Photonic Crystal System Design and Simulation for Biomolecule Detection

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ABSTRACT

Photonic crystals are periodic nano-structures used to control the propagation of electromagnetic waves. The variation in refractive index found in photonic crystal structures acts as a periodic potential for light propagating through the crystal, and if the refractive index contrast is large enough, a photonic bandgap is formed. Analogous to the bandgap energy region found in semiconductor crystals, photonic bandgaps in photonic crystals are frequency ranges of light that are forbidden from propagating within the structure. For three dimensional photonic crystal structures with complete photonic bandgaps, light of frequencies within the bandgap will be completely reflected, while light outside the bandgap will be completely transmitted. Introduction of defects that break the crystal's perfect periodic structure introduce localized modes within the photonic bandgap. Point defects can be used to create resonant cavities, and line defects can be used to create low loss waveguides. By introducing biomolecules in the point defects and exciting the photonic crystal with the defect frequency in the bandgap, light can be localized around the defect, enhancing fluorescence of the target molecule and aiding in the detection of the biomolecular events. Properly designed, the photonic crystal can support propagation of the fluorescence pump wavelength while line defect waveguides can be used for coupling of the resonant fluorescence emission energy from defects and out of the photonic crystal system .

Photonic crystals are generally complex two- and three-dimensional systems, which are described completely by four macroscopic Maxwell's equation. Complex numerical computations are required to solve these equations for the analysis and design of photonic crystals. The two main approaches to these numerical computations are frequency-domain and time-domain methods. The MIT Photonic Bands (MPB) software package is a freely available tool used to solve the photonic crystals in the frequency domain. Both the frequencies and modes are computed directly. Frequency domain methods like MPB are generally used to calculate band diagrams, which give the discrete, allowable frequency bands for a given structure and show any photonic bandgap ranges that are present. In contrast, the Optiwave OptiFDTD software is a finite difference time domain tool that iterates and solves Maxwell's equations in time and is generally used for computing things that involve fields changing in time, such as the resonant decay and quality factor of an optical cavity.

Numerical simulations of 2D and 3D photonic crystal systems that make use of both frequency and time domain approaches will be presented. We are optimizing systems for biosensor applications through simulation of structures of varying photonic crystal parameters such as the material, radii of rods or air holes, and slab thickness, in order to achieve effective bandgap design. Simulation results showing the effect of introducing line and point defects within the periodic structure, used for biomolecular detection, will also be presented, with a focus on Si and GaN materials.

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