Theoretical Design for a Plasmon-Polariton Photonic Crystal

R. M. Gelfand, L. Bruderer, and H. Mohseni

Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL

We explored a plasmon-polariton photonic crystal designed to have bandgap around 115-135 THz. With a cavity defect our structure strongly squeezes light, and with a Purcell's constant of 4.9×10^5 is suitable for single molecular detection.

Photonic [1] and more recently plasmonic [2] crystals have received increased attention for their abilities to control and manipulate electromagnetic radiation. Similarly metal dielectric metal sandwiches can manipulate light by squeezing it into a small two dimensional space [3]. By combining these two structures into a plasmon-polariton photonic crystal (PPPC) and exploiting the properties of nanoscale cavities we have been able to design and simulate a PPPC that can squeeze light in all three dimensions. A small volume and an intense field facilitate a large interaction between light and single molecules. Single molecule detection and terahertz spectroscopy is an important area of research for detecting the presence of explosive materials such as TNT and C4, biological materials such as proteins, drugs such as cocaine or methamphetamines, and both air and water pollutants [4]. However for any optical detection technique to be useful the interaction time between the light and the target molecule needs to be long and the spectral line width needs to be broad enough to allow for variations in the detected molecule's signature.

By controlling the geometry of a cavity and tuning the bandgap of the crystal one can manipulate the rate of spontaneous emission [5] by manipulating the interaction time between the cavity and the electromagnetic field. The strength of this effect can be characterized by Purcell's constant

$$p = \frac{3}{4\pi^2}\frac{Q}{V} * \lambda^3 .$$

A high p implies an intense interaction between the cavity, Q/V, and its resonant mode, λ, and would be required for any efficient optical sensor. Furthermore a wide spectral line width, Δf, is necessary for the operation and robustness of any single molecule sensor to ensure detection within slightly varying conditions such as temperature and cavity geometries. Since $\Delta f = f_0/Q$, a smaller Q relates to a wider line width. This implies that one needs to increase Purcell's constant without relying on extremely high Q-factors to build a practical sensor. In order to meet these two conditions, V the volume of the cavity must be as small as possible. The theoretical limit however for squeezing light into a confined space is about $(\lambda/2)^3$, but we will show that by using a PPPC we can confine light to such a magnitude that even a low Q-factor leads to an extremely high Purcell's constant. The best photonic crystals at a wavelength of 1.55 microns experimentally produce p values of 3.65×10^5 for a Q of 6×10^5 with theoretical maximums of 1.22×10^6 for a Q of 2 million and a Δf of 97 MHz [1]. Our device at a wavelength of 3.5 microns shows a p value of 4.9×10^5 with a Δf of 7.8 THz showing that we can squeeze a lot of light with a broad spectral range into a small volume though not for a long amount of time.

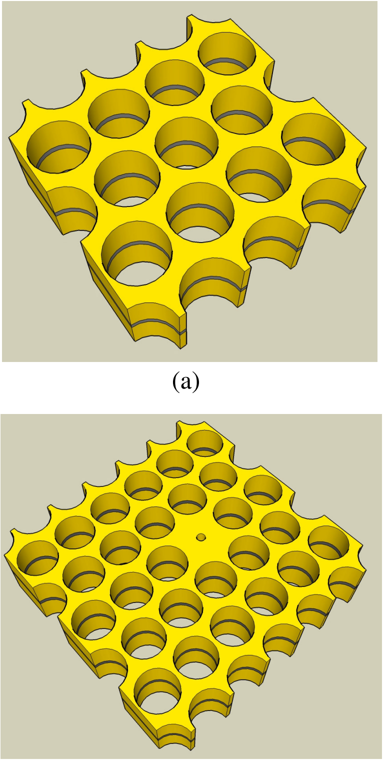
Figure 1-a presents our theoretical design for a PPPC. Using a commercial FDTD software package, we investigated the band structure of our PPPC. The gold metal cladding layers were simulated using the Drude model with sufficient Lorentz terms to match well with experiment. The thickness of the dielectric was 8 nm, with a dielectric constant of 9. When two metal dielectric interfaces are brought close together, the modes on each interface start to interact and get coupled. Even at very long wavelengths (away from the plasma frequency) the mode dispersion deviates strongly from the light line for very small gap thicknesses. On the other hand a nanometer size gap will push the field more into the metal, thus causing more loss and a shorter decay length. Depending on the relative phase of the two waves a symmetric or anti symmetric mode is formed. This research focuses on the antisymmetric mode, due to its superior characteristics in propagation distance and dispersion. Bloch-boundaries were introduced in each lateral direction and since the mode is anti-symmetric in the z-direction, an anti-symmetric boundary was placed in the middle of the slit. Due to the very high field effects of plasmons a small grid size of 3 nm was implemented in and around the slit. In the metal cladding, this grid size was gradually increased toward the top. Modes were stimulated using TM electric dipoles embedded in the middle layer and we took field measurements after the source field had dissipated. To measure the bands time monitors were placed throughout the simulation region and the FFT of the measured field was plotted versus intensity. Then we shifted k and iterated the simulation along a desired k path, from gamma point to M to K and back to gamma point. For each k-value the recorded time signals are read out and spectrally analyzed to find the resonances or modes of the crystal.

978-1-4244-1932-6/08/$25.00 ©2008 IEEE

Eventually, the peaks from all the k-iterations are assembled into a band plot where there is a clear bandgap between 115 THz and 135 THz (Figure 2).

The next step in the exploration of our structure was to construct and analyze a cavity defect within our PPPC (Figure 1-b). The defect is a hole that has a diameter of 100 nm and the other holes are 360 nm across with a period of 400 nm, the rest of the crystal structure remains the same. The cavity was excited using a broad electric TM dipole source and the frequency response was analyzed using the FFT of the measured field plotted versus intensity (Figure 3). After locating the first excited mode at 93 THz, its spectral line was determined at the full width half maximum of the peak, and from that Q can be calculated knowing that $Q = f_0/\Delta f$. With a spectral line width of 7.8 THz, the Q-factor for this crystal is 12. The volume of the cavity defect is 6.28×10^{-23} nm^3, far below the theoretical limit for 3.23 micron light, which is about 4.2×10^{-18} nm^3.

By using plasmon-polaritons one can squeeze light 4 orders of magnitude more than in conventional photonic crystals. The PPPC has a very intense field inside the cavity defect with a Purcell's constant of 4.9×10^5 rivaling the best photonic crystal cavities. We can therefore use this structure along with cavity ringdown spectroscopy to develop a highly efficient single molecule detection method in the terahertz frequency domain.



(a)

(b)

Figure 1. (a) Structure of a PPPC with upper and lower gold cladding layers sandwiching a thin, 8 nm, silicon dielectric film.
(b) Structure of a PPPC with a cavity defect.

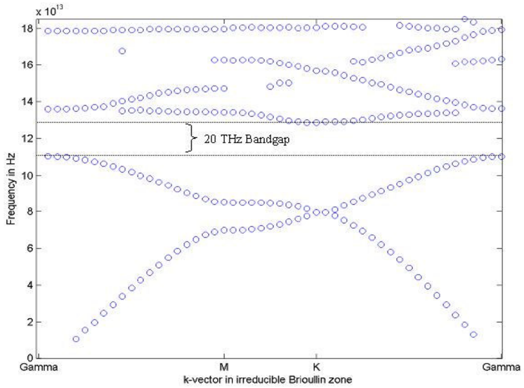


Figure 2. Band plot of the PPPC, hole diameter of 450 nm, period of 500 nm, shows a clear bandgap between 115 THz to 135 THz.

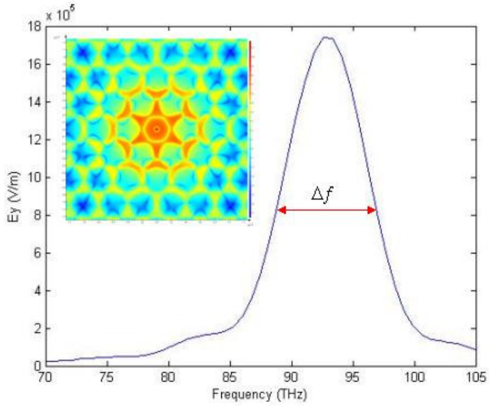


Figure 3. Fundamental mode of cavity defect in the PPPC. $f_0 = 93$ THz and $\Delta f = 7.8$ THz

References:

[1] Akahane, Noda, "High-Q photonic nanocavity in a 2D photonic crystal," *Nature*, vol. 425, pp. 944-947, (2003).

[2] Genet, Ebbesen, "Light in tiny holes," *Nature*, vol 445, pp. 39-46 (2007).

[3] Miyazaki, "Squeezing Visible Light Waves into a 3-nm-Thick and 55-nm-Long Plasmon Cavity," *Physical Review Letters*, vol. 96, 097401, (2006).

[4] Ferguson, "Materials for terahertz science and technology," *Nature Materials*, vol. 1, pp. 26-33, (2002).

[5] Krauss, "Photonic Crystals: Cavities without Leaks," *Nature Materials*, vol. 2, pp. 777 – 778, (2003).