

Effective optical properties of the one-dimensional periodic structure of TiO_2 and SiO_2 layers with a defect layer of nanocomposite consisting of silver nanoparticle and E7 liquid crystal

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Abstract. In this work, the dielectric property of a nanocomposite (NC) consisting of silver nanoparticle and E7 liquid crystal (LC) has been investigated theoretically at different temperatures. The study shows that the surface plasmon resonance (SPR) and filling fraction of the silver nanoparticle significantly change the dielectric property of the NC. To study the optical property of the defective periodic structure, the NC was considered as a defect layer in a semifinite one-dimensional periodic structure (1DPS) of TiO_2 and SiO_2 layers, i.e. $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$. The optical properties of the 1DPS with the NC as the defect layer have been studied by the simple transfer matrix method (TMM). Moreover, the transmission and absorption characteristics of the 1DPS in the presence of silver nanoparticle in the NC have been studied with different orientations of the LC molecule.

Keywords. Liquid crystal; silver nanoparticle; transfer matrix method; filling fraction; orientation.

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1. Introduction

A special class of optical periodic medium, commonly known as photonic crystals (PCs), has been developed. A PC consists of alternating stacks of dielectric materials in different directions. Therefore, PCs are classified into three types: one-dimensional PCs (1DPC), two-dimensional PCs (2DPC) and three-dimensional PCs (3DPC). PCs are very interesting due to the existence of a photonic band gap (PBG) in the transmission spectra of the optical periodic medium. PBGs are special regions in the transmission spectra of the PCs which prohibit the propagation of an electromagnetic wave in that region. PCs are capable of controlling the flow of electromagnetic wave due to the periodicity of dielectric materials. Due to their unusual properties, PCs find application in many optical devices, viz. optical filters, reflectors, switches, etc. [1–12]. Mostly, optical filter and reflector applications of PCs are based on the omnidirectional reflection and transmission properties of PCs. The metallic photonic crystal is used

as absorption-based optical devices such as sensors, microwave absorbers, etc. [13–21]. The third-order nonlinear optical properties of the silver nanocomposite (NC) have been studied experimentally and it was concluded that the control of optical nonlinearity may lead to novel device applications [22]. Certain optical anisotropic materials, known as liquid crystals (LCs), exhibit a transitional stage between liquids and solids. LC has both properties: flows like liquids while being crystalline as solid. LC has extraordinary and ordinary components of electric permittivity. Hence, electric permittivity of the LC can be expressed in tensor form which is dependent upon the molecular orientation of the LC. Such birefringent materials are used as tunable nonlinear optical devices [23–25]. The dielectric properties of the LC are tuned by the external electric field and temperature which affect the electric permittivity of the LC. The optical transmission of a photonic crystal with the LC as the defect layer can be regulated by varying the applied electric field and temperature. By coating the inverse opal with the LC, the

tunability of PBG in PCs can be controlled as suggested by Bush and John [26] and confirmed experimentally by Yoshino *et al* [27]. PCs with LC as the defect layer are used as tunable optical devices based on the external application of an electric field or magnetic field and temperature [28–41]. It is known that the LCs are anisotropic materials and the optical properties of the LC are dependent upon the orientation of the molecules. The dielectric tensor of the LCs, consisting of ordinary and extraordinary components of the electric permittivity and anisotropy (ε_a) [42] is expressed in the matrix form as

$$\tilde{\varepsilon} = \begin{pmatrix} \varepsilon_{\perp} + \varepsilon_a \sin^2 \phi & 0 & \varepsilon_a \sin \phi \cos \phi \\ 0 & \varepsilon_{\perp} & 0 \\ \varepsilon_a \sin \phi \cos \phi & 0 & \varepsilon_{\perp} + \varepsilon_a \cos^2 \phi \end{pmatrix}. \quad (1)$$

This dielectric tensor of the LC is a non-diagonal matrix containing an orientation-dependent matrix element which shows the anisotropic behaviour of the LC. The dielectric tensor of the LC is reduced to a diagonal matrix if we consider the orientation angle of the LC director (ϕ) to be either 0 or 90°. Hence, the transfer matrix method (TMM) [43] can be used to study the optical properties of the LC's director angle, $\phi = 0^\circ$ or 90°.

The dielectric permittivity of the E7 LC is temperature-dependent and it is also affected by external doping materials in the LC. NC material can be synthesised by the dispersion of nanoparticles into a host material (e.g. LC). Such NC material helps to produce new PBG regions in the transmission of the PC due to the change in dielectric constant. In addition to this, the optical characteristics of the PC are also observed to be affected by the filling fraction and the radii of the doped nanoparticles [44–48]. The effective dielectric function of the NC consisting of a doped nanoparticle (silver) in the LC host can be written by using the well-known Maxwell-Garnett model [49–51].

In the present work, we have investigated the effect of the inclusion of silver nanoparticle in the E7 LC mixture

at different temperatures. The optical properties of the one-dimensional periodic structure (1DPS) with the NC as the defect layer, i.e. $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$, are discussed at different temperatures and filling fractions. In our study, we have theoretically proposed to design a NC consisting of a silver nanoparticle of radius 5 nm and an E7 LC mixture. Here, the E7 LC is the mixture of four different LCs: 5CB ($\text{C}_{18}\text{H}_{19}\text{N}$), 7CB ($\text{C}_{20}\text{H}_{23}\text{N}$), 8OCB ($\text{C}_{21}\text{H}_{25}\text{NO}$) and 5CT ($\text{C}_{24}\text{H}_{23}\text{N}$) [52]. The ordinary and the extraordinary dielectric constants of the E7 LC are dependent upon the wavelength and the clearing temperature (T_C) of the LC [53]. For inclusions of the nanoparticle in the LC host, a spherical silver nanoparticle of radius 5 nm is considered and the optical properties of the NC (LC + AgNPs) as well as the defect periodic structure with such a NC defect $((\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5)$ have been studied.

2. Theoretical modelling

The periodic arrangement of the TiO_2 and SiO_2 layers in one direction has been considered for designing 1DPC with NC of silver nanoparticle with E7 LC as the defect layer, $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$, as shown in figure 1.

In our study, we have taken the refractive indices of SiO_2 and TiO_2 layers as 1.5 and 2.4, respectively, and the thicknesses of the SiO_2 and TiO_2 layers as 56.2 and 91.6 nm, respectively. The optical properties of the photonic crystal with NC as the defect layer are studied using the TMM. The extraordinary (n_e) and the ordinary (n_o) refractive indices of the E7 LC mixture are dependent on the temperature, and are represented as

$$n_e(T) = A - BT + \frac{2(\Delta n)_o}{3} \left(1 - \frac{T}{T_C}\right)^\beta, \quad (2)$$

$$n_o(T) = A - BT - \frac{(\Delta n)_o}{3} \left(1 - \frac{T}{T_C}\right)^\beta, \quad (3)$$

where A , B , (Δn) , β are the wavelength-dependent parameters of LC and T_C is the clearing temperature

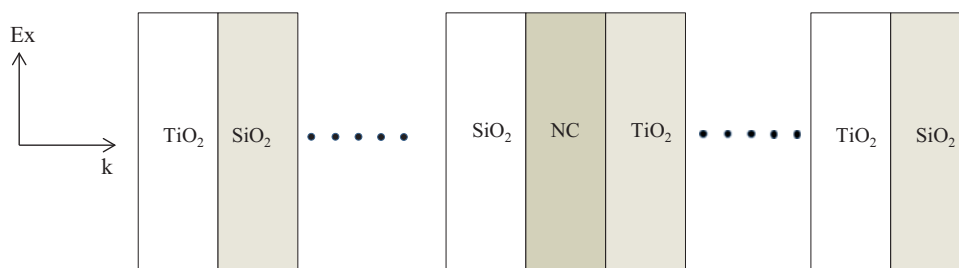


Figure 1. Schematic representation of the 1DPCs of the TiO_2 and SiO_2 dielectric layers with a defect layer of NC layer consisting of nanoparticle and E7 LC.

of the LC mixture. All constants are used to determine the refractive indices of the E7 LC mixture at $1.5 \mu\text{m}$ wavelength. The extraordinary dielectric permittivity ($\epsilon_{||}$) and ordinary dielectric permittivity (ϵ_{\perp}) of LC can be obtained by squaring the value of n_e and n_o using eqs (2) and (3), respectively.

The Maxwell–Garnett model is used to determine the refractive index of the NC consisting of silver nanoparticles and E7 LC. The silver nanoparticles are arbitrarily dispersed in the host LC. Consequently, the effective electric permittivity of NC can be written as

$$\epsilon_{\text{eff}} = \frac{2\epsilon_{\text{LC}}f(\epsilon_m - \epsilon_{\text{LC}}) + \epsilon_{\text{LC}}(\epsilon_m + 2\epsilon_{\text{LC}})}{2\epsilon_{\text{LC}} + \epsilon_m + f(\epsilon_{\text{LC}} - \epsilon_m)}, \quad (4)$$

where ϵ_{LC} , ϵ_m and f are the dielectric permittivities of the LC, silver nanoparticle and the volume fraction of nanoparticles inclusion in the LC, respectively. The dielectric permittivity of the silver nanoparticle can be considered using the Drude model:

$$\epsilon_m = \epsilon_0 - \frac{\omega_p^2}{\omega^2 + i\omega\eta}, \quad (5)$$

where ω_p , ϵ_0 and η are plasmon frequency, relative permittivity of the metal nanoparticles and damping frequency, respectively. The damping frequency is dependent upon the radius (r) of the nanoparticle and the velocity (v_f) of the electron at Fermi energy, which is described as

$$\eta(r) = \eta_0 + \frac{v_f}{r}, \quad (6)$$

where η_0 is the decay constant obtained by the scattering of free electron with phonons, electrons, etc.

3. Results and discussion

This section is divided into five subsections. In the first subsection, we have studied the refractive indices of the LC and the effective permittivity of the NC at different temperatures. The effective dielectric permittivities of the NC at different filling fractions are studied in §2. In §3, we have studied the optical property of the considered periodic structure without and with the defect layer LC. The transmission and absorption properties of the 1DPS with NC as the defect layer at different temperatures for filling fraction $f = 0.05$ are studied in §4. Lastly, the transmission and absorption characteristics of the 1DPS with NC as the defect at different filling fractions (f) for $T = 300 \text{ K}$ are studied in §5.

3.1 Refractive indices of LC and the effective refractive index of NC at different temperatures

First, the variation of refractive indices of the E7 LC mixture with temperature is investigated (figure 2). The extraordinary refractive index attains a minimum value of 1.55 when $T_C = 330 \text{ K}$. Similarly, the ordinary refractive index increases with temperature and attains the maximum value 1.55 which is equal to the minimum value of extraordinary refractive index at $T_C = 330 \text{ K}$. A further increase in temperature leads to a constant

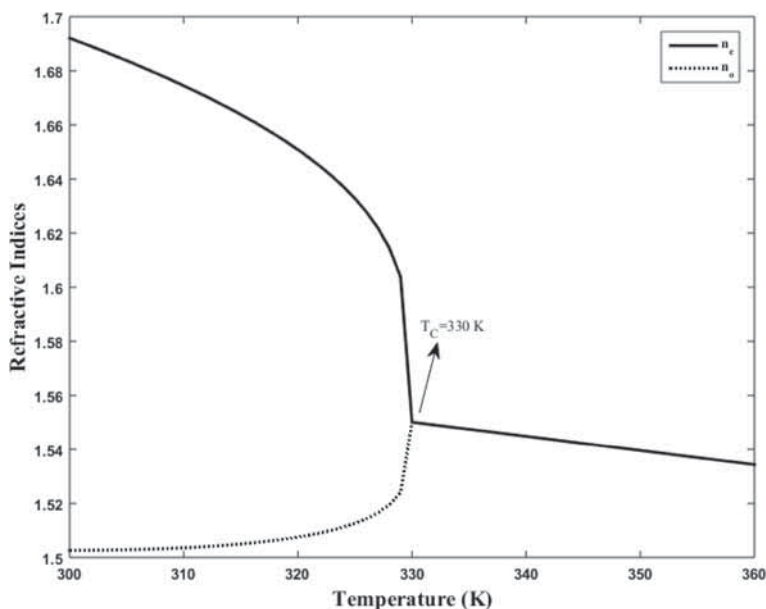


Figure 2. Variation of refractive indices of E7 LC mixture with temperature (K).

decrease in both refractive indices having the same nature. At $T_C = 330$ K, the phase of the E7 LC mixture changes and converts into an isotropic phase. Hence, both refractive indices vary with temperature in the same manner.

The optical properties of the 1DPS containing alternating layers of TiO_2 and SiO_2 with NC material (LC + AgNPs) as the defect layer were studied using the TMM. In our calculation, the refractive indices and the thicknesses of TiO_2 and SiO_2 layers are taken as discussed earlier in theoretical modelling. The thickness of the LC composite is 100 nm. The plasmon frequency ω_p and the decay constant of the silver particle are $2\pi \times 2.17 \times 10^{15}$ and $2\pi \times 4.8 \times 10^{12}$ Hz, respectively. The radius (r) of the spherical silver nanoparticle inclusion in the LC host is taken as 5 nm with $\epsilon_0 = 5$.

Next, the effective dielectric permittivity of the NC of the silver nanoparticle with the E7 LC mixture has been studied. For the composite structure, the spherical silver nanoparticle of 5 nm radius is dispersed in the E7 LC mixture with different filling fractions (f). The dielectric constants of the E7 LC mixture are temperature-dependent, and the effective permittivity of the NC structure (LC + AgNPs) changes with temperature also. So we have calculated the dielectric permittivity of the NC at 300 and 329 K (figure 3). The real part of the effective dielectric permittivity has both

positive and negative values, but the imaginary part has only positive values. The variations of ordinary and extraordinary dielectric permittivities of the NC at different temperatures are shown in figures 3 and 4.

Basically, the molecules retain the director distortion angle 0° below the Fréedericksz transition of the LC. It means that the ordinary or perpendicular component (ϵ_{\perp}) of dielectric permittivity of the NC dominates for all optical properties of the PCs. But, the molecules get switched above the Fréedericksz transition of the LC and finally attain the orientation angle 90° . At this transition, the extraordinary or parallel component of the dielectric permittivity (ϵ_{\parallel}) is responsible for changing the optical properties of the defective PC. At higher temperatures, the effective dielectric permittivity of the NC is shifted towards higher values as shown in figure 3.

The E7 LC mixture is known to be anisotropic. It changes its phase and converts into the isotropic phase at 330 K. The ordinary and extraordinary dielectric permittivities of the NC become equal at 330 K. The effective dielectric permittivity of the NC structure at 330 and 360 K are shown in figure 4. The anisotropy of the NC vanishes at clearing temperature T_C and it gets converted into the isotropic phase. In the isotropic phase, the effective permittivity of the NC shifts to lower values at higher temperatures.

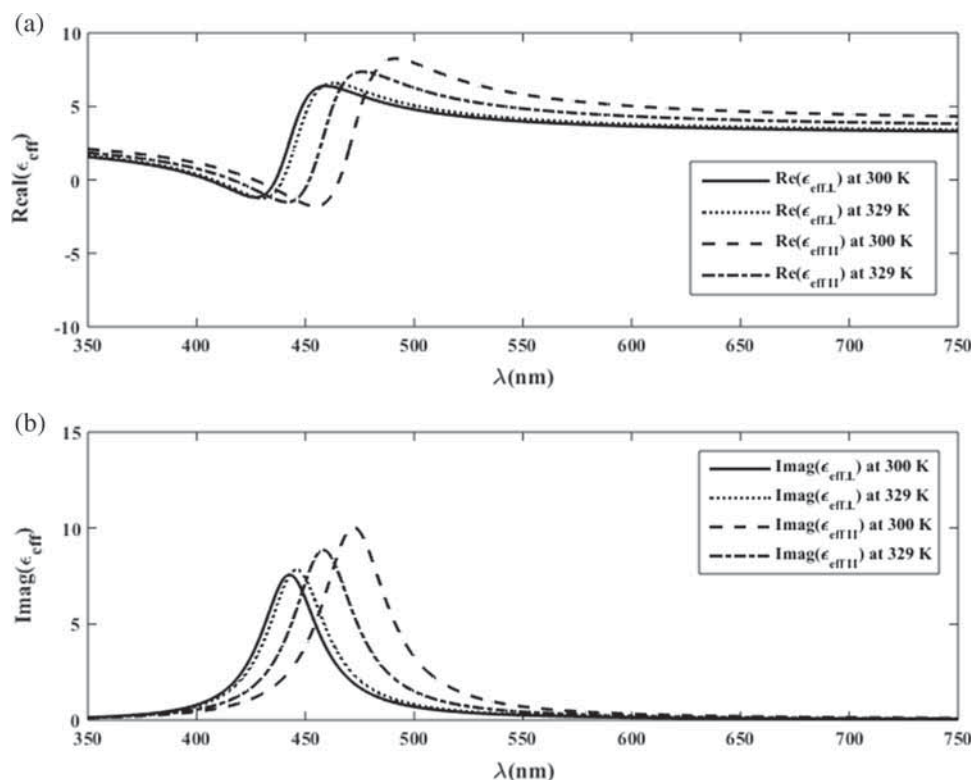


Figure 3. Real and imaginary parts of ordinary and extraordinary components of effective permittivity of the NC at different temperatures with $f = 0.1$.

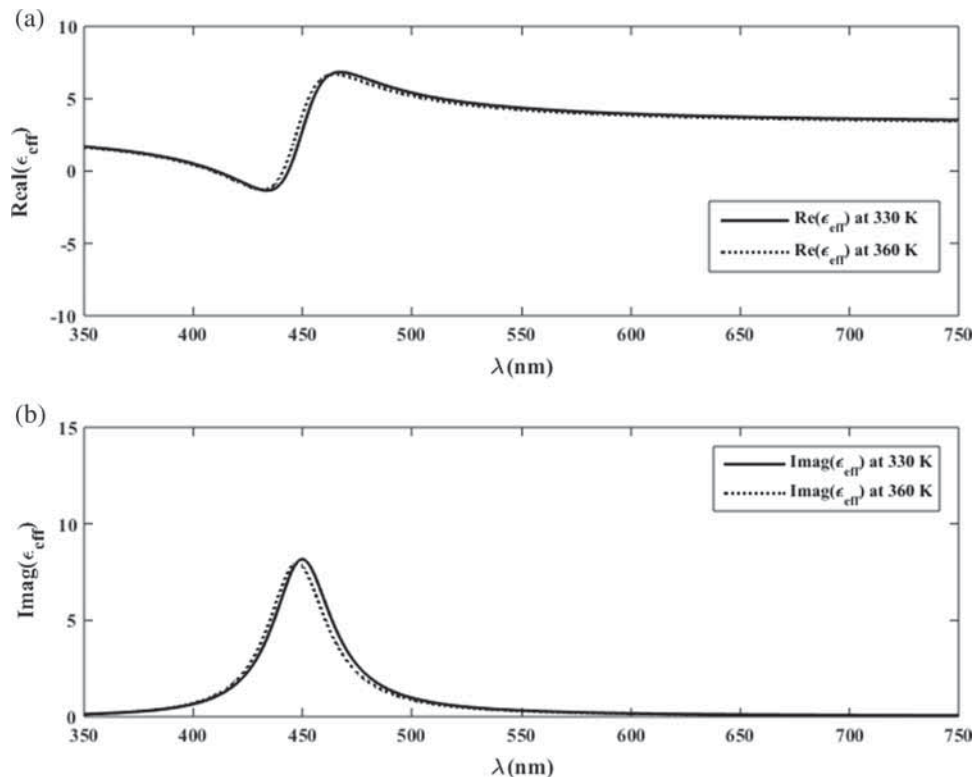


Figure 4. Real and imaginary parts of the effective permittivity of the NCs at different temperatures.

3.2 Effective dielectric permittivity of NC at different filling fractions f

In this subsection, the effective dielectric permittivity of the NC is calculated at different filling fractions and different director distortion angles (0° , 90°) of the LC. Figure 5 shows the effective dielectric permittivity of the NC at different filling fractions $f = 0.05, 0.10$ and 0.15 of silver nanoparticle inclusion in the host E7 LC with different orientations of LC. The filling fraction (f) affects the effective permittivity of the NCs as shown in figure 5. The effective permittivity shifts towards higher values for a high filling fraction as shown in figure 6. A comparison of the parallel and perpendicular components of the effective permittivity of the NC at the LC director distortion angles 0° and 90° is shown in figure 7.

3.3 Transmission and optical properties of the 1DPS without and with a defect of NC

The optical properties of the 1DPC of the TiO_2 and SiO_2 layers with a defect layer of the NC of silver nanoparticle in E7 LCs have been studied using the TMM. Figure 8 shows the optical transmission characteristics of the 1DPS of the TiO_2 and SiO_2 layers. Such a pure periodic structure of the TiO_2 and SiO_2 layers shows

a PBG region between the 467 and 669 nm region of the transmission spectra. Now, the same structure is symmetrically sandwiched by a defect layer NC that possesses a PBG region between the 451 and 712 nm wavelength range. A defect mode transmission peak of about 82.4% is obtained at 560 nm wavelength when the director distortion angle is 0° . When the distortion angle is 90° , the defect mode peak transmission is shifted at 574 nm wavelength with 72% transmission. The PBG region is also slightly changed towards the lower frequency range and the band region is found to be 454–712 nm. The transmission spectra of the 1DPS study show that the transmission of the defect mode peak is shifted towards a higher wavelength when the LC director distortion angle changes from 0° to 90° . Such a 1DPS with the NC as the defect layer can be used to design optical filters, switching devices, etc.

3.4 Transmission and absorption properties of the 1DPS with an NC at different temperatures when $f = 0.05$

Now, the optical properties of the periodic structure $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ with the NC defect layer at $f = 0.05$ have been studied for different temperatures for both 0° and 90° orientation angles. The

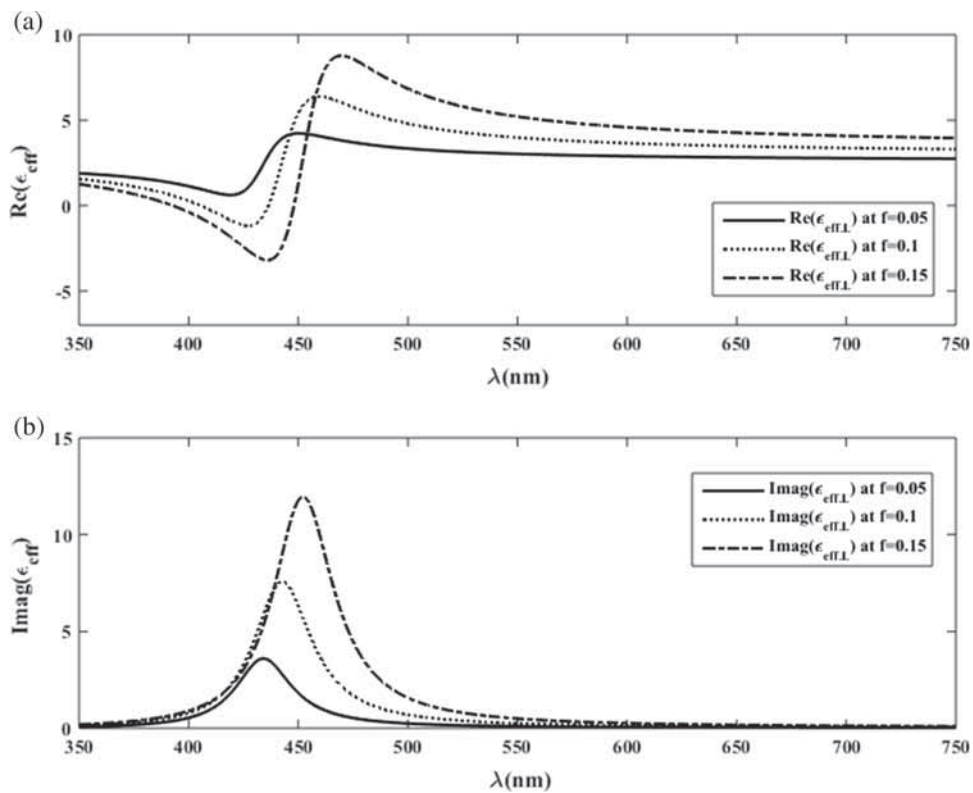


Figure 5. Real and imaginary parts of the ordinary effective permittivity of the NCs at different filling fractions.

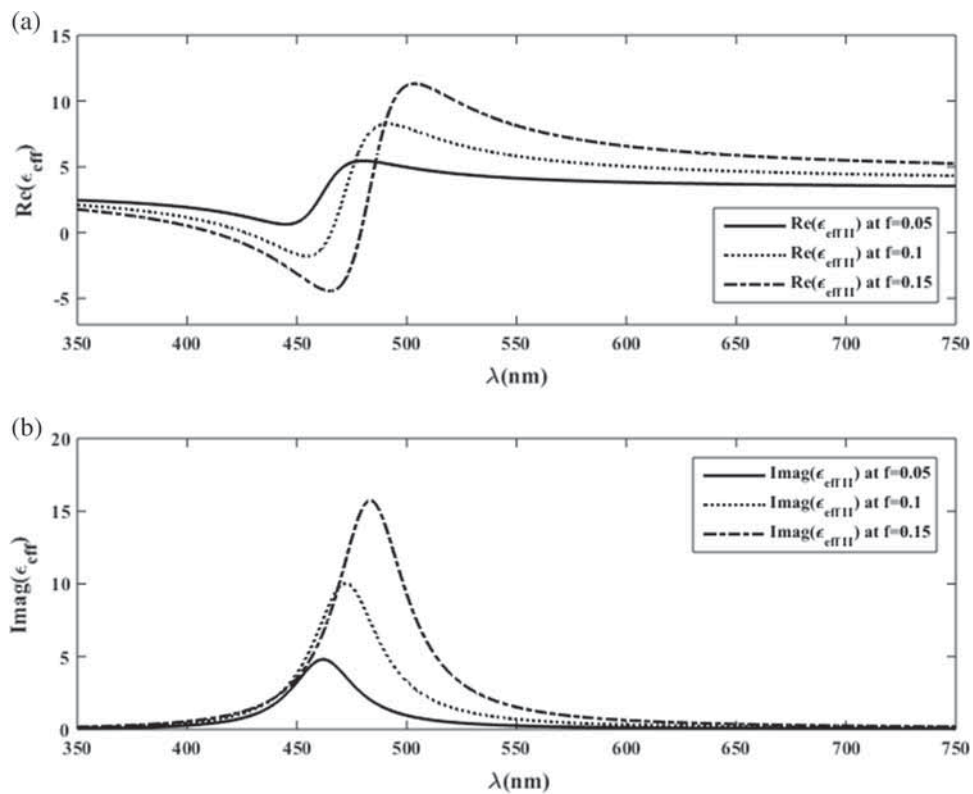


Figure 6. Real and imaginary parts of the extraordinary effective permittivity of the NCs at different filling fractions.

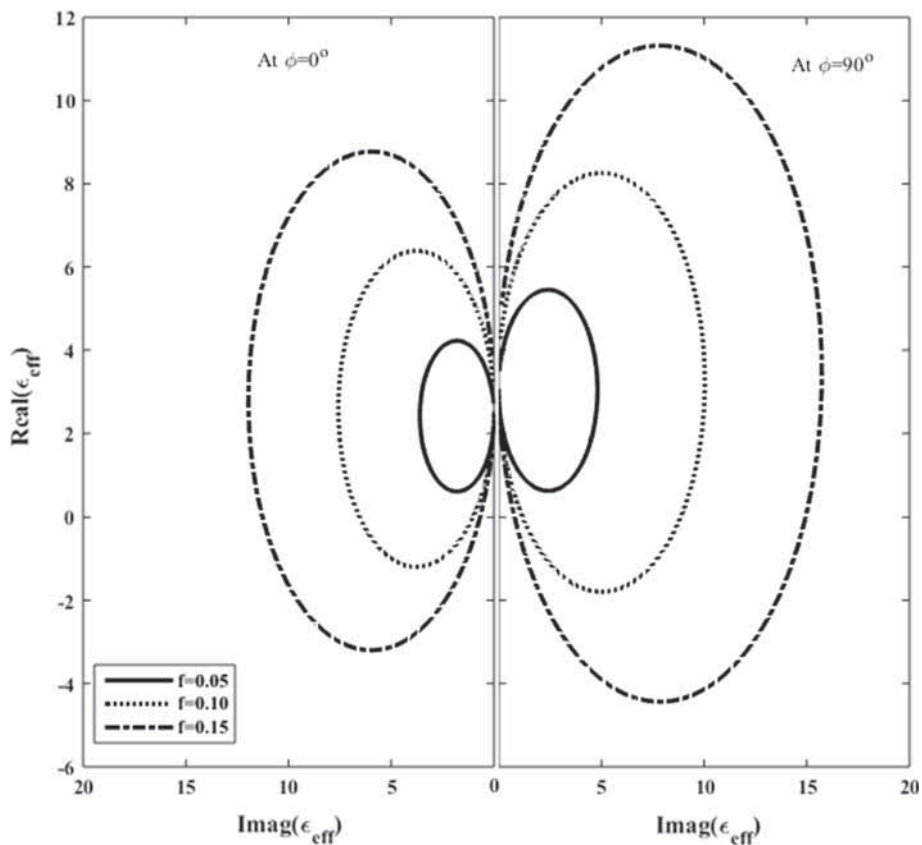


Figure 7. Real part vs. imaginary part of the effective permittivity of the NC at different filling fractions.

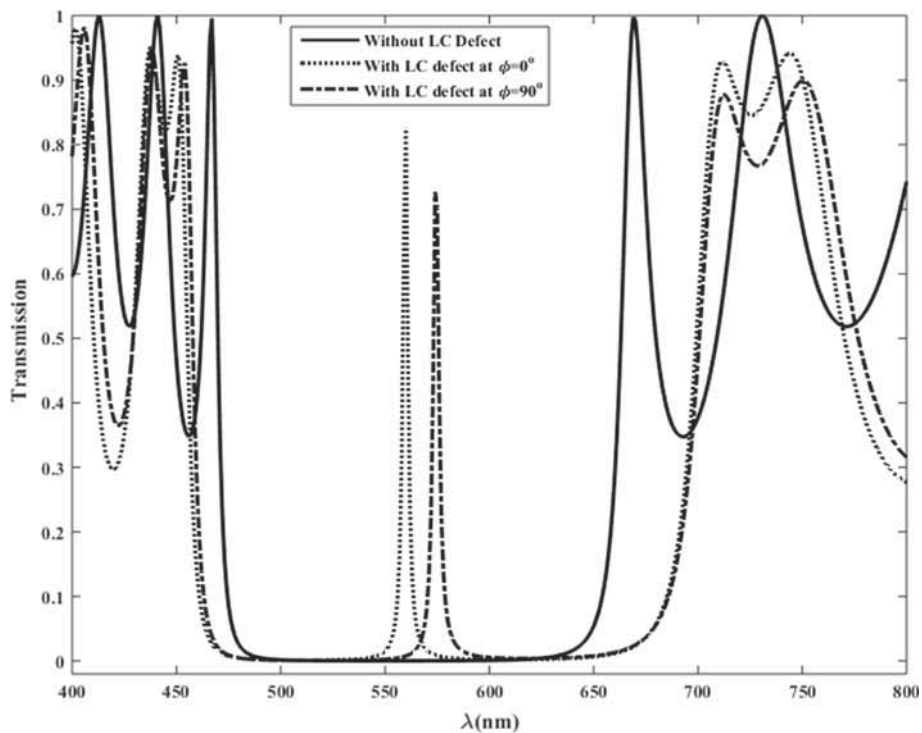


Figure 8. Transmission of the 1DPS without and with LC defect at different orientations (ϕ) of LC molecules.

transmission properties of the 1DPS $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ with a defect of the NC for 300 and 329 K at different orientation angles (0° and 90°) are shown in figure 9. The presence of silver nanoparticles in the NC affects the transmission of defect mode wavelengths. The obtained defect transmission peak lowers slightly and shows a redshift for an orientation angle of 90° . Such a periodic structure also shows absorption characteristics of the defect mode wavelengths at different orientation angles.

The absorption spectra of the periodic structure $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ are shown in figure 10 for both 0° and 90° orientations of the LC molecules at 300 and 329 K. Figure 10a shows the maximum value of absorption as 85.33% for 425 nm and the absorption of the defect mode peak is 26.74% for 576 nm at a director angle of 0° and temperature of 300 K. For 90° orientation angle, the maximum absorption is found to be 80.53 and 23.75%, at 456 and 595 nm wavelengths, respectively. Furthermore, we have also calculated absorption spectra at 329 K. The absorption value gets shifted by a small value. Figure 10b shows that the maximum absorptions are 85.93 and 85.23% at 426 and 452 nm for 0° and 90° director angles, respectively. The absorption of the defect peak is found

to be 25 and 24.93% at 579 and 586 nm for both director angles, respectively, as shown in figure 10b. The separation between defect transmissions or absorptions peaks obtained at 300 K for both director angles is greater than the separation between peaks obtained at 329 K.

Now, we have calculated the optical properties of the considered periodic structure at 330 and 360 K for $f = 0.05$. The anisotropy property of the NC vanishes because parallel and perpendicular components of the effective dielectric permittivity become equal at $T_C = 330$ K. As a result, transmission and absorption properties of the 1DPS are not affected by the orientation of the LC molecules but it is affected only by temperature. The transmission and absorption of the considered periodic structure $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ at 330 and 360 K are shown in figures 11 and 12, respectively. Figures 11a and 12a represent the transmission and absorption spectra of PC at 330 K. The transmission and absorption spectra observed at 360 K are shown in figures 11b and 12b. The maximum absorption is found to be 85.91 and 86.83% at 427 nm at 330 and 360 K, respectively. The absorption of the defect mode peaks is 25.71 and 25.77% at 581 and 579 nm at 330 and 360 K, respectively.

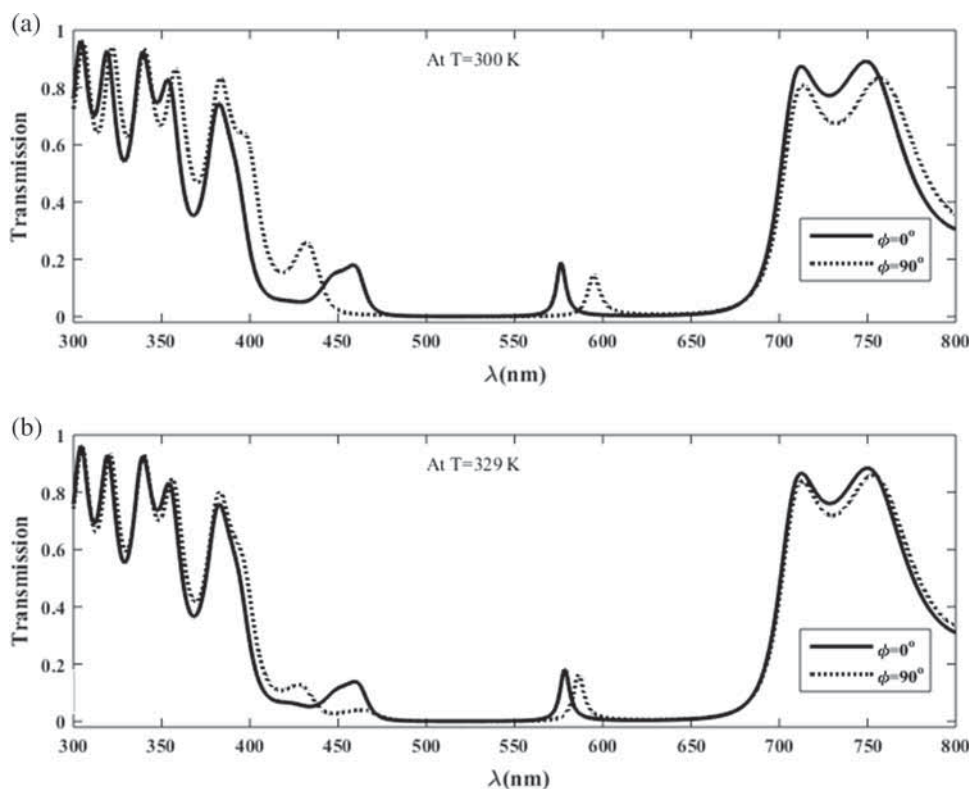


Figure 9. Transmission of the 1DPS with the NC at different orientations of molecules: (a) at $T = 300$ K and (b) at $T = 329$ K.

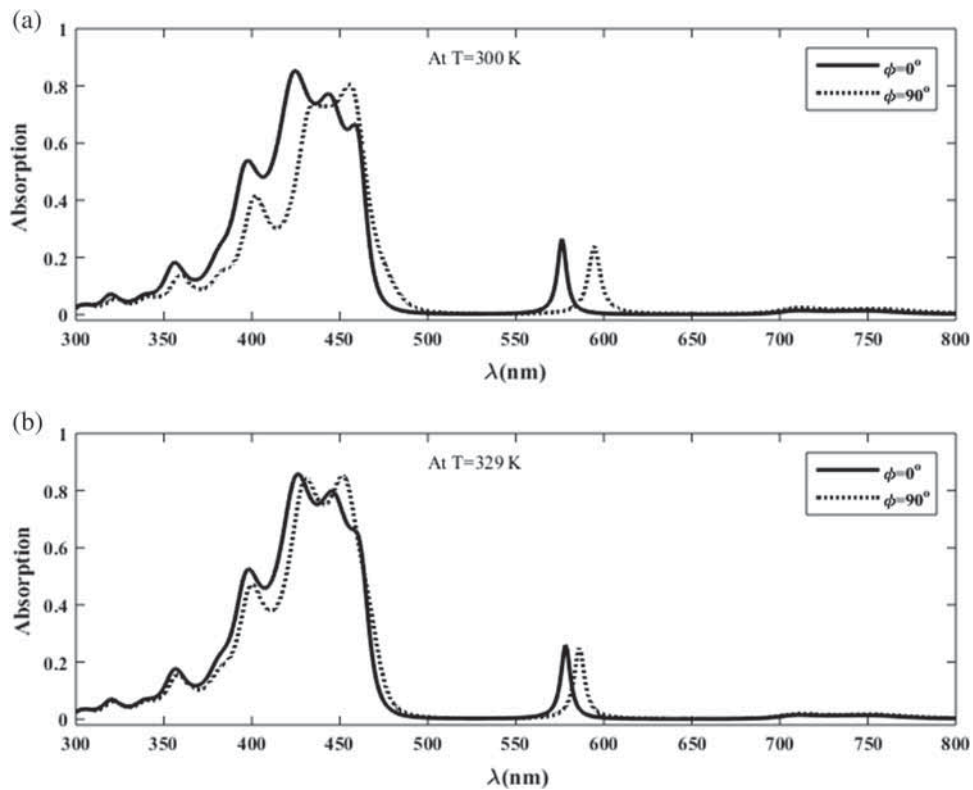


Figure 10. Absorption of the 1DPS with the NC at different orientations of LC: (a) at $T = 300$ K and (b) at $T = 329$ K.

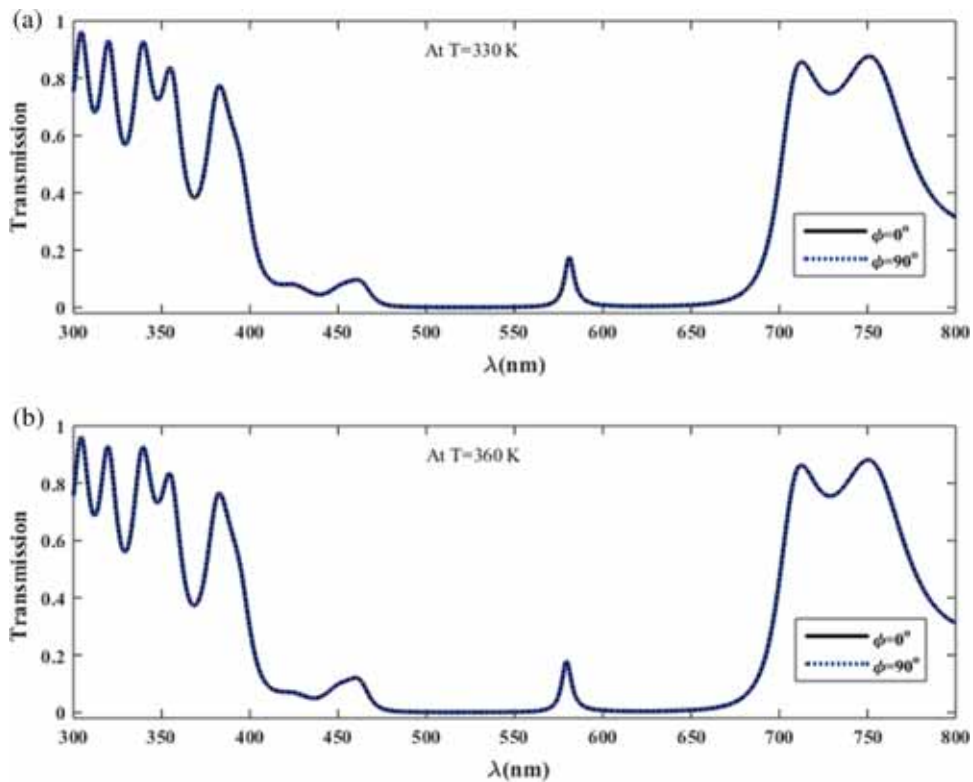


Figure 11. Transmission of the 1DPS with the NC defect: (a) at $T = 330$ K and (b) at $T = 360$ K.

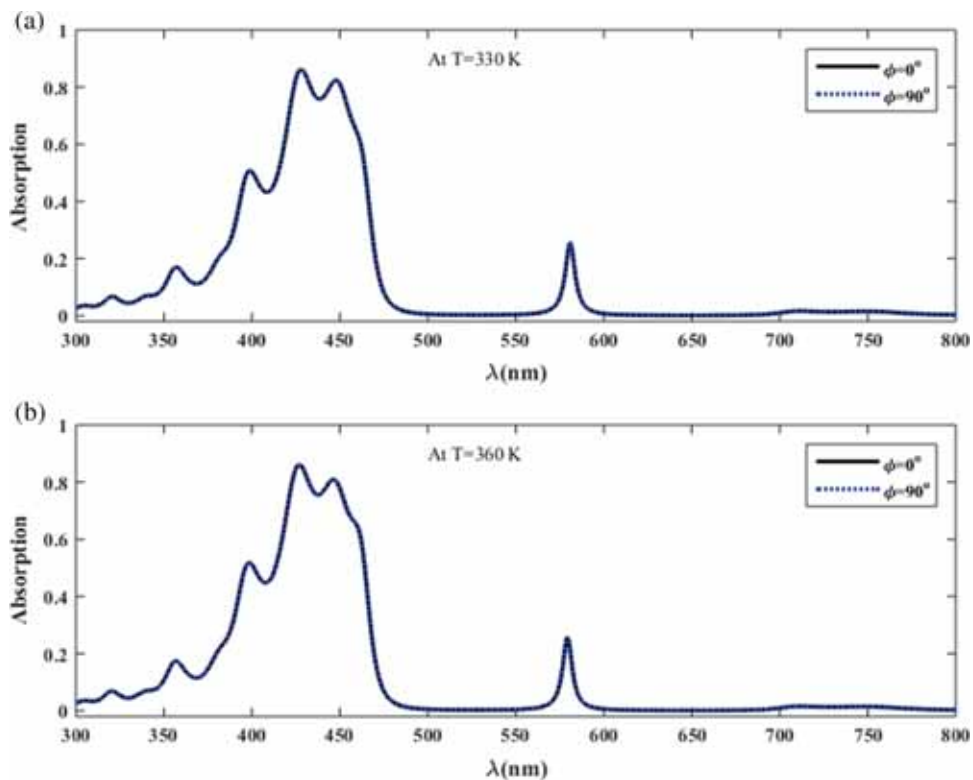


Figure 12. Absorption of the 1DPS with the NC defect: (a) at $T = 330$ K and (b) at $T = 360$ K.

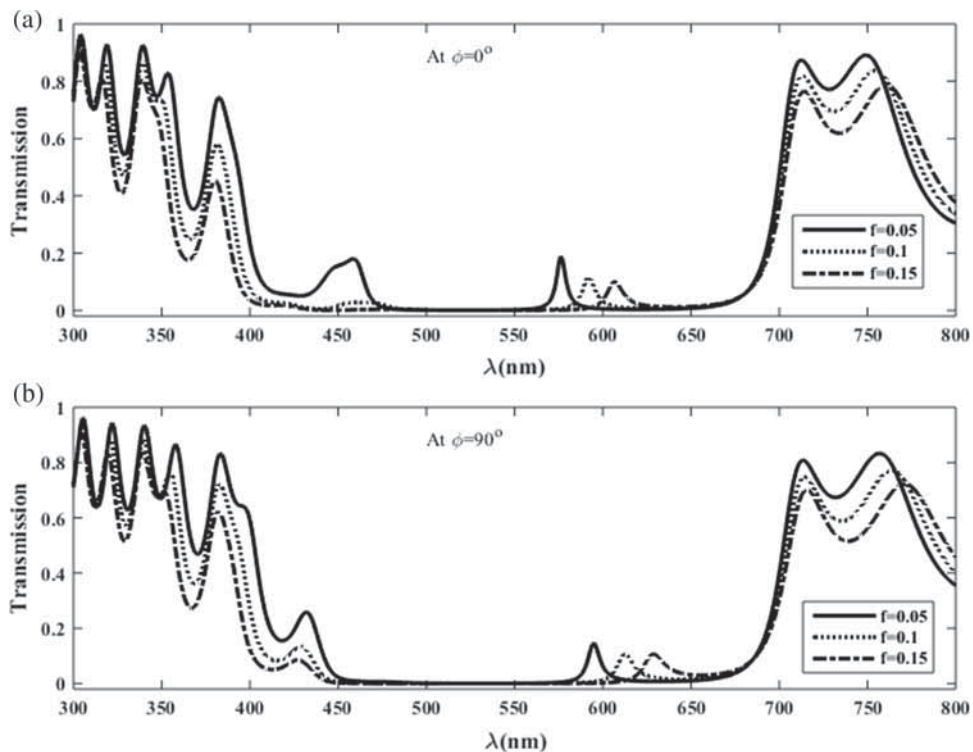


Figure 13. Transmission of the 1DPS with the NC at different filling fractions for the director angle: (a) at $\phi = 0^\circ$ and (b) at $\phi = 90^\circ$.

3.5 Transmission and absorption properties of the 1DPS with NC at different filling fractions (f) when $T = 300\text{ K}$

As discussed earlier, transmission and absorption of the considered periodic structure $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ are affected by temperature. The transmission of the periodic structure with a defect of NC with different filling fractions at 0° and 90° director angles are shown in figure 13. Similarly, the absorption of the periodic structure $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ with different filling fractions is

shown in figure 14. At different filling fractions (f), the absorption of PCs with NC can be seen in table 1.

The transmission and absorption properties of the 1DPS $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$ are studied with 0° and 90° director angles of the LC, for transitions above and below the Fréedericksz transitions. A comparative study of the optical properties at both LC director angles is shown in figures 15 and 16. It shows that optical transmission and absorption are affected by the filling fractions of the silver nanoparticle on the NC of E7 LC.

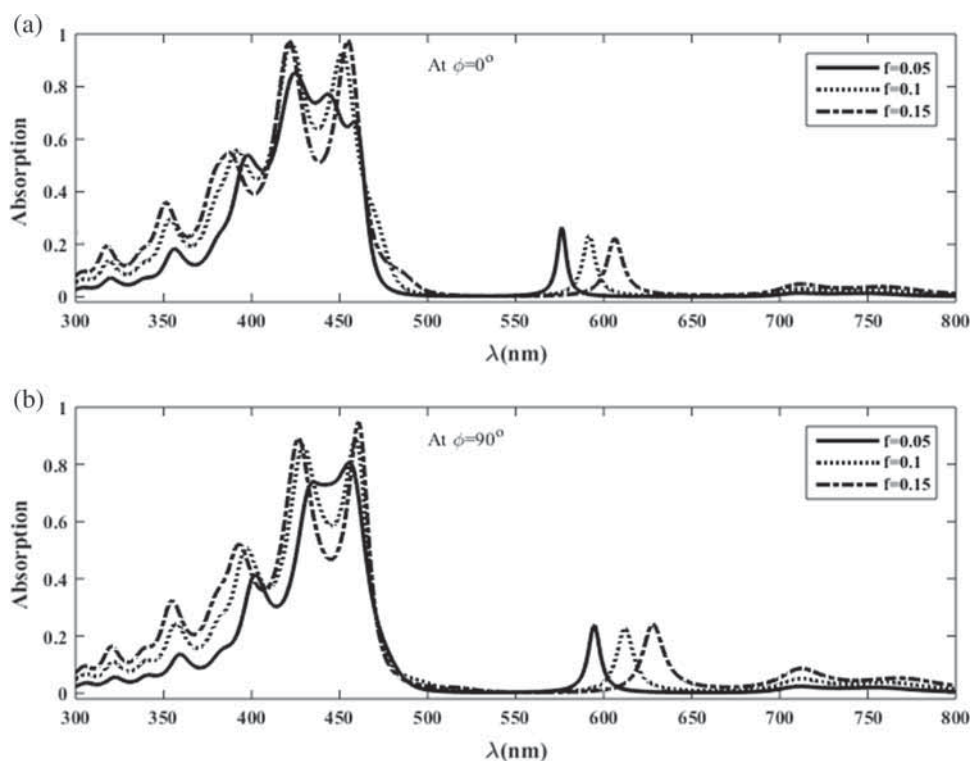


Figure 14. Absorption of the 1DPS with the NC at different filling fractions for the director angle: (a) at $\phi = 0^\circ$ and (b) at $\phi = 90^\circ$.

Table 1. Absorption detail of the 1DPS with NC defect layer at different filling fractions.

		Absorption					
		$f = 0.05$		$f = 0.10$		$f = 0.15$	
		Wavelength (nm)	Absorption (%)	Wavelength (nm)	Absorption (%)	Wavelength (nm)	Absorption (%)
$\phi = 0^\circ$	Defect peak	576	26.47	592	23.35	606	22.27
	Maximum value	1425	85.33	422	97.24	422	97.07
	Maximum value	2425	85.33	451	92.78	455	97.73
$\phi = 90^\circ$	Defect peak	595	23.35	612	22.67	628	24.22
	Maximum value	1456	84.74	430	86.22	427	89.10
	Maximum value	2434	73.56	451	88.69	461	94.88

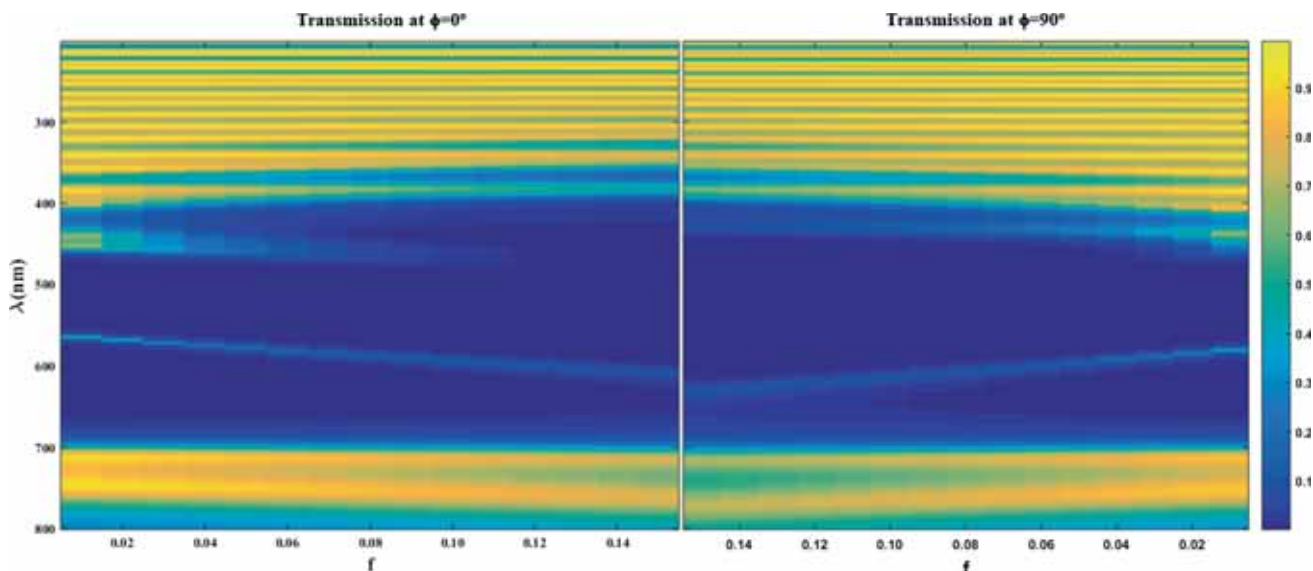


Figure 15. Transmission of the 1DPS with the NC as a defect layer vs. filling fractions at orientation angles of LC: (a) at $\phi = 0^\circ$ and (b) at $\phi = 90^\circ$.

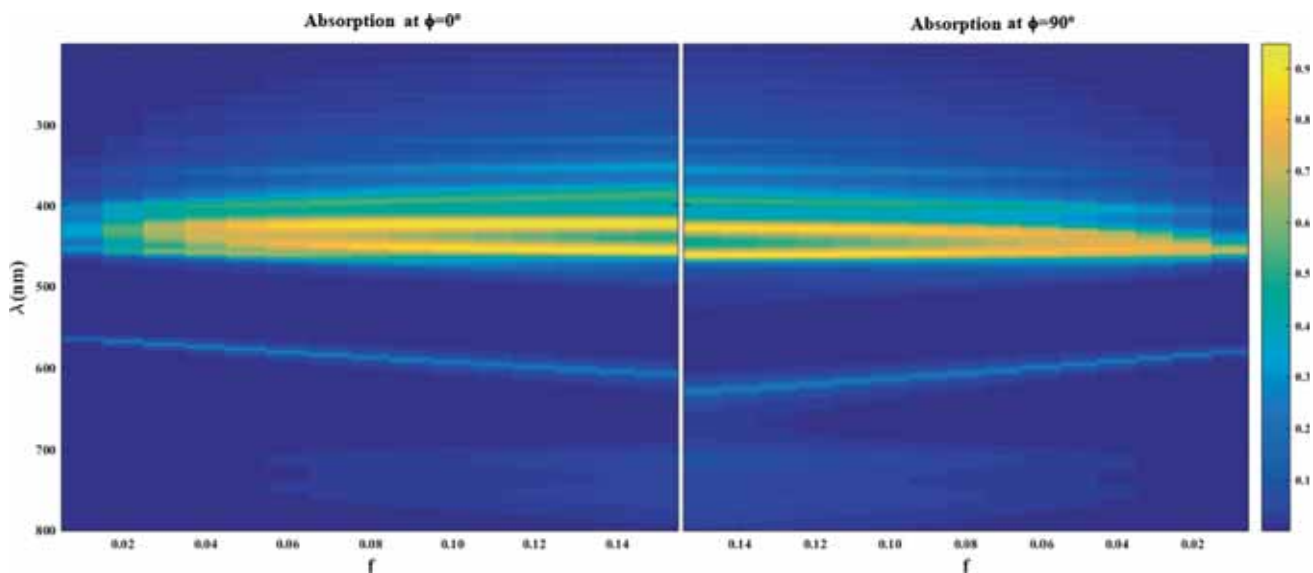


Figure 16. Absorption of the 1DPS with the NC as a defect layer vs. filling fractions at orientation angles of LC: (a) at $\phi = 0^\circ$ and (b) at $\phi = 90^\circ$.

4. Conclusion

In this paper, we have investigated the effective permittivity of the NC consisting of a silver nanoparticle and a E7 LC, i.e. the inclusion of a silver nanoparticle in E7 LC as the host material. The effective permittivity of the silver nanoparticle has been calculated using the Maxwell–Garnett model. Our study shows that the surface plasmon resonance of the nanosilver particle

is affected by the ordinary and extraordinary components of the effective dielectric permittivity of the NC at different temperatures. The study of transmittance and absorption of the 1DPS with the defect layer NC reveals that an NC with a defect layer in the 1DPS may be used to design optical devices because the effective permittivity of the NC is significantly changed at different filling fractions. The study also reveals that the optical properties of the 1DPS are affected significantly

at different filling fractions as well as at different orientations of the LC. Such periodic structure containing NC defect, $(\text{TiO}_2|\text{SiO}_2)^5|\text{NC}|(\text{TiO}_2|\text{SiO}_2)^5$, may be used to fabricate filters, switches, tunable devices, absorbers, sensors, etc.

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