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Optical properties of silver nanocomposites and photonic band gap – Pressure dependence

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ABSTRACT

We theoretically investigate the effect of photonic band gaps in one dimensional photonic crystals based on nanocomposite of silver nanoparticles. The dielectric permittivity is computed based on the pressure dependence of plasma frequency and damping constant of silver nanoparticle. It leads to the tuning of photonic band gap. We have also investigated the change in photonic band gap due to the influence of filling factor and the size of the nanoparticles. Our results provide a guideline for designing potential photonic devices.

1. Introduction

Photonic crystals (PCs) have attracted an important attention due to potential applications in optical sensors, optical filters and various optical integrated devices [1–3]. The main attraction of the PCs is the photonic band gap (PBG), which revealed the existence of forbidden band gaps in their transmission spectra. To achieve suitable band gaps, great efforts have been made to obtain tunability of the band gaps. To obtain a tunable PC, the dielectric constant depends on one of the constituent materials. It also depends on some external parameters, such as electric field [4], temperature and hydrostatic pressure [5], which can modify the response function of the PC materials.

Optical materials with a high refractive index have numerous applications in increasing the resolution of optical microscope [6], fabrication of miniature high quality lenses and other optical lenses. Nanoparticles (NPs) with size in the range $1-100$ nm are embedded in a host medium of metal, a semiconductor or a dielectric are of interest. The material properties of small sized particles are very interesting and are responsible for high surface to volume ratio, quantum size effect etc. The size controlled optical properties of silver nanoparticles have potential applications such as diffraction elements, optical filters, nanophotonic devices, biosensors and nonlinear media [7].

In metals, the free electron concentration is of the order of $10^{28}/m^3$ and the plasma frequency falls into the optical range. Because of the negative dielectric function for frequencies lower than the plasma frequency, the index of refraction is imaginary and the metals are plasmons. When $\omega > \omega_p$, the dielectric function becomes positive and the metals becomes transparent. Materials with dielectric permittivity at frequencies below their plasma frequency have a significant impact for the design and fabrication of novel hybrid materials [8]. The linear and nonlinear properties of composite materials are determined by Plasmon resonance of metal nanoparticles in transparent matrix. The increase in the dielectric function of the surrounding medium causes the Plasmon resonance position to shift to longer wavelength [9]. The wavelength shift can be used for sensing, because the relative shift of the Plasmon is a measure of the dielectric function of the material surrounding the metal structures. In the sensor applications, the sensitivity of the measurement is determined by the wavelength shift of the Plasmon per unit of refractive index change of the surrounding medium.

The effects of temperature and applied hydrostatic pressure on the photonic band structure of 1D PCs were investigated in Ref. [5]. In the present work, we propose to use composite structures to another class of PCs by applying hydrostatic pressure to tune the PBG. It depends on the dielectric permittivity of the composite materials that can be altered by applying pressure. For model calculations, we investigate the effect of silver NPs embedded in GaAs matrix with different filling factors in the composite layers. The position and width of PBG can be effectively tuned based on the pressure dependence of dielectric permittivity of the host matrix, filling factor and for different radii of the nanoparticles.

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2. Theoretical background

2.1. Dielectric permittivity of composite material

The nanocomposite metal nanoparticles are randomly distributed in transparent matrix. To determine the permittivity of the nanocomposite $\varepsilon_{mix}(\omega)$, we use the Maxwell–Garnett formula [10]

$$\frac{\varepsilon_{mix}(\omega)-\varepsilon_d}{\varepsilon_{mix}(\omega)+2\varepsilon_d}=f\frac{\varepsilon_m(\omega)-\varepsilon_d}{\varepsilon_m(\omega)+2\varepsilon_d} \tag{1}$$

where ε_d is the dielectric permittivity of the transparent matrix (GaAs), f is the filling factor of the nanoparticle, ε_m is the dielectric permittivity of the metal nanoparticle and ω is the optical frequency.

The dielectric function for GaAs is given by [11]

$$\varepsilon_d(\omega)=\varepsilon_\infty+\frac{(\varepsilon_0-\varepsilon_\infty)\omega_{TO}^2}{\omega_{TO}^2-\omega^2-i\omega\gamma} \tag{2}$$

where ω_{TO} is the frequency of the transverse optical phonons, ε_∞ and ε_0 are the high frequency and static dielectric constants respectively. Here γ is the damping factor ($\gamma = 2.4\ \mathrm{cm}^{-1}$) [12].

The dielectric constant and optical phonon frequency varies with pressure [11]

$$\varepsilon(P)=\varepsilon(0)\exp\left(\frac{d\log\varepsilon}{dp}P\right) \tag{3}$$

where $\varepsilon_0=13.18$, $\varepsilon_\infty=10.89$ at zero pressure, $\frac{d\log\varepsilon_0}{dp}=-17.3\times10^{-3}\ \mathrm{GPa}^{-1}$ and $\frac{d\log\varepsilon_\infty}{dp}=-14\times10^{-3}\ \mathrm{GPa}^{-1}$.

The pressure dependence of ω_{TO} is given by

$$\omega_{TO}(P)=\left(268.1+3.95P-0.032P^2\right)\mathrm{cm}^{-1} \tag{4}$$

The dielectric constant of metal nanoparticles is calculated according to Drude theory

$$\varepsilon_m(\omega)=\varepsilon_0-\frac{\omega_P^2}{\omega(\omega+i\gamma)} \tag{5}$$

where ε_0 is a constant (ε_0=5 for silver [13], ω_P is the plasma frequency and γ is a damping constant of plasma oscillations (the inverse of the relaxation time).

The spherical NPs are distributed randomly and homogenously in a transparent matrix. The pressure dependence of plasma frequency [14]

$$\omega_P^2(P)=\frac{\omega_P^2(0)}{\left(1+q\frac{\Delta V}{V_0}\right)} \tag{6}$$

where $\omega_P(0)=9$ eV [15]. $\omega_P^2(P)$ is proportional to the electron density which scales with volume as $\frac{1}{V}$ and then $q=1$ for all pressures.

The radius of the nanoparticle with pressure

$$R_P=R_0[1-3P(S_{11}+2S_{12})]^{\frac{1}{3}} \tag{7}$$

where R_0 is the radius of the NP at zero pressure, S_{11} and S_{12} are the compliance constants of silver NP ($=23\times10^{-12}\ \mathrm{Pa}^{-1}$, $S_{12}=-9.8\times10^{-12}\ \mathrm{Pa}^{-1}$ [16]).

The fractional change in volume associated with the hydrostatic pressure [17]

$$\frac{\Delta V}{V_0}=-3P(S_{11}+2S_{12}) \tag{8}$$

where $\Delta V=V_P-V_0$ is the volume reduction with pressure with $V_P=\frac{4}{3}\pi R_P{}^3$ and $V_0=\frac{4}{3}\pi R_0{}^3$.

The free electron density in a metal is given by $=\frac{n}{V}$, where n is the concentration of electrons and V is the volume. If the free electron density at zero pressure be N_0 (N_0=5.85×10^{28} m^{-3} [18]), then the total number of free electrons in the metal NPs is

$$n=N_0V_0=N_PV_P \tag{9}$$

The Plasmon damping constant can be expressed as [19]

$$\gamma=\gamma_\infty+A\frac{v_F}{R_0} \tag{10}$$

where R_0 is the radius of the NP and γ_∞ is the size-independent damping constant caused by scattering of free electrons, phonons and lattice defects. The value of $A=1$ [19] and v_F is the Fermi velocity in bulk metal (v_F=1.39×10^8 m/s in bulk silver metal [18]). The surface to volume ratio of NP increases dramatically when their size is reduced as $\frac{1}{R_0}$. This means that the smaller the size, the larger the contribution of the surfaces to the properties of materials [20].

The relaxation time

$$\tau=\frac{m}{\rho Ne^2} \tag{11}$$

where m is the mass of an electron, ρ is the resistivity of silver (ρ = 1.61×10^{-6} ohm cm [18]), N is the concentration of electrons and e is the charge of the electron.

Substituting the value of the dielectric constant of metal nanoparticle ε_m and of GaAs ε_d in Eq. (1), we can deduce the real and imaginary parts of the composite material which is given by

$$\epsilon_{mix}(\omega)=\epsilon'_{mix}+i\epsilon''_{mix} \tag{12}$$

The real and imaginary parts of $\varepsilon_{mix}(\omega)$ characterize the refractive properties of the material. Around the resonant frequency ω, ε'_{mix} behaves as an anomalous manner and exhibits strong absorption. The ε'_{mix} is negative in a particular frequency range to be denoted as ω_{10} and ω_{20}. In this interval, the nanocomposite has metallic optical properties.

2.2. Transmission properties of photonic crystals

The transmission properties of one dimensional PC of N elementary cells of lattice constant 'a' consisting of spherical silver NPs embedded in a host matrix of GaAs may be obtained now. Each cell consists of one nanocomposite layer of width d_1 and another layer of air of width d_2. We assume that the lattice constant $a=2\lambda_P$ where λ_P is the plasma wavelength corresponding to the plasma frequency at zero pressure (ω_p=9 eV) such that λ_P=138 nm. The width of the layers are $d_1=0.75a$ and $d_2=0.25a$.

To calculate the thickness of the nanocomposite layer d_1 due to change in volume associated with hydrostatic pressure, we assume that the GaAs layer is of spherical shape of radius ($r=\frac{d_1}{2}$) embedded with silver NP of radius R_0. The volume of the composite layer can be computed as

$$V_{comp}=V_1\left(1+\frac{\Delta V_1}{V_{01}}\right)(1-f)+V_2\left(1+\frac{\Delta V_2}{V_{02}}\right)f \tag{13}$$

where $V_1=\frac{4\pi r^3}{3}-\frac{4\pi R_0{}^3}{3}$ is the volume of the GaAs layer and $V_2=\frac{4\pi R_0{}^3}{3}$ the volume of the silver NP and f is the filling factor. The values of $\frac{\Delta V_1}{V_{01}}$ and $\frac{\Delta V_2}{V_{02}}$ are calculated as per Eq. (7) and the compliance constants of GaAs are $S_{11}=11.6\times10^{-12}\ \mathrm{Pa}^{-1}$, $S_{12}=-3.66\times10^{-12}\ \mathrm{Pa}^{-1}$ [5]. The thickness of the nanocomposite layer is reassigned as $d_1=\sqrt{V_{comp}}$.

To compute the PBG in the transmission spectra due to pressure dependence, we employ the transfer matrix method (TMM)