved if the terahertz wave has low group velocity. Moreover the field amplitude and profile is also important. It is desired that the electric-field maxima are confined inside the holes within the PC where the biological materials is placed. PC's with judicious design can provide all these features.

Many biological materials have significant frequency dependence to their index of refraction. Therefore, it is important to consider the frequency dependence of the electromagnetic response of biological samples. Here, the dispersive effect of the DNA molecules in PC's is investigated by using the FDTD method with recursive convolution.[2] The computational domain is terminated by perfectly matched layer (PML) . Each unit cell is divided into 30x30 grid points. The PC studied has a triangular array of holes in a dielectric background (Fig. 1). We assume that the dielectric background is non-absorbing, and has constant index of refraction $n = 3.46$. The radius of the air holes is $r = 0.4a$, where a is the lattice periodicity. The transmission spectrum shows that this structure possesses a wide band gap for TE polarization (Fig. 2).

The PC waveguide (PCW) is obtained by increasing or reducing the radius of air holes to $r = 0.45a$ (PCW-A) and $r = 0.3a$ (PCW-B), respectively, thereby permitting a propagating mode inside the PBG. It's important to have a propagating mode which has very high transmission and low group velocity. The spectroscopic change in the transmission spectrum with the sample inserted into the air holes in the line defect is monitored to ascertain the effect of and the electromagnetic-matter interaction. The guided propagating signal interacts with the dispersion and absorption of the PC structure containing the biological material, which provides the sensing mechanism. Figure 2 also shows the interaction of the propagating mode with the Lorentz media. The propagating signal in the sensing region is decreasing exponentially due to the absorption and it's shown in Fig. 3. The linear dependence of the absorption to the imaginary part of the

dielectric constant of the DNA molecule is observed and shown in Fig 4. These results are for the PCW-A, and further results for the PCW-B will be presented at the conference.

- [1] E. Yablonovitch, "Inhibited Spontaneous Emission in Solid-State Physics and Electronics," Phys. Rev. Lett. 58, 2059 (1987).
- [2] B. M. Fischer *et al.*, "Far-infrared vibrational modes of DNA components studied by terahertz time-domain spectroscopy," Phys. Med. Biol. 47, 3807 (2002).
- [3] A. Taflov, "Computational electrodynamics," The Finite-Difference Time-Domain Method, Artech House, Boston, London, (1995).

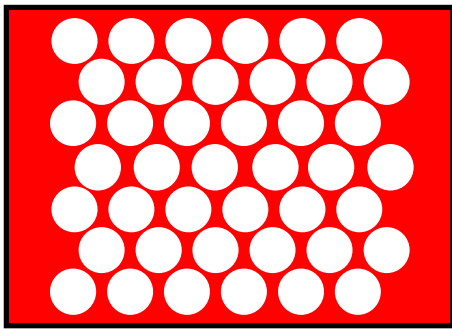


Fig. 1: Schematic of the analyzed photonic crystal structure.

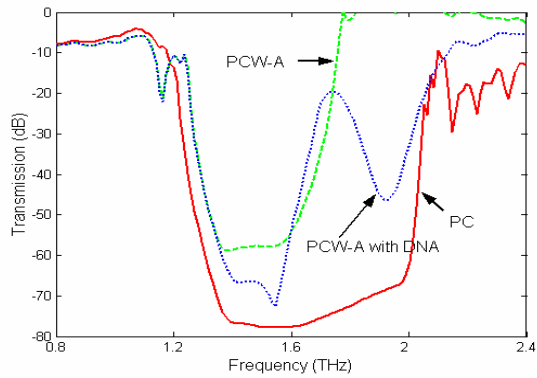


Fig. 2: Transmission spectrum of the photonic crystal, photonic crystal waveguide with and without absorption at 1.9 THz.

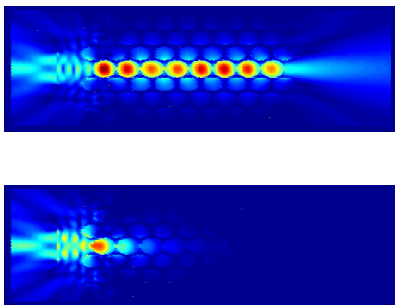


Fig. 3: Single frequency propagation through PCW with Lorentz absorption center frequency at 1.9 THz.

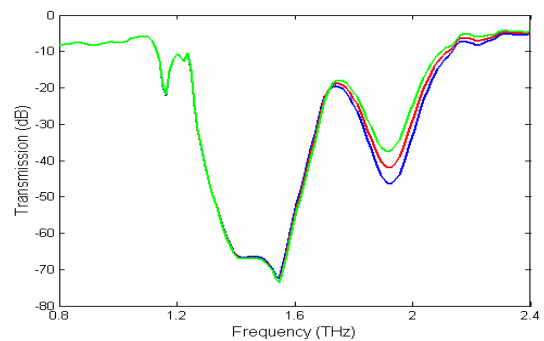


Fig. 4: Transmission spectrum variation for different values of imaginary part of the dielectric constant of DNA.