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Investigation on the dependence of optical spectra of silver chiral nanostructures on shape, dimensions and incident light by discrete dipole approximation

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Abstract

Extinction spectra of chiral silver nanostructures are calculated by means of Discrete Dipole Approximation (DDA). Dependence of Plasmonic peaks to both structural parameters of nanostructures and direction of the incident light are obtained. This dependence is investigated on variation of chiral dimensions, chiral shape and direction of incident light. We have observed a resonance peak of transverse mode (TM) for the extinction spectra of chiral structure at normal incidence. However, for oblique angle incident light, in addition to the TM mode, a longitudinal mode (LM) appears at longer wavelengths. The latter undergoes a shift to longer wavelengths with increasing the diameter of chiral arm. When the cross-section of chiral is changed to an oval this resonance peak disappears, while some other peaks appear at longer wavelengths that were not present for a chiral with circular cross-section. Extinction spectra of chiral nanostructure with different structural parameters and different rise angles (slanted chirals) showed dependence on the incident light direction.

1. Introduction

Surface plasmons are the results of reaction of light with surface of metallic nano-particles that cause collective motion (oscillation) of surface electrons. These oscillations in turn cause resonances in the extinction of light at a certain frequency, which depends on the particle characteristics and the incident light (extinction is the result of absorption and scattering) [1-6].

Plasmon resonance strongly depends on composition [7-9], morphology [10-17] and surrounding medium [18-20] of nano-particle. Optical properties of gold and silver because of their application in Plasmonic have been under investigation by researchers for a long time.

Since these electronic oscillations are caused by the increase of the local electric field, hence with changing the size and shape of nano-particle and incident light characteristics, the electric field distribution around the nano-particle changes, which in turn results in the change of resonance frequency [10-16]. An increase in the oscillation amplitude decreases the resonance frequency and vice versa [21].

These properties of nano-particles have many applications in chemical and biological sensors [22-27].

Glancing angle deposition (GLAD) provides facilities for production of oblique columnar structure and with rotation of substrate it is possible to produce two and three dimensional structures of different shapes. One of these structures is the chiral nano-sculptured structure which is obtained by rotation of substrate about its surface normal in the GLAD. These structures are of interest due to optical rotation and circular Bragg phenomenon. They have different responses to right-handed and left-handed incident lights. Left-handed chiral transmits right-handed light, while right-handed chiral transmits left-handed light [28]. Owing to the high porosity of these sculptured structures that can be controlled, they may be used in optical sensors for fluids, biological and chemical media [29].

Discrete dipole approximation method is a useful technique for solving light scattering problems from objects with arbitrary geometries. In this theory, the object is in arbitrary shape but its size is of the order of wavelength or smaller than the wavelength of the incident light [30,31]. In DDA the object is replaced by an array of point dipoles and

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the interaction of these dipoles with the electric field of the incident light is considered. The dipoles react with each other too. Therefore, the applied/external electric field produces a local electric field at a position of each point dipole, in addition the rest of dipoles also produce an electric field at this point, hence each dipole is effectively consists of an electrical dipole momentum due to the local electric field of the process just mentioned. Therefore, calculation of this dipole momentum will provide the appropriate facility for obtaining answers to the scattering problems [32,33]. For larger objects one should also consider the high-multipolar excitations [2].

The distance between dipoles, d in the array can be obtained as:

$$V = Nd^3 \quad (1)$$

$$d = (V/N)^{\frac{1}{3}}$$

where, N is the number of point dipoles and V is the volume of the object.

In order to solve this problem by replacing the object with an assembly of point dipoles both position of N dipoles ($r_i, i = 1, \dots, N$) and dipoles momentums P_i must be determined. After determining this dipole momentum one can calculate the absorption, scattering and extinction cross sections of light.

According to Clausius-Mossotti equation, polarizability of an electrical dipole i , at a position r_i with a dielectric constant of ϵ_i is given as [34]:

$$\alpha_i^{CM} = \frac{3d^3 \epsilon_i - 1}{4\pi \epsilon_i + 2} \quad (2)$$

Since in Eq. (2) the radiation interaction effects are not considered, Clausius-Mossotti equation does not satisfy the energy conservation law. Hence, inclusion of radiation interaction effects modifies Eq. (2) and the polarizibility of electrical dipole is [34]:

$$\alpha_i = \frac{\alpha_i^{CM}}{1 - (2/3)ik^3\alpha_i^{CM}} \quad (3)$$

In Eq. (3), α_i^{CM} is Clausius-Mossotti polarizibility, and k is the wavenumber. Then electrical dipole momentum is obtained as:

$$p_i = \alpha_i \cdot E_{loc}(r_i) \quad (4)$$

In Eq. (4), $E_{loc}(r_i)$ is the local electric field (i.e., the electrical field at the position of i^{th} dipole) which is the sum of incident electric field and the electric field due to

the rest of point dipoles in the suggested array for the object under examination [35]:

$$E_{loc}(r_i) = E_{inc,i} - \sum_{j \neq i} A_{ij} P_j \quad (5)$$

where E_{inc} is the incident electric field. If E_{inc} is a plain wave field with a wave number k , then by omitting its time dependence, its dependence on the position is:

$$E_{inc}(r) = E_0 \exp(ik \cdot r) \quad (6)$$

P_i is the electrical dipole momentum of i^{th} dipole and A_{ij} is the vector potential that is given as:

$$A_{ij} = \frac{\exp(ikr_{ij})}{r_{ij}} \times \left[k^2 (\hat{r}_{ij} \hat{r}_{ij} - I_3) + \frac{ikr_{ij} - 1}{r_{ij}^2} (3\hat{r}_{ij} \hat{r}_{ij} - I_3) \right] \quad (7)$$

where $r_{ij} = r_i - r_j$, $\hat{r}_{ij} = \frac{r_i - r_j}{|r_i - r_j|}$ and I_3 is a 3 x 3 identity matrix.

Using the definition $A_{ii} = \alpha_i^{-1}$, the electrical dipole momentum may be obtained as:

$$\sum_{j=1}^N A_{ij} p_j = E_{inc,i} \quad (8)$$

Then one can calculate the absorption, scattering and extinction cross sections as:

$$C_{ext} = \frac{4\pi k}{|E_0|^2} \sum_{i=1}^N \text{Im}(E_{inc,i}^* \cdot P_i) \quad (9)$$

$$C_{abs} = \frac{4\pi k}{|E_0|^2} \sum_{i=1}^N \left\{ \text{Im} \left[P_i \cdot (\alpha_i^{-1})^* P_i^* \right] - \frac{2}{3} k^3 |P_i|^2 \right\} \quad (10)$$

$$C_{sca} = C_{ext} - C_{abs} \quad (11)$$

Owing to the ability of DDA theory in solving the scattering problem from complex objects of different shapes it has attracted the attention of many researchers during the last few years. Sosa et al. [2] in 2003 calculated the extinction spectra for silver nano-particles in spherical, ellipsoidal and cubic shapes. In 2006, Zhang and Zhao [36] reported their results for extinction spectra of silver rods of different shapes (i.e., needle, periodical nano-rod, L shaped nano-rod and Y shaped nano-rod). They also investigated the dependence of extinction spectra on the nano-rod height and their results showed that extinction spectra shifts towards long wavelengths with increasing the height of the nano-rod [37,38]. Later Zhang and Zhao [39] investigated the extinction spectrum of a U shaped

silver structure with varying dimensions. Their results showed that the extinction spectra are strongly dependent on the dimensions (size) of this structure; for large scale U shaped structure they obtained numerous resonance peaks that increased with size. They concluded that, in addition to electrical dipole effects one should also include many/multiple dipole effects in the calculations [39]. They also in another work [21] reported their findings for a silver chiral structure with varying structural parameter and azimuthal incident angle, while they compared these results with those of a multi-ring.

In this work, as mentioned in Section 1 (Background) we report our results on the influence of different parameters, such as size, shape and incident light direction (angle) on the extinction spectra of silver chiral nanostructure, using DDA theory.

2. Results and discussion

In this study the chiral nanostructure was chosen with the following dimensions: inner radius of 5 nm, outer radius of 6 nm, structural period of 5 nm and a height of 25 nm that is constructed with 124 point dipoles that were in a distance of 1.89 nm from each other. The extinction spectrum of this chiral nanostructure was investigated for the p-polarized light. For p-polarized light, the electric field is in the incident light plane and chiral axis (Figure 1).

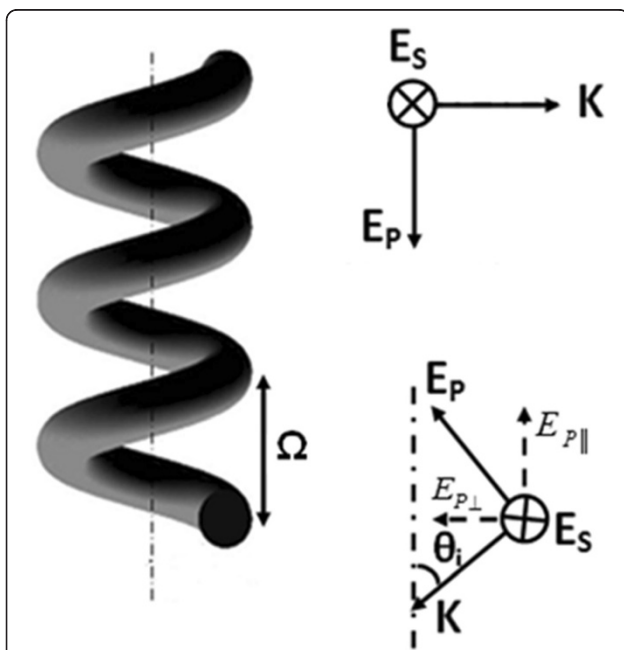


Figure 1 Schematic of chiral nanostructure and positions of p- and s-polarization direction of incident light relative to the chiral axes.

Extinction spectrum of chiral nanostructure for p-polarized light and at 90° polar angle (θ) and 90° azimuthal angle (ϕ) (i.e., electric field is along chiral axis) shows one peak at 349 nm wavelength. This resonance peak is related to the transverse mode (TM) (Figure 2-a).

At off normal incident angles, the electric field decomposes to a component along the chiral axis and a component normal to the chiral axis. Hence the extinction spectrum consists of one more resonance peak at longer wavelength, identified as longitudinal mode (LM). In Figure 2-b, the extinction spectra of chiral structure are given for 90° azimuthal angle and different polar angles (i.e., $\theta = 30^\circ, 70^\circ$ and 90°). It can be clearly distinguished that with decreasing the incident angle, intensity of LM peak increases and the intensity of TM peak decreases and there is a shift towards longer wavelength due to increase in the oscillation amplitude.

Figure 3 shows the influence of diameter of chiral arm from 1 to 3 nm on the extinction spectrum of chiral

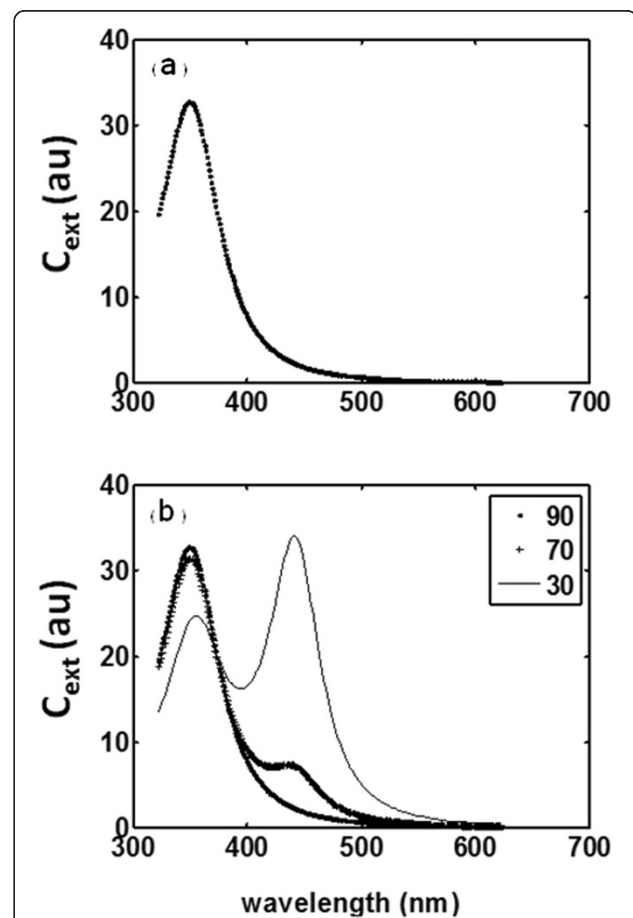
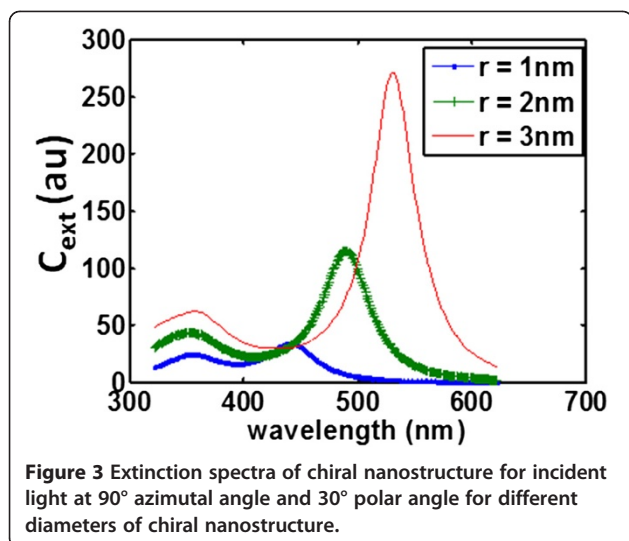


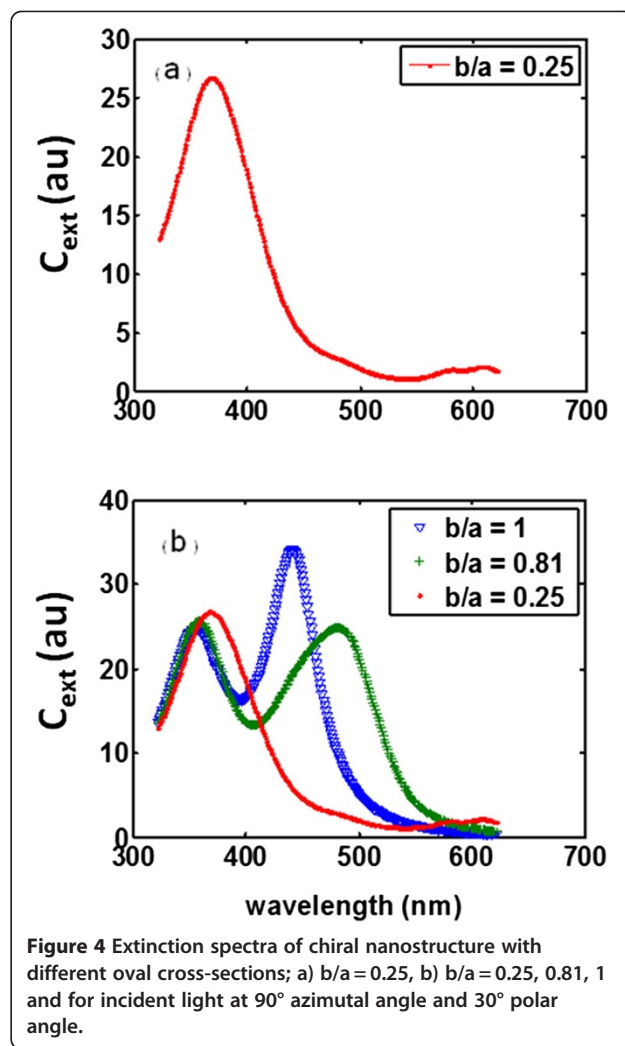
Figure 2 Extinction spectra of chiral nanostructure for incident light at 90° azimuthal angle and different polar angles; a) 90° , b) $30^\circ, 70^\circ$ and 90° .



nanostructure. It can be seen that LM peak shifts towards longer wavelengths which is due to increase of oscillation amplitude. Results also show that the intensity of both LM and TM peaks increases with diameter of chiral arm. This is because of increased number of dipoles due to increase of diameter of chiral arm which should contain higher number of oscillating dipoles, hence peak intensity is increased.

We next investigated the effect of change of chiral cross section from circular to oval shape on the extinction spectra. Figure 4-a shows that this change of cross section causes a shift of the TM peak towards longer wavelengths which is due to increase of oscillation amplitude and the intensity of LM peak decreases considerably. Assuming that a and b are the half of diameters of oval in the x and y axes, respectively, then by decreasing the ratio of b/a while the area of the cross section remains unchanged, reduction ratio in the intensity of LM increases. We can also observe a few more resonance peaks at long wavelengths that were absent in the extinction spectra of chiral nanostructure with circular cross section (Figure 4-b).

Effect of variation of structural period of chiral nanostructure on the extinction spectrum as a function of polar angle (θ) ranging from 0° to 90° is shown in Figures 5(a-e). It can be seen that not only the extinction spectrum changes with structural period but also the direction of incident light influences the extinction spectrum. For incident angles at polar angles less than 45° (Figures 5-a to 5-c) with increasing the structural period TM oscillation shifts towards longer wavelengths and the LM peak shifts towards shorter wavelengths. This means that two peaks get closer to each other. Also due to increase in the dipole numbers by increasing the structural period and because the intensity of peaks is directly related to the number of



oscillating dipoles, the intensity of peaks varies accordingly. For incident angles at polar angles more than 45° (Figures 5-d to 5-e) with increasing the structural period both TM and LM oscillations shift towards shorter wavelengths.

The other interesting parameter to be investigated is the slanted chiral nanostructure. In Figure 6-a it can be observed that for incident light at polar and azimuthal angles of 0° (i.e., incident light is in the direction of the axis of chiral), when the chiral is tilted to $-\alpha$ and $+\alpha$ angles no change is occurred in the extinction spectra, even when the tilt angle is changed. When the direction of incident light is in the x -axis of chiral (i.e., incident light is at polar angle of 90° and azimuthal angle of 0°), the extinction spectra for both $-\alpha$ and $+\alpha$ angles are the same (Figure 6-b), while they change by changing the tilt angle, and by increasing the tilt angle the intensity of LM peak increases and the intensity of TM peak decreases, while the TM peak shifts towards longer wavelengths.

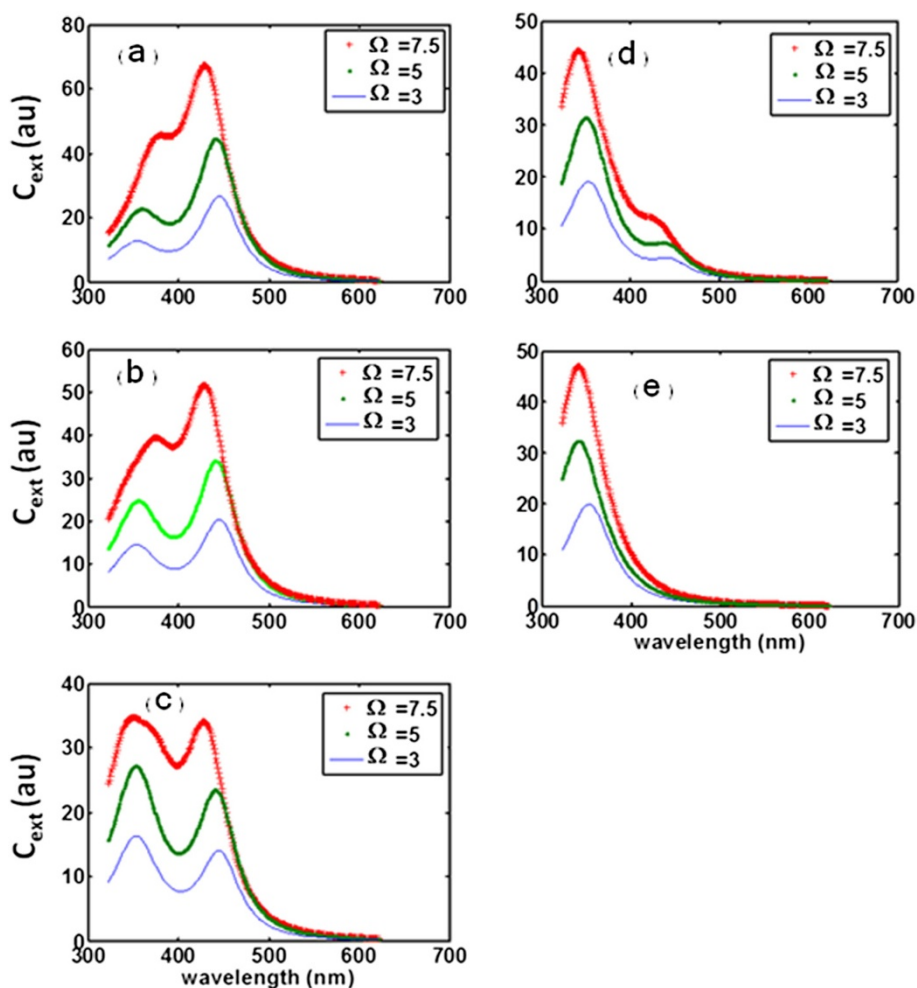


Figure 5 Variation of extinction spectrum of chiral nanostructure at different polar angles (θ); a) 0° , b) 30° , c) 45° , d) 70° , and e) 90° .

Figure 6-c shows the extinction spectra of slanted chiral for incident light at 90° polar angle and 90° azimuthal angle. In this case, again the extinction spectra for the same angles $-\alpha$ and $+\alpha$ are the same, while by increasing the tilt angle of the chiral from the z-direction the intensity of LM peak increases and that of TM peak decreases and the TM peak shifts towards longer wavelengths. Therefore it may be suggested that slanted chiral structures provide the facility for controlling the intensity of extinction spectra at chosen wavelengths.

It is worthwhile to point out that for the incident light at polar angle of 90° and azimuthal angle of 90° (i.e., electric field in the direction of chiral axis) for the upright chiral (0° tilt) LM peak was not observed, while by increasing the tilt angle the LM peak also appears in the extinction spectrum. This is because the electric field decomposes to two components in two normal directions as discussed before.

In Figures 6-d and 6-e the extinction spectra for the incident light at two directions of ($\theta = 30^\circ$ and $\phi = 0^\circ$; incident light in xz plane) and ($\theta = 30^\circ$ and $\phi = 90^\circ$; incident light in yz plane) are given, respectively. For the former case, by increasing the chiral tilt angle, the intensity of LM peak increases and that of TM peak decreases. For the latter case, by increasing the chiral tilt angle in the negative direction relative to the z-axis the intensity of TM peak increases and shifts towards longer wavelengths, while the intensity of LM peak decreases. If the chiral is tilted towards positive direction relative to the z-axis the intensity of TM peak decreases and shifts towards longer wavelengths, while the intensity of LM peak increases.

The extinction spectra of chiral structure slanted at -30° and for the incident light at 90° polar angle (incident light is in the y-axis direction) and for varying azimuthal angles (ϕ) are given in Figure 7-a. It can be seen that variation of

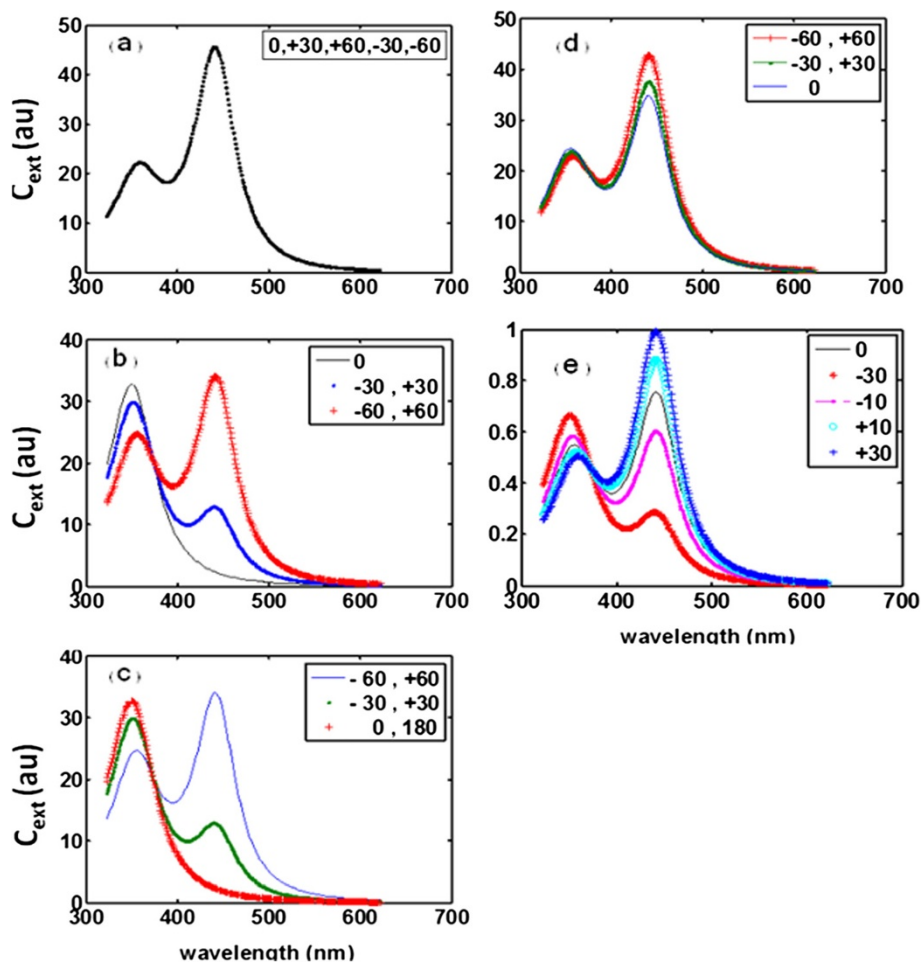


Figure 6 Variation of extinction spectrum of slanted chiral nanostructure with its tilt angle relative to the z-axis; a) $\theta = 0^\circ$, $\phi = 0^\circ$, b) $\theta = 90^\circ$, $\phi = 0^\circ$, c) $\theta = 90^\circ$, $\phi = 90^\circ$, d) $\theta = 30^\circ$, $\phi = 0^\circ$, e) $\theta = 30^\circ$, $\phi = 90^\circ$.

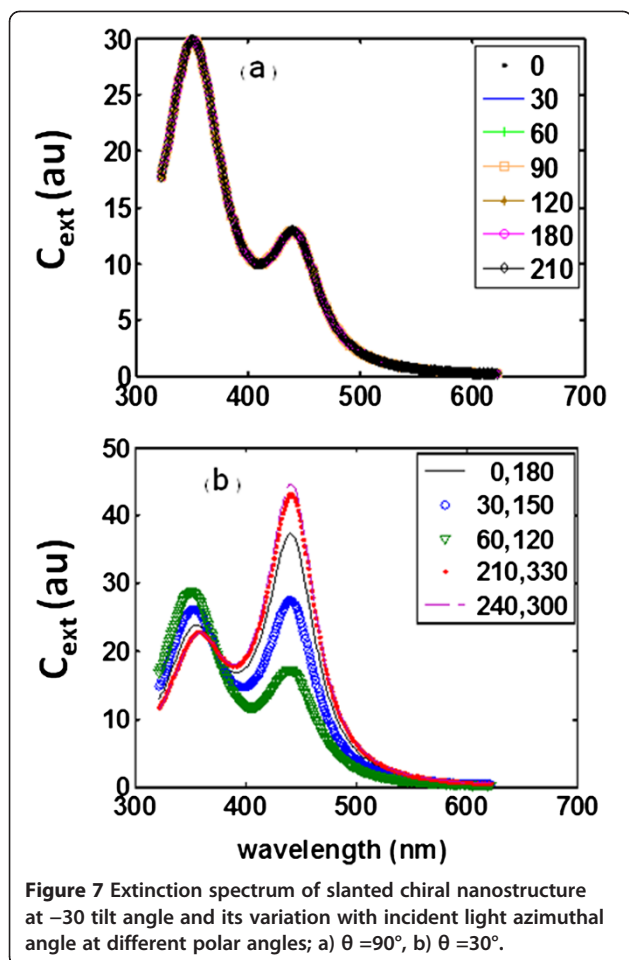
azimuthal angle has no effect on the extinction spectra in this case.

The extinction spectra of chiral structure slanted at -30° relative to z-axis and for the incident light at 30° polar angle and for varying azimuthal angles are given in Figure 7-b. It can be seen that the extinction spectra show strong dependence on the variation of azimuthal angle. The intensity of TM peak increases with azimuthal angle ($\phi = 0^\circ$ to 180° ; light is incident on the chiral nanostructure from behind) and shifts towards shorter wavelengths and the intensity of LM peak decreases. When the light incidences on the chiral structure from front side of it (180° to 360° azimuthal angle) the intensity of LM peak increases with azimuthal angle and that of TM decreases and shifts towards longer wavelengths.

3. Conclusions

We used the DDA theory to investigate the dependence of the extinction spectrum of chiral nanostructure on chiral

nanostructural period, diameter of chiral arm, change of circular cross section to oval cross section, incident light polar angle, tilt angle of chiral structure relative to z-axis, and azimuthal angle. It was found that extinction spectrum for normal incident light consists of one resonance peak that is related to the TM oscillation. When the incident light is off normal direction another resonance peak at longer wavelengths appears as the LM peak. The LM peak shifts towards longer wavelengths with increasing the diameter of the chiral arm, while this peak disappears when the chiral cross section is changed to an oval shape. However, with this change in the shape of chiral cross section a few other resonance peaks appear at longer wavelengths that do not exist in the spectra of chirals with circular cross section. It was observed that for incident light at polar angles below 45° , by increasing the structural period TM peak shifts towards longer wavelength and LM peak shifts towards shorter wavelengths, while for polar angles above 45° both TM and LM peaks shift towards



shorter wavelengths. The slanted chirals may be used to control the intensity of TM and LM peaks. Results showed that for a fixed polar angle, extinction spectrum of slanted chiral structure depends on the incident light azimuthal angle. It is also shown that for incident light in the forward direction of chiral structure with increasing the azimuthal angle the intensity of LM peak decreases and that of TM peak increases while for light incidence at the opposite direction LM and TM behavior are also opposite.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

All authors read and approved the final manuscript.

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