ZnO 나노막대 광결정의 광밴드갭

Photonic band gaps of ZnO nanorod photonic crystals

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Nanostructures with high aspect ratio, such as nanotubes, nanowires, and nanorods have attracted much attention since they are expected to improve the performance of electronic devices, data-storage, bio-chemical and chemical sensors, optoelectronic devices, and so on. Very recently, the successful fabrications of periodic arrays of InAs nanowires and carbon nanotubes have been reported [1,2]. Well aligned zinc oxide (ZnO) nanorods and Ag nanowires have also been synthesized [3,4]. These periodically aligned nanostructures are very attractive optical materials because they have the periodic modulation of dielectric constant. The artificial structures with periodic dielectric modulation, i.e., photonic crystals, can exhibit frequency ranges in which the propagation of photons is prohibited, i.e., photonic band gaps, and highly dispersive properties causing the anomalous refraction phenomena such as super-prism effects and negative refraction. It has been demonstrated that are useful in controlling the propagation and emission of photon [5,6]. Thus photonic crystals based on the nanostructures could offer unprecedented properties playing a crucial role in developing future nanophotonics [7,8].

In this presentation, we investigate the optical properties of periodic arrays of aligned ZnO nanorods, which are attractive efficient ultraviolet light emitting materials, ZnO nanorod photonic crystals. We show that the ZnO nanorod photonic crystals can exhibit the photonic band gaps from the photonic band calculations using the modified plane wave expansion method that treats effectively frequency dependent materials. The photonic band gaps can be tuned to the interesting spectral range by varying the radius of ZnO nanorod and the period of the array. We also show from the finite difference time domain simulations that the luminescence of ZnO nanorod can be altered by the photonic band gap effect.

The height of ZnO nanorod is in general very longer than its diameter [4]. Thus the periodic array of well aligned ZnO nanorods can be treated as a two-dimensional photonic crystal. In a two-dimensional photonic crystal, there are two independent modes, i.e., transverse magnetic (TM) mode $E \parallel c$ and transverse electric (TE) mode $E \perp c$, where $E$ is the electric field of the mode and $c$ is the axis of ZnO nanorod. In general, a two-dimensional photonic crystal composed of dielectric rods in air exhibit large photonic band gaps for TM mode. Thus we consider TM modes only here. The refractive index for polarization parallel to the $c$-axis of ZnO, $n_{\parallel}$, has been in recent measured in the energy range between 1.0 to 3.0 eV and well fit to the a three-term Cauchy approximation type formula [9]. Since $n_{\parallel}$ is frequency dependent, we employed the modified plane wave expansion method that treats effectively frequency dependent materials in the photonic band calculations [10].

Figure 1(a) shows the lowest three photonic bands for TM modes in a two-dimensional triangular lattice of ZnO nanorods when the period of the nanorod array $a$ is 240 nm and the diameter of rod $2R$ 120 nm, where $R$ is the radius of rod. The inset denotes the first Brillouin
zone of a two-dimensional triangular lattice. One can see that there is a photonic band gap between the first and the second bands. The band gap range is about from 2.0 to 2.4 eV (514 ~ 617 nm). The band gap range can be varied by changing the radius of ZnO nanorod. The dependence of the band gap range on $R/a$ is represented in fig. 1(b). $a$ is kept 240 nm. The band gap range is hatched. The band gap is opened (closed) when $R/a$ is about 0.1 (0.45). The band gap size reaches the maximum value, 0.46 eV around $R/a=0.25$.

Fig. 1. a) the lowest three photonic bands for TM modes in a triangular lattice of ZnO nanorods when the period of the nanorod array $a$ is 240 nm and the diameter of the rod $2R$ is 120 nm. ZnO nanorod photonic crystal exhibits the photonic band gap in the range from 2.0 to 2.4 eV. The inset denotes the first Brillouin zone of a two-dimensional triangular lattice. (b) the dependence of the band gap on $R/a$ when $a=240$ nm. The hatched area denotes the band gap.

The photonic band gap can affect the emission from ZnO nanorods. For example, ZnO shows a visible luminescence band with a spectral maximum around 2.35 eV (~ 530 nm) due to oxygen or zinc vacancies [11]. If the spectral maximum frequency of the luminescence lies around the center of a photonic band gap, the luminescence could be strongly suppressed. The simulated yellow luminescence from ZnO nanorod photonic crystals by the finite difference time domain method will be presented.

Reference