Polarization effects in the diffraction of light by a planar chiral structure

S. L. Prosvirnin¹ and N. I. Zheludev^{2,*}

¹Institute of Radio Astronomy, National Academy of Sciences of Ukraine, Kharkov, 61002, Ukraine

²EPSRC NanoPhotonics Portfolio Centre, School of Physics and Astronomy, University of Southampton, SO17 1BJ, United Kingdom

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We analyze polarization changes of light diffracted on a planar chiral array from the standpoint of the Lorentz reciprocity lemma and find biorthogonality in the polarization eigenstates for waves diffracting though the grating in the opposite direction. Both reciprocal and nonreciprocal components in the polarization azimuth rotation of the diffracted light are identified. The structural chirality of the array arrangement and the chirality of individual elements of the array give rise to polarization effects.

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Recently we reported that planar two-dimensional (2D) chiral structures affect the polarization state of light in an enantiomeric fashion, similarly to three-dimensional chiral media [1]. However, polarization phenomena of diffraction from planar chiral structures have never been studied theoretically before, leaving the fundamental properties of 2D chirality not fully understood. Here we report on the results of a theoretical investigation of polarization changes for light diffracted by regular arrays of planar chiral metallic structures from the standpoint of the Lorentz reciprocity theorem. By analyzing the propagation of light in two opposite directions we have identified a strong component in the polarization effect on diffraction that can be induced either by the chirality of the individual elements of the array or by arranging nonchiral elements of an array in a chiral fashion.

Let us consider a planar-square periodic array of metallic elements of thickness *t* with equal pitch *d* along the axes *x* and *y* placed between planes z=0 and z=-t (see Figs. 1 and 2). If a plane electromagnetic wave

$$\mathbf{E}_i = \mathbf{A}_i e^{-i\mathbf{k}_i \cdot \mathbf{r}} \tag{1}$$

of unit amplitude and polarization vector \mathbf{A}_i is incident on the array from the region corresponding to z > 0, the transmitted field may be written as a summation over all diffracted waves, numbered by integer indices q and p:

$$\mathbf{E}_{t} = \sum_{q,p=-\infty}^{\infty} \mathbf{a}_{qp} e^{-i\mathbf{k}_{qp} \cdot (\mathbf{r} + \mathbf{e}_{z} t)}, \quad z < -t,$$
(2)

where \mathbf{a}_{qp} and \mathbf{k}_{qp} are the amplitudes and wave vectors partial to diffracted waves and

$$\mathbf{k}_{qp} = \mathbf{g} + \mathbf{h}_{qp} - \mathbf{e}_z \sqrt{k^2 - |\mathbf{g} + \mathbf{h}_{qp}|^2},$$
$$\mathbf{h}_{qp} = 2\pi (q\mathbf{e}_x + p\mathbf{e}_y)/d.$$

Here \mathbf{e}_x , \mathbf{e}_y , and \mathbf{e}_z are unit vectors along the axes x, y, and z, \mathbf{g} is the component of \mathbf{k}_i transverse to the axis z, and $k = |\mathbf{k}_i|$. Let us now consider a "reversed" wave with polariza-

tion vector \mathbf{A}_r approaching the array from the opposite side of the structure (z < -t) along the direction of one of the partial diffracted waves of the "direct" scenario, with indices *s* and *l* and wave vector $\mathbf{k}_r = -\mathbf{k}_{sl}$:

$$\mathbf{E}_r = \mathbf{A}_r e^{-i\mathbf{k}_r \cdot (\mathbf{r} + \mathbf{e}_z t)}.$$
 (3)

In the region z>0 this wave will produce diffracted waves with amplitudes \mathbf{b}_{qp} . This corresponds to the reversed scenario of diffraction. The Lorentz reciprocity lemma [2] applied to the field superposition in the volume bounded by surface *S*, which consists of planes $x=\pm d/2$, $y=\pm d/2$, $z=z_1>0$, and $z=z_2<-t$, may be written in the following form:

$$\oint_{S} \{ [\tilde{\mathbf{E}}_{i} \times \tilde{\mathbf{H}}_{r}] - [\tilde{\mathbf{E}}_{r} \times \tilde{\mathbf{H}}_{i}] \} d\boldsymbol{\sigma} = 0, \qquad (4)$$

where $\tilde{\mathbf{E}}_i$, $\tilde{\mathbf{H}}_i$ and $\tilde{\mathbf{E}}_r$, $\tilde{\mathbf{H}}_r$ are electric and magnetic fields created by waves incident from opposite directions. By using the corresponding field expressions it may be shown from formula (4) that



FIG. 1. Coordinate systems and waves in the direct (a) and reversed (b) diffraction scenarios.

^{*}Electronic address: n.i.zheludev@soton.ac.uk; URL: www.nanophotonics.org.uk



FIG. 2. Structural elements of the arrays: planar straight cross tilted against the array greed on the tilt angle ψ and chiral right-handed gammadion with bending angle φ .

$$\sqrt{k^2 - |\mathbf{g}|^2} (\mathbf{A}_i \cdot \mathbf{b}_{sl}) = \sqrt{k^2 - |\mathbf{g} + \mathbf{h}_{sl}|^2} (\mathbf{A}_r \cdot \mathbf{a}_{sl}).$$
(5)

Equality (5) constitutes the universal relation between the amplitudes of partial waves in the direct and reversed diffraction scenarios. Scattering processes are often described in terms of 2×2 transformation matrices, relating Cartesian components of electric fields in coordinate frames of incident and scattered waves. For the direct (\hat{D}) and reversed (\hat{R}) scenarios these matrices for the incident and partial diffracted waves can be introduced as follows: $\mathbf{a}_{sl} = \hat{D}\mathbf{A}_i$, $\mathbf{b}_{sl} = \hat{R}\mathbf{A}_r$. It may be shown from Eq. (5) that these matrices are linearly related and mutually transposed:

$$R_{nm} = c(2\delta_{mn} - 1)D_{mn},\tag{6}$$

where δ_{mn} is the Kroneker index and $c = \sqrt{k^2 - |\mathbf{g} + \mathbf{h}_{sl}|^2} / \sqrt{k^2 - |\mathbf{g}|^2}$. For the purpose of analyzing the polarization eigenstates of the diffraction process it is instructive to present both scattering matrices in the coordinate frame of the direct scenario [see Fig. 1(a)] where the operator of the reversed scattering process acts on the complex-conjugated field amplitudes. Here the polarization eigenstates are simply two linearly independent eigenvectors of



FIG. 3. Schematic representation of diffraction on the Poincaré sphere. For a chiral grating polarization eigenstates in the direct scenario (1d and 2d) and reversed scenario (1r and 2r) are elliptical. Polarization eigenstates (underlined) for nonchiral gratings are mutually perpendicular linear polarization.

matrices \hat{R}^* and \hat{D} . The relation between them may be derived from Eq. (6), which, when converted to the coordinate frame of the direct scenario, gives $R_{nm}^* = cD_{mn}^*$. It follows from the theory of matrix operators that eigenvectors of the Hermitian-conjugated matrices with elements D_{nm} and D_{mn}^* , and therefore of matrices \hat{R}^* and \hat{D} , are biorthogonal or, in terms of polarization eigenstates, are represented by antipode points on the Poincaré sphere, as shown in Fig. 3. In general, the point representing the first eigenstate in the direct scenario 1d is an antipode to one of the points, which represents

TABLE I. Polarization eigenstates (PES's) for various diffraction processes presented in the direct scenario coordinate frame (all angles are measured in degrees; subscripts d and r denote direct and reversed scenarios).

	Direct scenario		Reversed scenario		
Structure	1st PES (deg)	2nd PES (deg)	1st PES (deg)	2nd PES (deg)	Type of diffraction
Straight crosses	θ_{1d} =0.00	$\theta_{2d} = 90.00$	$\theta_{1r} = 0.00$	$\theta_{2r} = 90.00$	No chiral effect
$\psi = 0; \ \beta = 0$	$\eta_{1d} = 0.00$	$\eta_{2d} = 0.00$	$\eta_{1r} = 0.00$	$\eta_{2r} = 0.00$	$\theta_{1d} = \theta_{1r}, \ \eta_{1d} = \eta_{1r}$
Straight crosses	$\theta_{1d} = -14.4$	$\theta_{2d} = 77.1$	$\theta_{1r} = -12.9$	$\theta_{2r} = 75.6$	Chiral effect is present
$\psi = +15; \ \beta = 0$	$\eta_{1d} = -0.05$	$\eta_{2d} = 0.08$	$\eta_{1r} = -0.08$	$\eta_{2r} = 0.05$	$\theta_{1d} - \theta_{1r} = -1.5, \ \theta_{2d} - \theta_{2r} = 1.5$
Straight crosses	$\theta_{1d} = 14.4$	$\theta_{2d} = -77.1$	$\theta_{1r}=12.9$	$\theta_{2r} = -75.6$	Chiral effect is present
$\psi = -15; \ \beta = 0$	$\eta_{1d} = 0.05$	$\eta_{2d} = -0.08$	$\eta_{1r} = 0.08$	$\eta_{2r} = -0.05$	$\theta_{1d} - \theta_{1r} = 1.5, \ \theta_{2d} - \theta_{2r} = -1.5$
Right gammadions	$\theta_{1d} = 6.1$	$\theta_{2d} = -26.6$	$\theta_{1r} = 63.5$	$\theta_{2r} = -83.9$	Chiral effect is present
$\varphi = 120; \ \beta = 0$	$\eta_{1d} = 4.38$	$\eta_{2d} = -0.02$	$\eta_{1r} = 0.12$	$\eta_{2r} = -4.42$	$\theta_{1d} - \theta_{1r} = -57.4, \ \theta_{2d} - \theta_{2r} = 57.3$
Left gammadions	$\theta_{1d} = -6.1$	$\theta_{2d} = 26.6$	$\theta_{1r} = -63.5$	$\theta_{2r} = 83.9$	Chiral effect is present
$\varphi = 120; \ \beta = 0$	$\eta_{1d} = -4.38$	$\eta_{2d} = 0.02$	$\eta_{1r} = -0.12$	$\eta_{2r} = 4.42$	$\theta_{1d} - \theta_{1r} = 57.4, \ \theta_{2d} - \theta_{2r} = -57.3$
Right gammadions	θ_{1d} =9.9	$\theta_{2d} = -80.0$	$\theta_{1r}=9.9$	$\theta_{2r} = -80.0$	Chiral effect is present
$\varphi = 120; \beta = \beta_2$	$\eta_{1d} = 5.2$	$\eta_{2d} = 5.2$	$\eta_{1r} = -5.2$	$\eta_{2r} = -5.2$	$\theta_{1d} = \theta_{1r}, \ \eta_{1d} = -\eta_{1r}$
Left gammadions	θ_{1d} =-9.9	$\theta_{2d} = 80.0$	θ_{1r} =-9.9	$\theta_{2r} = 80.0$	Chiral effect is present
$\varphi = 120; \beta = \beta_2$	$\eta_{1d} = -5.2$	$\eta_{2d} = -5.2$	$\eta_{1r} = 5.2$	$\eta_{2r} = 5.2$	$\theta_{1d} = \theta_{1r}, \ \eta_{1d} = -\eta_{1r}$



FIG. 4. Polarization azimuth rotation $\Delta = \theta - \alpha$ on diffraction from chiral arrays as a function of incident polarization azimuth. Straight line: direct scenarios. Dashed line: reversed scenarios (all results are presented in the direct scenario coordinate frame). The influence of chirality is manifested as a split between corresponding solid and dashed lines: (a) Array of straight crosses. The insert shows the chiral difference in polarization azimuth for the two polarization eigenstates as a function of the tilt angle of the crosses. (b) Array of left (L) and right (R) gammadions. The inset shows the chiral difference in polarization azimuth for the two polarization eigenstates as a function of gammadion bending angle.

the eigenstates of the reversed scenario (this point is designed as 2r in Fig. 3). However, eigenstate 1d does not necessary coincide with eigenstate 1r of the reversed scenario, nor eigenstate 2d coincide with 2r. Therefore, the polarization eigenstates in the direct and reversed scenarios presented in the coordinate frame of the direct scenario could be different. Such a situation takes place if the complex matrix \hat{D} is an asymmetric or even a nondiagonal matrix.

We found that scattering matrices of nonzero order diffraction by periodic planochiral arrays, where chirality is due to either structural chirality or chirality of individual elements of the array, are either asymmetric or nondiagonal. Below we will illustrate these properties by numerical modeling the diffraction process for various planar chiral gratings. We calculated the fields and polarization characteristics of light diffracted on gratings numerically using the method described in Ref. [3]. It is based on a vector integral equation for the surface current induced by the light wave on the array particles. The equation is derived with boundary conditions for ideal metallic structures that assume a zero value for the tangential component of the electric filed on the metal. The integral equation is then reduced to an algebraic equation set by use of the Galerkin technique.

In our modeling we concentrated on planar chiral arrays of the 442 symmetry wallpaper group and calculated the polarization eigenstates of the diffraction process and polarization changes occurring in the diffracted wave for different incident polarizations.

We studied diffraction for two different incident angles β , at $\beta_1=0$ and at $\beta_2=\arcsin(\pi/kd)$. In the first case, the diffracted wave (q=1,p=0) propagates at angle $\xi=\xi_1$ $=\arcsin(2\pi/kd)$ to the array. In the second case the diffracted wave (q=-1, p=0) the same angle makes to the array as the incident wave $\xi = \xi_2 = -\beta_2$ (for definitions of angles see Fig. 1). The wave's polarization azimuth θ and degree of ellipticity η were calculated from the Cartesian field amplitudes using the standard definitions: $\tan 2\theta = s_2/s_1$, $\sin 2\eta = s_3/s_0$, where s_i are the Stokes parameters. The results of our analysis for $d=4 \ \mu m$, $\lambda = 2\pi/k = 1520 \ nm$, $\beta_1 = 0$, $\xi_1 = 22.3^\circ$, $\beta_2 = 11.0^\circ$, and $\xi_2 = -11.0^\circ$ are summarized in Table I and Fig. 4. We considered an array without a substrate. The width of the metal strips was equal to 0.05 μm .

In optics polarization elements are often classified as reciprocal or nonreciprocal depending on whether their effect on the polarization state of the transmitted light is the same or different for light propagating in the opposite directions. This understanding of optical reciprocity which we will use below is somewhat different from the general, more tolerant definition of reciprocity based on the Lorentz lemma. For the purpose of comparison of the polarization transformations for opposite directions of light propagation, in the table and figures the polarization parameter of the waves are converted into the coordinate frame of the direct scenario. In such a presentation, if the values of polarization azimuth rotation in the direct and reversed scenarios are the same, the rotation is truly nonreciprocal like, for instance, in the optical Faraday effect in magnetic field. On the contrary, a difference between the values of polarization azimuth rotation in the direct and reversed scenarios would represent a reciprocal component of the polarization change that is analogous to the optical activity effect in a chiral liquid.

The calculations revealed the following.

(i) For all diffraction processes involving twisted or nontwisted arrays, equalities (6) are held to within the numerical accuracy of the method. They are thus compatible with the Lorentz lemma.

(ii) For the arrays of straight crosses polarization azimuth rotation in opposite directions have opposite signs due to the difference in the efficiency of diffraction for perpendicular polarization components [line *C* in Fig. 4(b)]. This nonreciprocity of polarization azimuth rotation is analogous to the polarization rotation nonreciprocity in dichroic media due to anizotropic dissipation.

(iii) No polarization rotation is seen in the nondiffracted part of the beam at the normal incidence. Its polarization eigenstates are the same in both directions and for any type of array.

(iv) From Table I, one can see that for nonzero order asymmetrical diffraction $(|\xi| \neq |\beta|)$ when individual structural elements of the array are chiral gammadions polarization azimuths of eigenstates for the direct and reversed sce-

narios are resolutely different. The difference between the polarization azimuths of the eigenstates depends on the rosette curvature angle φ and reaches a maximum of about 57° at $\varphi = 120^{\circ}$. The difference in the eigenstates vanishes at rosette bending angle $\varphi = 95^{\circ}$.

(v) When individual structural elements of the array are chiral gammadions, polarization azimuth rotation on diffraction has both reciprocal and nonreciprocal components. The nonreciprocal component of the polarization azimuth rotation is due to a difference in the efficiency of diffraction for perpendicular polarization components. The corresponding oscillating dependence of the nonreciprocal rotation on the incident angle is shifted in respect of line *C* corresponding to straight crosses. It is shifted along the incident polarization azimuth axis towards left for left rosettes and towards right for right rosettes. The split between corresponding solid and dashed lines in Fig. 4 indicates the reciprocal component of the polarization azimuth rotation analogous to optical activity.

(vi) Nonreciprocity of polarization rotation in the diffraction process is evident when a diffracted light wave is reflected straight back towards the twisted planar structure by a mirror, and then diffracts again. The polarization state of the returning light after the second diffraction is different from that of the incident light, even if the incident light was an eigenstate in the forward direction. For an array of rosettes with $\varphi = 120^\circ$, the two incident eigenstates and corresponding returning polarizations have azimuths different by 27° and 21° .

Therefore, polarization effects on diffraction from planar chiral grating can be induced by either structural chirality or the chirality of individual elements of the array. However, in contrast with findings reported in Ref. [4], no polarization rotation compatible with the Lorentz lemma is possible for a wave transmitting through or reflected from a planar chiral structure at normal incidence, as the scattering matrices are diagonal in this case.

Finally, we shall note that our analysis is underpinned by the Lorentz lemma while our computational method is compatible with it. It shall be noted, however, that the recent true three-dimensional finite elements calculations revealing chirality-related nonreciprocity of polarization conversion for the light transmission through a chiral hole [5] may well call for reexamining the validity of the Lorentz lemma for planar chiral structure.

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