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Enhanced Circular Dichroism of Z-Shaped Nanorod in Rectangular Nanohole Arrays

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Abstract

Chiral nanostructures have attracted much attention due to the valuable applications in biochemistry, medicine industries, and photonic devices. In this study, we propose an ease-of-fabrication planar nanostructure that consists of rectangular nanohole arrays in which the Z-shaped nanorod is arranged. Theoretically, such chiral nanostructure supports significant absorption circular dichroism (CD) compared with the Z-shaped nanorod because charge distributions are tuned after the introduction of the rectangular frame. Meanwhile, the Z-shaped nanorod directs the flow of current on the rectangular frame, thereby generating the effective quadruple electron oscillation in the Z-shaped nanorod. A novel mode also emerges when an identical Z-shaped nanorod is added into the rectangular hole. The studies will provide a novel approach to enhance the CD effect of planar structures.

Keywords

Absorption Circular Dichroism, Surface Plasmon, Chiral Nanostructure

1. Introduction

Chirality, including spiral, propeller, and polymolecular chirality, is a general characteristic of objects lacking mirror symmetry property [1] [2] [3] [4], which can generate remarkable optical effects, such as optical rotation and circular dichroism (CD) [5] [6]. In particular, CD is defined as the discrepancy of left- and right-handed circularly polarized lights (LCP and RCP, respectively) as it irradiates a chiral medium and has indispensable technological applications in photoelectric detection [7], ultrasensitive biosensing [8], high-resolution imaging [9], and ultrathin broadband optical element [10].

The chiroptical responses of natural chiral materials are exremely weak because the wavelength of incident light does not match the size of the molecule.

Therefore, artificial chiral metamaterials with mutiple designs which include helix [11] and letter-shaped structure [12] have been investigated to generate considerable transmission CD effect. However, in addition to the difference of transmission, the investigation of absorption discrepancy is non-negligible and many relevant studies have been conducted [13]. Bilayered or multilayered structures, such as double-layered nanowires, double-layered forks, double-layered loops, double-layered split ring [14], and rotating structures have evident optical chiral properties. Dipole hybridization can produce a strong CD effect between layers. For example, a three-layer metal-dielectric-metal structure as a chiral metasurface absorber has been proposed to generate a large absorption CD [15]. However, the complexity of fabrication is a weakness for multilayered structures. By contrast, planar structures, as a category of chiral metamaterials [16], are easy to prepare and have considerable absorption CD effect simultaneously.

In this paper, with the aim to produce an enhanced absorption CD response, as well as to avoid the fabrication challenges, we propose an ease-of-fabrication planar nanostructure that consists of the Z-shaped nanorod which is arranged in rectangular nanohole (ZNRN) arrays. Such chiral nanostructure supports significant absorption circular dichroism because the rectangular frame tunes charge distribution and the Z-shaped nanorod simultaneously directs current flow on the film. The underlying mechanism of the enhanced absorption CD is the effective quadruple electron oscillation in the Z-shaped nanorod. When two identical Z-shaped nanorods are introduced, an additional new mode is created. This work not only proposes a planar nanostructure which can generate a giant absorption CD but also provides a novel approach to enhance chiroptical response through placing planar structure into rectangular nanohole arrays.

2. Structure and Computational Method

The schematic and the unit cell with the associated parameters of the ZNRN arrays are shown in **Figure 1**. The ZNRN consists of one rectangular nanohole and Z-shaped nanorod. The periods of ZNRN arrays are 500 nm along x and y directions. The rectangular nanohole has a length L = 400 nm and width W = 200 nm, whereas the Z-shaped nanorod has a width d = 20 nm. The length of the nanorod that is connected in the middle is defined as l. The thickness of the film is 40 nm. The circular polarization light is incident in the negative z-direction.

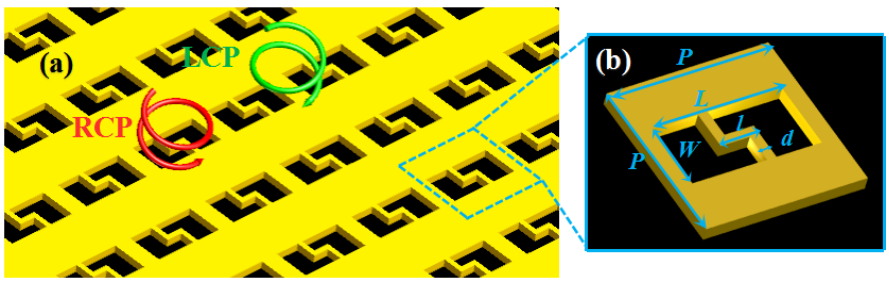

Figure 1. (a) Schematic model of ZNRN arrays and (b) the unit cell with the associate parameters.

The material of the film is gold, and the dielectric constant of gold can be obtained from Ref. [17].

The three-dimensional finite element method software COMSOL Multiphysics is used for numerical simulation and to study the optical properties of the ZNRN arrays. The excitation source is circularly polarized light irradiating the gold film along the negative z-direction. The periodic boundary conditions are set along the x and y directions and the minimum mesh size is one tenth of the minimum width of the structure according to the COMSOL stability criterion. The perfectly matched layers are set at the top and bottom of the computational domain to reduce the reflection. The absorption A is calculated as the volume integral of resistive losses in the metal domain. The absorption difference is defined as CD = A− − A+, where A+ and A− are the absorption under RCP and LCP excitations, respectively.

3. Results and Discussion

As shown in **Figure 2**, the absorption under circular polarization excitation and CD spectra of the Z-shaped nanorod and the ZNRN arrays are compared. **Figure 2(a)** shows the spectra of Z-shaped nanorod arrays. The parameters of the Z-shaped nanorod are the same as those of ZNRN arrays. A peak appears at the wavelength λ = 630 nm under LCP and RCP illuminations, the red and black dotted lines refer to the charge distribution of the Z-shaped nanorod arrays at the resonance wavelength for RCP and LCP lights, respectively. It forms the quadruple electron oscillation, however, the discrepancy of LCP and RCP absorption is extremely small, thereby forming an exceedingly faint CD. The absorption and CD spectra of ZNRN arrays are simulated in **Figure 2(b)**, with the following parameters: P = 500 nm, L = 400 nm, W = 200 nm, l = 100 nm, and d = 20 nm. Comparing **Figure 2(a)** and **Figure 2(b)** shows that after the introduction

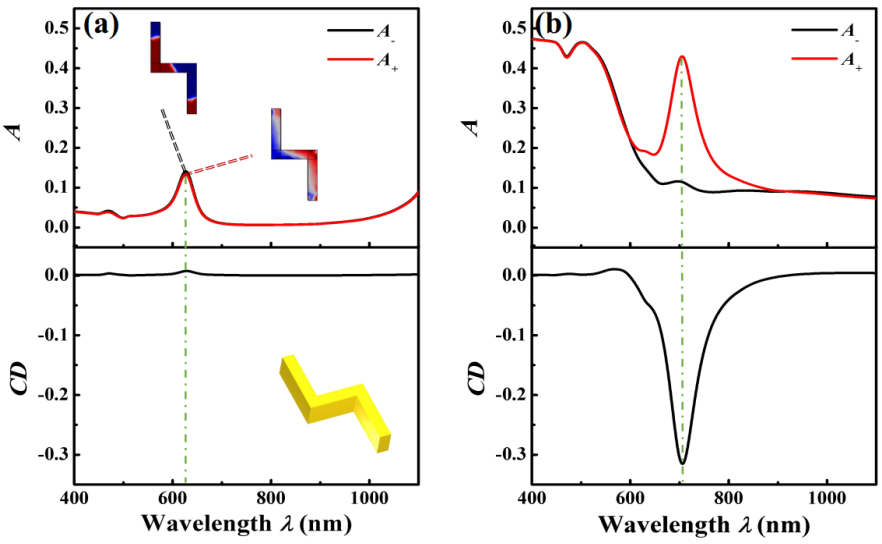

Figure 2. The absorption spectra and CD spectra under LCP and RCP excitations of (a) Z-shaped nanorod arrays and (b) ZNRN arrays.

of the rectangular frame, the absorption of RCP will be significantly enhanced, while the absorption of LCP remains essentially unchanged, thus, an intense CD enhancement effect will occur. The spectra shows that the remarkable absorption CD results from the absorption difference in peaks. CD reaches the peak value of 32% at resonance wavelength λ = 710 nm. Therefore, the ZNRN arrays will produce a significant chiroptical response under circularly polarized light excitation.

To further investigate CD mechanisms, the charge distribution and the power dissipation density distribution of ZNRN arrays at the resonance wavelength are simulated in **Figure 3**. As shown in **Figure 3(a)** and **Figure 3(b)**, the Z-shaped nanorod directs the flow of current on the film, and the charge mainly flows along the nanorod. Strong coupling is observed in the Z-shaped nanorod, where the resonance oscillation occurs, thereby forming the effective quadruple electron oscillation. The formation of the resonance mode is due to localized surface plasmon (LSP) resonance, which is more intense than that of the Z-shaped nanorod arrays. The power dissipation density distribution of ZNRN arrays is simulated in **Figure 3(c)** and **Figure 3(d)**. Significant enhancement effect occurs under RCP excitation dramatically, while there is no visible resonance for the LCP excitation, which results in the remarkable CD response.

With the aim to study the role of parameters on the chiroptical response of ZNRNs, we change the parameters l, d, W, L, and P regularly. The parameters of the control group are as follows: l = 100 nm, d = 20 nm, W = 200 nm, L = 400 nm, and P = 500 nm. We change the parameters individually, while the other parameters are fixed. As shown in **Figure 4(a)**, with the increase in the value of l, a red shift is observed for the resonance mode mainly because the effective resonance length become longer after increasing the value of L, thereby leading to a red shift in resonance mode. **Figure 4(b)** shows that resonance mode blue

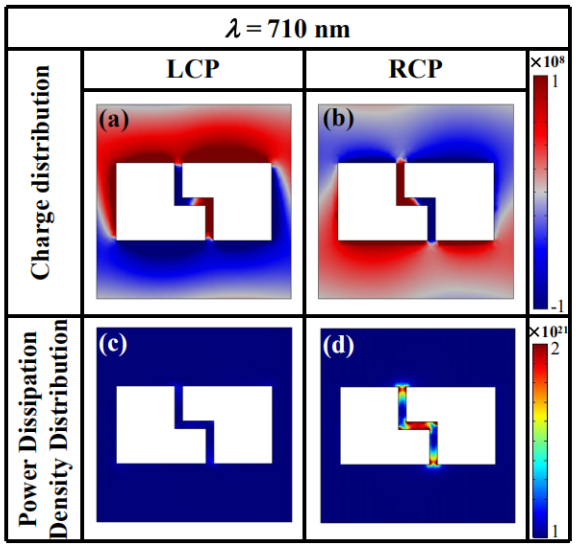

Figure 3. The charge distribution and the power dissipation density distribution at the resonance wavelength for ZNRN arrays under the LCP and RCP excitations.

shifts apparently with the increase in *d*. The increase in the width of nanorod reduces the effective aspect ratio at the resonance domain, thus, the resonance mode has a blue shift. **Figure 5(a)** shows that when the width of the rectangular hole is reduced, the resonance mode blue shifts, which is the result of the decrease in effective resonance length due to shorter vertical nanorod.

As shown in **Figure 5(b)**, when parameter *L* increases, the resonance mode has a slight red shift. The increase of *L* leads to the path of the current flow longer, resulting in a slight red shift of resonance mode.

As shown in **Figure 6**, changing the P has no effect on the resonance mode because the variation of period affects the oscillation of surface plasmon polaritons

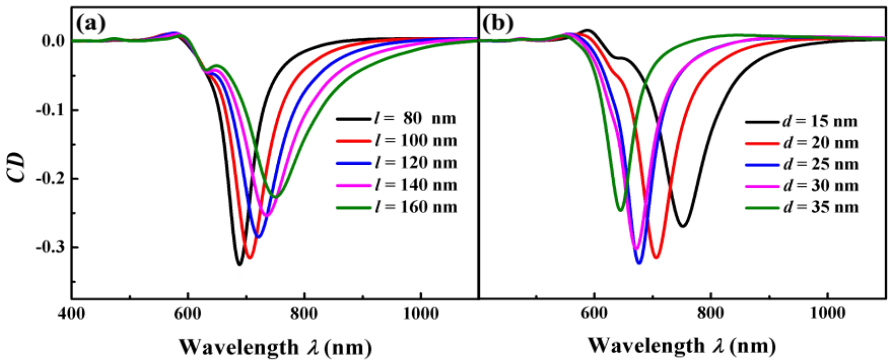

Figure 4. CD spectra of ZNRN arrays with different values of (a) l, and (b) d.

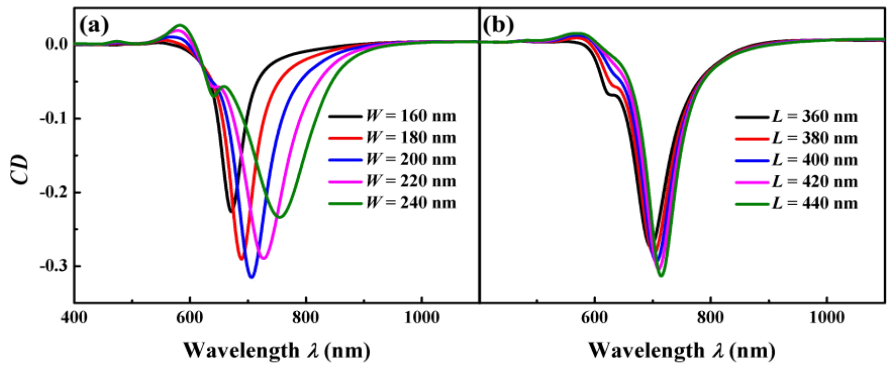

Figure 5. CD spectra of ZNRN arrays with different values of (a) W, and (b) L

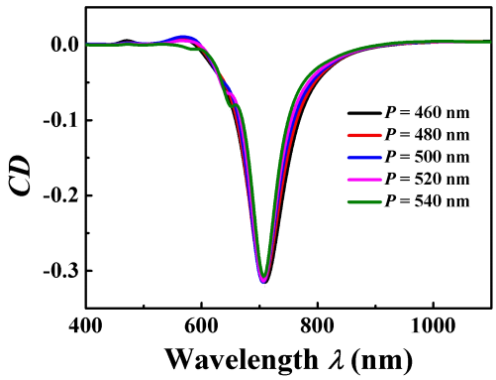

Figure 6. CD spectra of ZNRN arrays with different values of P.

(SPPs). However, the formation of resonance mode of ZNRN arrays is due to LSP effective quadruple electron oscillation, and the period does not affect the effective resonance length.

Furthermore, when two identical Z-shaped nanorods are introduced, a remarkable phenomenon occurred. The absorption under LCP and RCP excitations and the CD spectra of the double Z-shaped nanorods in rectangular nanohole (DZNRN) arrays are shown in **Figure 7**. The distance between two Z-shaped nanorods is defined as D. The parameters of the Z-shaped nanorods are constant, while the value of D is 260 nm. Two remarkable modes, that is Modes I and II, are observed in the absorption spectra at λI = 740 nm and λII = 1280 nm, respectively. The evident CD valley is observed around Mode I with a relatively large value of 26%, and another CD valley is observed at Mode II with the values of 7%. The spectra show that the absorption difference at valleys leads to a remarkable CD effect.

In contrast to ZNRN arrays, it is obvious that DZNRN arrays induce a novel mode. We observe the charge distribution of DZNRNs under LCP and RCP in resonance mode. The resonance of Mode I is similar to ZNRNs, whereas the charge distributions of Mode II are distinguishing due to the interaction between two nanorods instead of the resonance inside the single nanorod. As shown in **Figure 8**, a red shift for Mode II is observed with the value of D increasing. This result is mainly due to the fact that the increase in D increases the interaction distance, which results in the increase of the effective resonance length and Mode II has a red shift.

4. Conclusion

In summary, we placed the Z-shaped nanorod into rectangular hole arrays. Such chiral nanostructure induces remarkable CD effect because the rectangular frame tunes the charge distributions, and the Z-shaped nanorod directs the flow of current on the rectangular frame. We demonstrate that the underlying physical

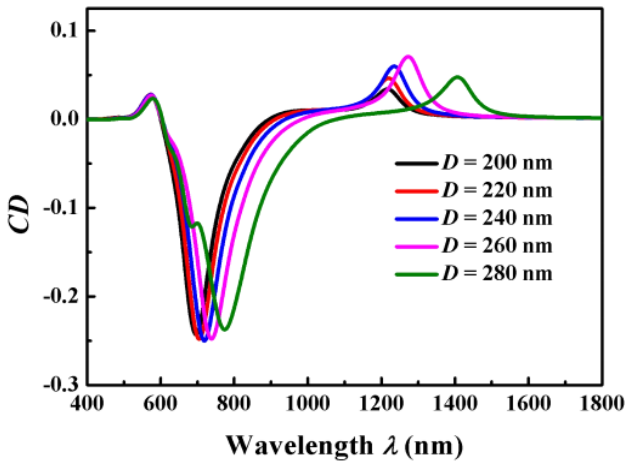

Figure 7. The absorption spectra and CD spectra under LCP and RCP excitation of DZNRN arrays.

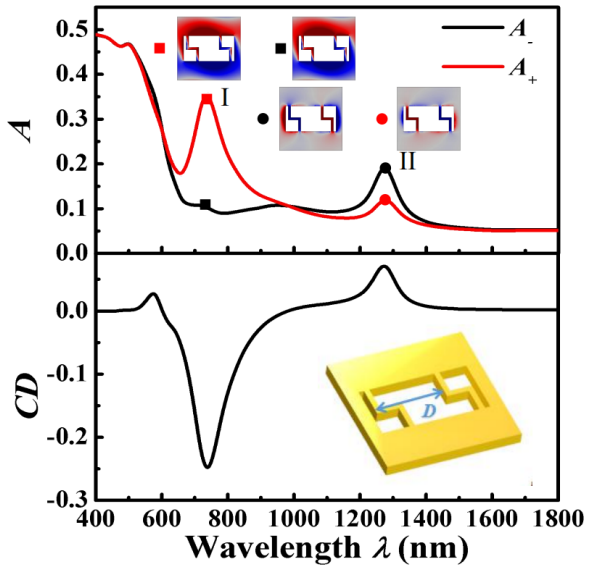

Figure 8. CD spectra of DZNRN arrays with different values of D.

mechanism of the CD effect generation is the effective quadruple electron oscillation in the Z-shaped nanorod. When two identical Z-shaped nanorods are introduced, an additional novel mode is created. The calculated consequence also shows that the response of CD is closely related to the value of the structural parameters. The studies are beneficial for providing novel approach to enhance the CD effect of planar nanostructures.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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