Research on Circular Dichroism of Double L-shaped Metal Block Composite Structure

The rapid development of surface plasmon photonics has promoted the application of optical chirality, expanding chirality research from traditional chiral molecules to artificial chiral nanostructures. Chirality refers to the characteristic that a substance does not have a coincidence with its mirror structure. The unique optical properties of chiral micro nano structures under circularly polarized light excitation have attracted increasing attention. Due to its different absorption of left-handed circularly polarized light and right-handed circularly polarized light, it can produce Circular Dichroism (CD) effect, which has a wide range of applications in life sciences, biochemistry, and medical diagnosis. Single planar nanostructures with simple structures often only produce weak CD signals, while three-dimensional chiral nanostructures, although having stronger CD effects compared to two-dimensional structures, have the disadvantage of being difficult to prepare. Therefore, the study of planar nanostructures that can generate significant CD responses has become particularly important. This article designs a double L-shaped metal block combination nanostructure by combining simple planar nanostructures to increase circular dichroism signals. By placing two L-shaped metal blocks close to each other, a CD enhancement effect is generated, and its inherent mechanism is the strong coupling effect between dipole resonances. A single L-shaped metal block can generate dipole oscillation modes. After combining them, a strong coupling effect between dipole resonances can be achieved, which adjusts the surface plasmon resonance characteristics and excites local field enhancement in the gaps of the composite structure. This field enhancement effect produces different responses to left-handed circularly polarized light and right-handed circularly polarized light excitation, thus forming a significant CD enhancement effect compared to a single L-shaped metal block structure.

1 Introduction

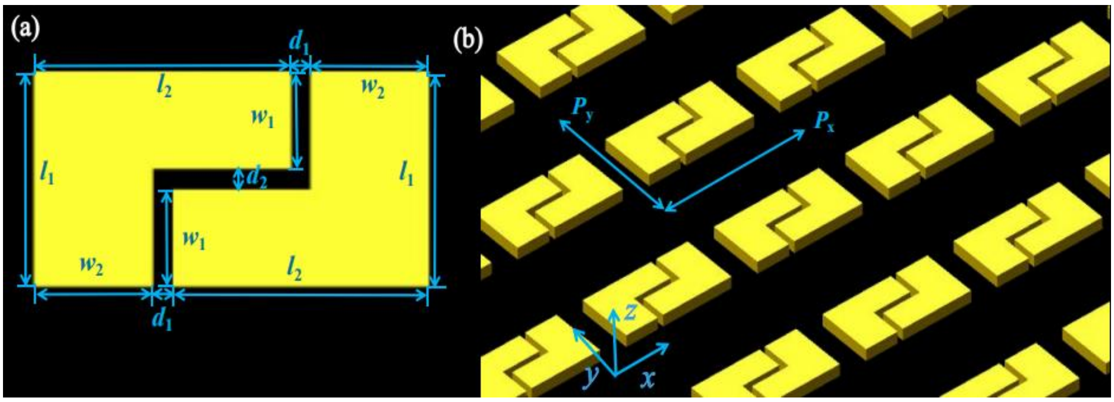
Chiral metamaterials are artificial structures that cannot overlap with their mirror images. Their structural chirality can result in different responses to left-handed circularly polarized light (LCP) and right-handed circularly polarized light (RCP), leading to different absorption under the two types of circularly polarized light, thereby achieving circular dichroism (CD) effect. Compared with natural chiral molecules such as DNA and proteins, chiral metamaterials can achieve significant improvements at the CD level. In addition, chiral metamaterials can achieve special optical properties [1] by introducing artificial design, with strong tunability and flexibility. Therefore, they have been widely used in negative refraction [2], optical polarization manipulation [3,4], CD switching [5,6], second harmonic generation [7], and super chiral field biosensing [8,9].

Researchers have proposed different artificial chiral plasma nanostructures to study the mechanism of CD, among which breaking symmetry is a typical method for achieving CD signals [10]. The higher the degree of asymmetry, the stronger the chirality [11,12]. According to the structure, symmetry breaking can be classified into the following categories. Firstly, adding or reducing a portion of the structure to achieve symmetry breaking and obtain CD signals [13-15], such as etching chiral shapes on the surface of gold nanofilms [16] and sloping nanostructures with gradient depth. Secondly, symmetry breaking can be achieved by combining non chiral components. The non chiral components in chiral arrangements can be coupled together, and their non resonant coupling leads to optical response, thereby obtaining the CD signal of the system [17,18]. In this combination, optical response is generally generated by forming mixed plasma modes between nanostructures. The strongest reaction occurs when the nanostructure approaches another structure [19,20]. This type of structure composed of two or more simple shapes is called composite micro nano structure. Compared with single nano structures with simple shapes, composite nano structures can achieve more significant surface plasmon resonance characteristics due to the special nature of the structure. They will form strong coupling between multiple structures, producing strong near-field effects, which in turn lead to enhanced circular dichroism effect.

In this chapter, a composite nanostructure was designed by placing two L-shaped metal blocks close to each other, and its chiral optical properties were studied through numerical simulation methods. Compared with a single L-shaped metal structure, this composite structure achieves significant CD signal enhancement, and its inherent mechanism is the coupling effect between multiple dipoles. A single L-shaped metal block can generate dipole oscillation modes. After combining them, a strong coupling effect between dipole resonances can be achieved, and due to the presence of gaps, local field enhancement can be formed in the gaps. This field enhancement effect produces different responses to the excitation of left-handed circularly polarized light and right-handed circularly polarized light, resulting in a significant CD enhancement effect compared to a single L-shaped metal block structure. The CD signal can be adjusted by changing the gap between the two metal structures.

2 Structure and calculation method

The nanostructure designed in this chapter consists of two identical L-shaped metal blocks, and rotating one L-shaped structure 180 degrees yields the other L-shaped structure. Figures 1 (a) and (b) show the schematic diagrams of a single period and an array of L-shaped composite structures, respectively. The geometric parameters of a single structure are defined as shown in Figure 1 (a). The parameters of two L-shaped structures are exactly the same. The length of the shorter side of the L-shaped metal block is defined as l_1, the length of the longer side is defined as l_2, and the width of the shorter side on both sides of the L-shaped block is defined as w_1, and the width of the longer side is defined as w_2. The horizontal spacing between the two L-shaped structures is defined as d_1, and the vertical spacing is defined as d_2. The schematic diagram of the composite structure array is shown in Figure 1 (b), with a fixed period of $P_x = P_y = 500$ nm. The material of the nanostructure is gold, with an overall thickness of 40 nm. The excitation light source is left-handed circularly polarized and right-handed circularly polarized along the z-direction.



The absorption values, charge distribution, and electric field distribution of nanostructures were simulated using the three-dimensional finite element numerical simulation software COMSOL Multiphysics. Firstly, set the light source to circularly polarized light that is vertically incident along the negative z-axis direction. Add periodic boundary conditions for the x-z and y-z planes, as well as absorption boundary conditions on the x-y plane, and set perfect matching layers above and below the structure to achieve non reflective effects. The absorbance of nanostructures under circularly polarized light is obtained by integrating the resistance heat loss of the effective calculation area, represented by A_- and A_+, respectively. The difference in absorption between left-handed circularly polarized light and right-handed circularly polarized light is represented by CD, CD = A_- - A_+。

Figure 1 (a) Single period and related parameter definitions of the double L-shaped metal block combination structure; (b) Schematic diagram of periodic array of double L-shaped metal block combination structure.

Fig. 1 (a) Double L-shaped composite structure with the associated parameters definition, (b) Double L-shaped composite structure arrays.

3 Results and discussion

3.1 Absorption circular dichroism of double L-shaped metal block composite structure

To demonstrate the significant optical properties of this composite structure, the absorption spectra and circular dichroism spectra of individual L-shaped metal block structures and double L-shaped composite structures under circularly polarized light were compared in Figure 2. The side length l_1 of the shorter side on the outer side of the single L-shaped metal structure is 200 nm, the side length l_2 of the longer side is 260 nm, the width w_1 of the shorter side is 90 nm, and the width w_2 of the longer side is 120 nm. The parameters of the L-shaped structure in the double L-shaped metal composite structure are exactly the same as those of the single L-shaped structure, where the horizontal spacing d_1 between the two L-shaped metal blocks is 20 nm and the vertical spacing d_2 is 20 nm.

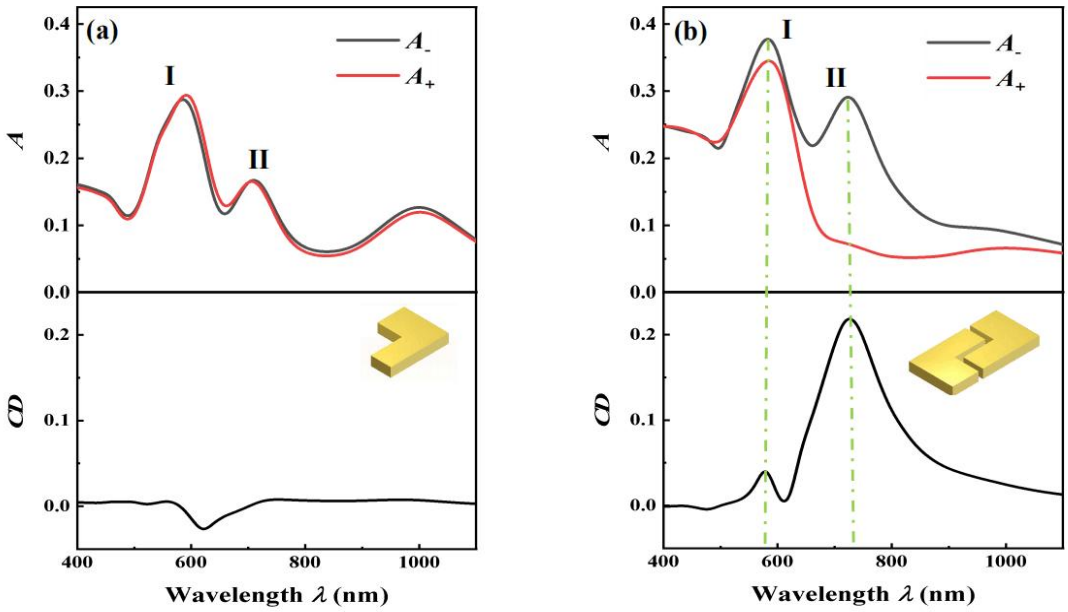


Figure 2 (a) Absorption and CD spectra of a single L-shaped metal block structure array under LCP and RCP incidence; (b) Absorption and CD spectra of a dual L-shaped metal block composite structure array under LCP and RCP incidence.

Fig. 2 The absorption spectra under LCP and RCP excitation and the CD spectra of (a) L-shaped structure and (b) Double L-shaped composite structure arrays.

According to the absorption spectrum shown in Figure 2 (a), the single L-shaped metal structure forms two absorption peaks at wavelengths of λ=580 nm and λ=720 nm, respectively. Compared with the spectral lines of the double L-shaped metal block combination structure in 2 (b), these two absorption peaks appear at similar wavelengths, and these two resonance positions are defined as mode I and mode II, respectively. By observing the absorption values at these two resonance modes, it can be found that the difference in absorption values between the single L-shaped metal structure under left-handed circular polarization and right-handed circular polarization is very weak, forming a negligible CD signal with very small values. However, the absorption spectrum of the double L-shaped metal block combination structure has changed. At mode I, the absorption values of both left-handed and right-handed circularly polarized light have increased to a certain extent. However, the increase in left-handed circularly polarized light is slightly larger than that of right-handed circularly polarized light, forming a positive CD signal with a value of 5.2%. For Mode II, the absorption value significantly increases under left-handed circularly polarized light, while the absorption value decreases under right-handed circularly polarized light, thereby increasing the difference between the two and forming an enhanced CD effect with a value of 22%. From this, it can be concluded that compared to the single L-shaped metal structure, the CD value of the double L-shaped metal block combination structure has been significantly enhanced on a scale of magnitude.

3.2 Mechanism of circular dichroism in the combination structure of double L-shaped metal blocks

In order to investigate the mechanism behind the generation of this resonance mode, as shown in Figure 3, the charge distribution of a single L-shaped metal structure and a double L-shaped composite structure at the resonance mode was simulated and calculated separately. Figures 3 (a) - (d) show the charge distribution of mode I and mode II of a single L-shaped metal block structure under LCP and RCP excitations, respectively. Figures 3 (e) - (g) show the charge distribution of mode I and mode II of a double L-shaped metal block combination structure under LCP and RCP excitations, where positive and negative charges are represented by red and blue, respectively, and yellow arrows indicate the direction of dipole vibration.

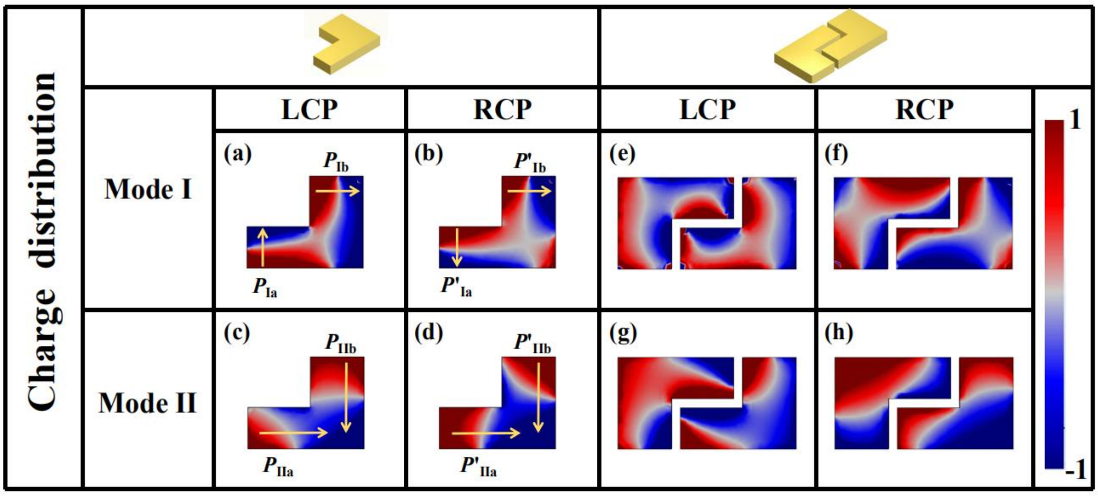


Figure 3 shows the charge distribution at the resonance wavelength of the single L-shaped metal block structure and the double L-shaped metal block combination array structure under LCP and RCP excitation.

Fig. 3 The charge distribution at the resonance wavelength of the L-shaped structure and double L-shaped composite structure arrays under the LCP and RCP excitation.

As shown in Figures 3 (a) and 3 (b), at Mode I, the two arms of the L-shaped metal block have different types of charge distributions, forming dipole P_{Ia} and dipole P_{Ib} that vibrate along the short sides of both arms, which can be regarded as quadruple dipole oscillation. The charge distribution at Mode II is shown in Figures 5-3 (c) and 3 (d). Only one type of charge is distributed at the ends of the two arms of the L-shaped metal block, but opposite charges are distributed at the middle corner, forming even sub oscillations P_{IIa} and P_{IIb} along the long sides of the two arms, resulting in the formation of resonance peaks. The charge distribution pattern of the double L-shaped metal block structure is shown in Figure 3 (e) - (g). It can be seen that compared with the single L-shaped metal structure, the charge distribution of its original L-shaped structure remains basically unchanged, so the direction of dipole vibration formed by a single L in the composite structure remains unchanged. However, it is worth noting that the charge distribution of the introduced L-shaped structure is completely opposite to the distribution of the original L-shaped metal block results. Through comparison, it can be observed that two charges with completely opposite signs are distributed at the same position of the two L-shaped metal block structures, and both structures have dipole oscillations, indicating that there is mutual coupling between the dipole oscillations of these two structures, which can be regarded as a bonding coupling mode.

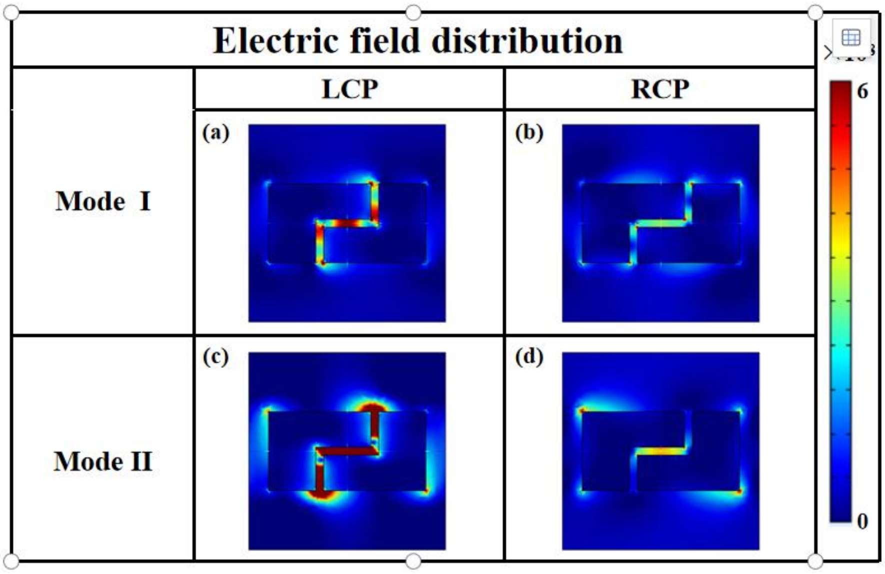


Figure 4 shows the electric field distribution at the resonance wavelength of the double L-shaped metal block combination array structure under LCP and RCP excitation.

Fig. 4 The electric field distribution at the resonance wavelength of the double L-shaped composite structure arrays under the LCP and RCP excitation.

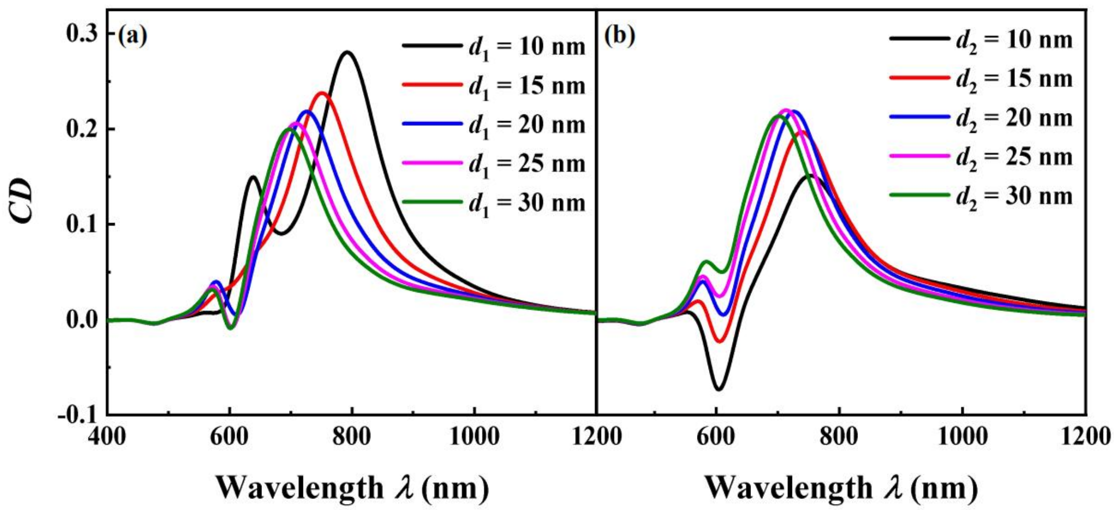
In order to further reveal the intrinsic nature of the enhanced circular dichroism, simulations were conducted on the electric fields at resonance modes I and II. As shown in Figure 4 (a) and (b), at the short wavelength resonance, there is an enhanced electric field mainly in the horizontal and vertical gaps of the two structures near the inner side. The electric field generated by LCP excitation is significantly stronger than that of RCP, which leads to the formation of the resonance peak at mode I. Figures 4 (c) and (d) show the electric field distribution at the long wavelength resonance mode. It is observed that under LCP excitation, there is a very significant electric field enhancement occurring at the horizontal and vertical gaps and the two tips of the L-shaped metal structure connected to them. However, under RCP excitation, only a relatively weak electric field is generated at the horizontal gap, resulting in different absorption values at the resonance peak. This indicates that the combination of two L-shaped metal block structures causes a coupling effect between the dipoles generated inside the two structures, resulting in a localized field enhancement effect in the structural gaps. Moreover, this field enhancement effect produces different responses to the excitation of left-handed circularly polarized light and right-handed circularly polarized light, thus forming a CD enhancement effect.

3.3 The influence of structural parameters on circular dichroism

The significant reason for the enhanced circular dichroism effect is the combination of two L-shaped metal blocks and the formation of gaps. So relevant research has been conducted on the impact of gaps on CD. As shown in Figure 5 (a), the spectral line of CD variation with a change in spacing d_1. Where d_1 is the horizontal distance between two L-shaped metal block structures. The horizontal distance between two structures increases from 10 nm to 30 nm, while the vertical spacing remains unchanged. Other parameters of the L-shaped metal block structure remain unchanged. It can be observed that at mode I, as the distance in the horizontal direction increases, mode I shifts blue. The distance between two L-shaped metal blocks increases, the coupling effect weakens, the effective resonance distance decreases, and the mode undergoes a blue shift. Similarly, at Mode II, the spacing between the horizontal directions reduces the effective resonance distance of the dipole, resulting in a blue shift. Moreover, when the spacing d_1 is reduced to 10 nm, there is a significant enhancement effect on the CD intensity at both mode I and mode II. Figure 5-5 (b) shows the spectral lines of CD as the spacing d_2 changes. d_2 is the distance between two L-shaped metal block structures in the vertical direction. As d_2 increases, mode I undergoes a red shift and mode II undergoes a blue shift. This is because the dipole resonance distance at mode I increases, while the effective resonance distance at mode II decreases.

Figure 5 shows the CD spectral lines of the double L-shaped metal block combination array structure when parameters d_1 and d_2 are changed.

Fig. 5 CD spectra of double L-shaped composite structure arrays with different values of (a) d_1, and (b) d_2.



The curve in Figure 6 (a) shows the variation of CD with the length and side length l_1 of the L-shaped metal block. It can be seen that when the parameters l_1 of two L-shaped structures are increased simultaneously, mode I undergoes a blue shift, while mode II undergoes a red shift. This is because the dipole of mode I vibrates along the short side direction of the L-shaped metal block, and the increase of l_1 reduces the aspect ratio of the dipole vibration, resulting in a blue shift of mode I. The resonance at Mode II occurs by the dipole vibrating along the long side of the L-shaped metal structure. As the length of l_1 increases, the effective resonance distance becomes longer, resulting in a redshift in Mode II. The influence of parameter l_2 on CD is shown in Figure 6 (b). When the other long side length l_2 of the L-shaped metal block increases, both mode I and mode II will experience a redshift phenomenon. This is because when l_2 is increased, the two modes The effective resonance distance of dipoles increases, resulting in mode redshift.

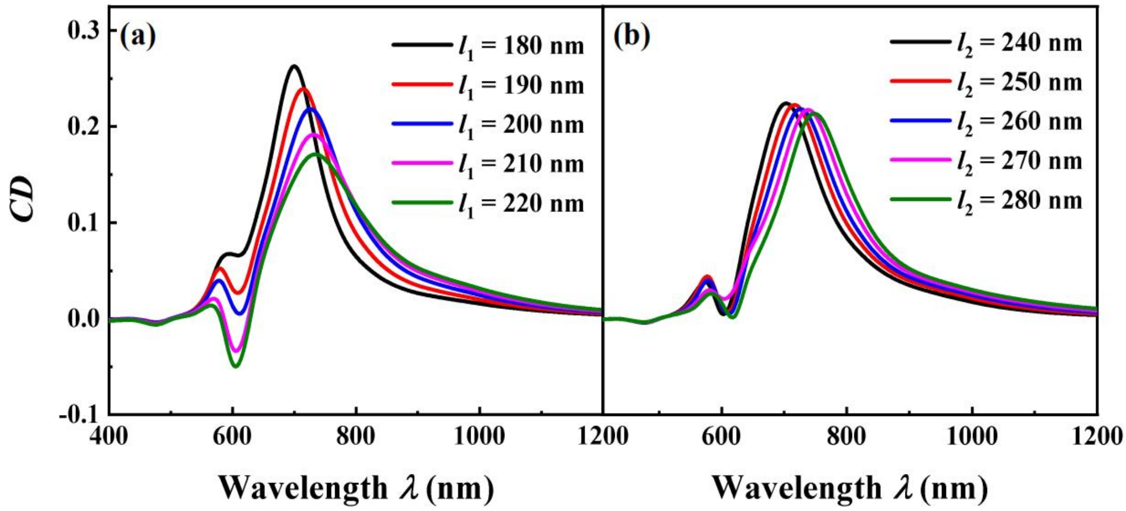


Figure 6 shows the CD spectral lines of the double L-shaped metal block combination array structure when changing parameters l_1 and l_2.

Fig. 6 CD spectra of double L-shaped composite structure arrays with different values of (a) l_1, and (b) l_2.

As shown in Figure 7, the variation of CD spectral lines when changing the two short side lengths w_1 and w_2 of the L-shaped metal block combination structure. As shown in Figure 5-7 (a), when one of the short side lengths w_1 is increased, there is a slight redshift in mode I. This is because as w_1 increases, the effective resonance distance of dipoles vibrating along the short side of the L-shaped metal block structure increases, resulting in a redshift in mode I. At the same time, Mode II also exhibits redshift phenomenon, because as w_1 increases, the length of the upper and lower vertical slits also increases, which enhances the coupling effect between the two structures and increases the effective resonance distance, resulting in redshift of Mode II. As shown in Figure 5-7 (b), with the increase of the length of the other short side w_2, mode I exhibits a red shift, while mode II exhibits a blue shift phenomenon. The resonance mode of Mode I vibrates along the short side of the L-shaped metal block structure, and increasing w_2 increases the effective resonance distance, resulting in a redshift of Mode I. On the contrary, the resonance of Mode II is a dipole vibration along the long side of the L-shaped metal block structure. Increasing the length of w_2 reduces the effective resonance aspect ratio, resulting in the blue shift of Mode II.

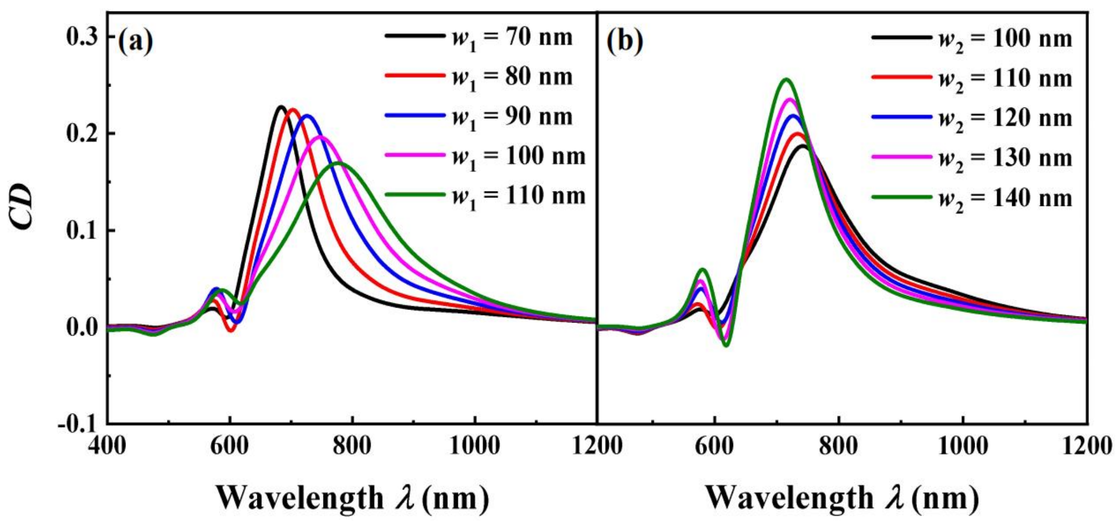


Figure 7 shows the CD spectral lines of the double L-shaped metal block combination array structure when parameters w_1 and w_2 are changed.

Fig. 7 CD spectra of double L-shaped composite structure arrays with different values of (a) w_1, and (b) w_2.

4 sections

In this chapter, the optical properties of two L-shaped metal block composite structures were studied using numerical simulation methods. The calculation results showed that the composite L-shaped metal block structure can produce significant circular dichroism compared to a single L-shaped metal structure. A single L-shaped metal block structure can generate dipole oscillation modes. After combining them, a strong coupling effect between dipole resonances can be achieved, and a local field enhancement effect is formed in the gap. This field enhancement effect produces different responses to the excitation of left-handed circularly polarized light and right-handed circularly polarized light, thus forming a significant CD enhancement effect compared to a single L-shaped metal block structure, and the CD signal can be adjusted by changing the gap. This study provides new ideas for improving the CD effect of planar structured nano optical devices.

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