

Analytical theory of resonance diffraction and transformation of light polarization

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(Received 18 April 2001; published 22 April 2002)

This paper presents an analytical theory of resonance diffraction in the conical mount. The resonance is caused by plasmon polariton excitation via diffraction from a high reflecting shallow grating. The dependence of polarization, intensity, and phase of specular and resonance waves on the parameters of the problem is presented in explicit form and examined for arbitrary polarization of the incident wave as a function of the angle of incidence and the grating period, orientation and depth. The results obtained enable us to indicate gratings with specific properties, for instance, gratings, ensuring transformation of arbitrarily polarized incident wave into the linearly polarized specular wave. The properties of two-dimensional transformation matrix relating polarization amplitudes of the incident and the specular reflected waves are analyzed. It is shown that the transformation matrix is antisymmetric (in accordance with the reciprocity theorem) for an arbitrary grating profile in the main approximation. The comparison of the results obtained shows remarkable agreement (without any parameters fitting!) with data of the polarization conversion experiments. Both concrete results and the approach presented may be of use in constructing gratings with the predetermined parameters and, therefore, in solving problems of designing optical devices selective with respect to the polarization, wavelength, and orientation.

DOI: 10.1103/PhysRevB.65.195406

PACS number(s): 42.25.-p

I. INTRODUCTION

This work presents results of the simple analytical theory of Wood-type anomalies for diffraction in the general geometry (see Refs. 1,2 and works cited therein) in connection with the experimental work.³ In the work³ there was demonstrated that diffraction of p -polarized laser radiation at a shallow harmonic grating for some angles of incidence θ and orientations of the grating leads to strong changes in polarization of the specular reflected wave in comparison with the case of a flat surface. This effect is caused by the resonance excitation of the surface electromagnetic wave (SEW), cf. Refs. 4,5. In Ref. 3, the polarization conversion efficiency (PCE) was under investigation and in the next works⁶ both the conversion efficiency and reflection coefficient were investigated both numerically and experimentally.

Here we show that computations for the problems discussed in these works can be fulfilled analytically and radically simplified in comparison with Ref. 6 without the loss of accuracy. The analytical approach presented allows to us deepen our understanding of the problem as a whole, and especially to investigate carefully the dependence on parameters. In addition to this we present results for more general problem, assuming that polarization of the incident wave is arbitrary. For this case we obtain the explicit form of the corresponding transformation matrix and discuss its properties. As a result we present general symmetry properties and formulate corresponding reciprocity theorem for the $s \rightarrow p$ and $p \rightarrow s$ conversion. We also demonstrate some additional unique properties of the resonance diffraction for special values of parameters that may be used in optical devices design.

The fact that light diffraction on the reflecting grating formed at high conducting (metal) surfaces may lead to great

changes in the properties of diffracted waves for some values of parameters is well known from the famous Wood's work.⁷ These effects are known in optics as Wood anomalies and were investigated theoretically in a number of works starting from Rayleigh's one,⁸ see reviews in Refs. 4,5. To the reviews we may add the recent book⁹ where the reader will find the necessary literature information. We emphasize here two older works^{10,11} that made essential contribution to up-to-date understanding of the problem in whole.

Note that in the framework of explanation of the stimulated scattering at the surface waves and the surface structures generation, there was developed rather simple analytical method for solving resonance diffraction problems for shallow grating, see, for instance Refs. 1,12. The following consideration is based on the results presented in Ref. 1.

The crucial point for us is the fact that due to the resonance with SEW the amplitude of the corresponding diffracted order becomes great for rather shallow grating (height h to period d ratio smaller than $1/10$). But for a shallow grating the analytical investigation gives accurate results that may be presented in the explicit form. This allows to consider the problem in details in the cases of specific interest.

The structure of the paper is as follows. In Sec. II, we formulate the problem and present a brief summary of the necessary results, cf. Ref. 1. The main results are presented in Secs. III and IV. In Sec. III A, we present transformation coefficients (TC) in the main approximation and discuss their fast (resonance) dependence on parameters of the problem. Next Sec. III B deals with TC symmetry properties. Section III C is devoted to investigation of the slow dependence of TC on the parameters and presents resonance TC values. Here we present also some interesting special cases of the

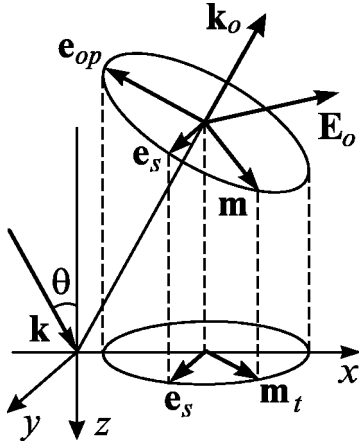


FIG. 1. Geometry of diffraction.

resonance diffraction. The detailed investigation of the conversion efficiency and comparison with experimental data are presented in Sec. IV. The conclusions are presented in Sec. V.

II. GENERAL SETUP

Let a plane electromagnetic monochromatic wave¹³

$$\vec{E}(\vec{r}, z) = \vec{E} \exp[i(\vec{k}_t \vec{r} + k_z z)] \quad (1)$$

fall on a cosine profiled surface,¹⁴

$$z = \zeta(\vec{r}) = a \cos(\vec{g} \vec{r}) \quad (2)$$

of a highly reflecting medium. Here $\vec{g} \equiv g(\cos \varphi, \sin \varphi)$ is the grating (2) wave vector ($d = 2\pi/g$ is the grating period), $-\pi < \varphi \leq \pi$ presents azimuthal angle of the grating relative to the incidence plane, $\vec{k}_t = k(\sin \theta, 0)$, $k_z = k \cos \theta$, $k = 2\pi/\lambda$, θ denotes angle of incidence, z -axis is directed inward the material (Fig. 1), $\vec{r} \equiv (x, y)$. We assume the dielectric permittivity ε to be high, $|\varepsilon| \gg 1$ and, consequently, the surface impedance $\xi = 1/\sqrt{\varepsilon}$ to be small, $|\xi| \ll 1$. Supposing the grating grooves depth to be small, $a \ll \lambda$, d , we may use Rayleigh's hypothesis⁸ and represent the free space field $\vec{E}(\vec{r}, z)$ as a sum of the incident wave and outgoing (and evanescent) waves

$$\vec{E}(\vec{r}, z) = \vec{E}(\vec{r}, z) + \sum_{j=-\infty}^{\infty} \vec{E}_j(\vec{r}, z). \quad (3)$$

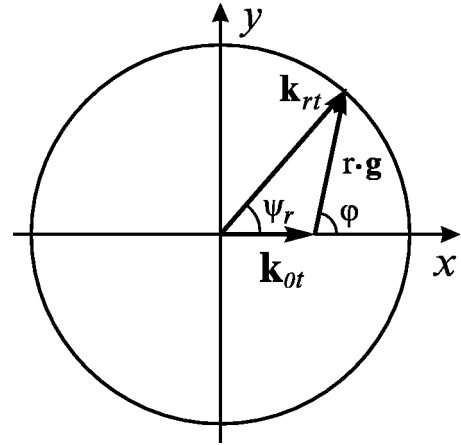
Here

$$\vec{E}_j(\vec{r}, z) = \vec{E}_j \exp[i(\vec{k}_{jt} \vec{r} + k_{jz} z)], \quad (4)$$

$$\vec{k}_{jt} = \vec{k}_t + j\vec{g}, \quad k_{jz} = -\sqrt{k^2 - \vec{k}_{jt}^2}, \quad \text{Re}(k_{jz}) \leq 0,$$

$$\text{Im}(k_{jz}) \leq 0, \quad j = 0, \pm 1, \pm 2, \dots \quad (5)$$

The amplitudes of diffracted waves may be obtained from the Leontovich boundary condition at the surface (2), see details in Ref. 1. Resonance corresponds to small z -component value of some wave vector,


FIG. 2. Resonance in the r th diffraction order.

$$|\vec{k}_{rt}| \approx k, \quad |k_{rz}| \ll k, \quad (6)$$

and r th-order wave is close to SEW, (Fig. 2). The resonance in the order higher than the first one is weak for the harmonic grating, therefore, we suppose that the resonance condition (6) may be fulfilled for $r = \pm 1$ (separately or simultaneously). In that case the result is as follows:

$$E_{rz} = -2ir\mu_r \frac{B_{\bar{r}}[\vec{\kappa}, \vec{H}]_z}{(B_r + B_{\bar{r}})D}, \quad \bar{r} \equiv -r, \quad (7)$$

$$|\vec{E}_{rt}| = |k_{rz} E_{rz}| / |\vec{k}_{rt}| \ll |E_{rz}|, \quad r = \pm 1, \quad (8)$$

$$B_r = \beta_r + \xi + A|\mu_r|^2/\beta_{2r}, \quad A = (\vec{\alpha}_r \vec{\kappa})^2 = \beta_0^2 \kappa^2 + (\vec{\alpha}_0 \vec{\kappa})^2, \quad (9)$$

$$D = (1/B_r + 1/B_{\bar{r}})^{-1} + A|\mu_r|^2/\beta_0, \quad (10)$$

$$\begin{aligned} \vec{E}_{0t} &= -\vec{E}_t + i\vec{\kappa}(\mu_{\bar{1}} E_{1z} - \mu_1 E_{\bar{1}z}) \\ &\equiv -\vec{E}_t + 2\vec{\kappa}|\mu_r|^2 D^{-1}[\vec{\kappa}, \vec{H}]_z, \quad E_{0z} = (\vec{\alpha}_0 \vec{E}_{0t})/\beta_0, \end{aligned} \quad (11)$$

where \vec{H} denotes magnetic field amplitude of the incident wave and following designations are introduced:

$$\begin{aligned} \mu_1 &= \mu_{\bar{1}} \equiv \mu = ka/2, \quad \vec{\kappa} = \vec{g}/k, \quad \vec{\alpha}_j = \vec{k}_{jt}/k, \\ \beta_j &= -k_{jz}/k, \quad \text{Re}, \text{Im} \beta_j \geq 0, \quad \beta_0 = \cos \theta. \end{aligned} \quad (12)$$

Formulas (7)–(10) describe both single resonance for $|\beta_r| \ll |\beta_{\bar{r}}| \sim 1$, $r = \pm 1$ and double degenerate geometry resonance for $|\beta_r| \approx |\beta_{\bar{r}}| \ll 1$.¹⁵ These particular expressions follow strictly from the more general results presented in the paper,¹ [formulas (3.12), (3.1)–(3.3) and (3.6), (2.8)], after some algebraic manipulations. The resonance waves are grazing along the boundary and therefore are close to the eigenmodes of the highly conducting surface—SEW. The last is evanescent wave with large z and the small tangential component of the electrical field, magnetic field is perpendicular to the propagation direction and parallel to the boundary.

The results presented are obtained in the main approximation. The latter means that we take into account scattering processes up to the second order and neglect the higher ones. This leads to the quadratic terms in the B_r corresponding to the shift and broadening of the resonance. The procedure of solving the problem allows us to present the diffracted wave amplitudes as fractions with numerator and denominators that are series in the grating depth. The results presented correspond to the first nonvanishing terms in the series. As we shall see, the main approximation is sufficient in order to compare the theoretical and the experimental results.

Note also that we neglect here ξ in comparison with β_0 and β_{2r} in Eqs. (7)–(10). This allows to simplify and make expressions more transparent, but it is not principal. The numerical results presented below take these terms into account.

For the single resonance case, $|\beta_r| \ll |\beta_r^-|$, expressions (7) may be simplified:

$$E_{rz} = -2ir\mu_r[\vec{\kappa}, \vec{H}]_z / \vec{\beta}_r, \quad \vec{\beta}_r \equiv \beta_r + \xi + A|\mu_r|^2(1/\beta_0 + 1/\beta_{2r}), \quad r = \pm 1. \quad (12)$$

From the last expression, it follows that resonance center lies at the point $\text{Im}(\beta_r) = -\xi'' + A\mu^2/|\beta_{2r}|$. At this point the resonance wave amplitude achieves peak value

$$E_{rz}|_{peak} = -2ir\mu[\vec{\kappa}, \vec{H}]_z / \Delta, \quad \Delta = \xi' + A\mu^2/\beta_0. \quad (13)$$

Here and below prime ' and two primes '' denote the real and imaginary parts of a quantity, respectively. The width of the resonance in terms of β_r may be estimated as $\delta\beta = \xi' + A\mu^2/\beta_0$, where the quadratic in the grating height term presents the broadening of the resonance.

$|E_{rz}|_{peak}$ depends nonmonotonically on the grating depth and achieves maximum at

$$\mu = \mu_{opt} \equiv \sqrt{\xi' \beta_0 / A}, \quad (14)$$

and corresponding E_{rz} value equals

$$E_{rz}|_{max} = -i \sqrt{\frac{\xi'}{\beta_0 A}} [\vec{\kappa}, \vec{H}]_z. \quad (15)$$

The maximum excitation of the resonance wave corresponds to the extremes in the specular reflected wave, discussed in the following sections.

III. RESONANCE POLARIZATION TRANSFORMATION

Let us decompose the vector amplitudes of incident and specular reflected wave into s - and p -polarization components

$$\vec{E} = \sum_{\sigma=\pm 1} E^\sigma \vec{e}^\sigma, \quad \vec{H} = \sum_{\sigma=\pm 1} \sigma E^{-\sigma} \vec{e}^\sigma, \quad (16)$$

$$\vec{E}_0 = \sum_{\sigma=\pm 1} E_0^\sigma \vec{e}_0^\sigma, \quad \vec{H}_0 = \sum_{\sigma=\pm 1} \sigma E_0^{-\sigma} \vec{e}_0^\sigma. \quad (17)$$

Here \vec{e}^+ , \vec{e}^- and \vec{e}_0^+ , \vec{e}_0^- are s - and p -polarization orthonormal bases of incident and specular waves correspondingly:

$$\begin{aligned} \vec{e}^+ &= \vec{e}_0^+ \equiv \vec{e}_y, & \vec{e}^- &= [\vec{e}_y, \vec{k}]/k = \beta_0 \vec{e}_x - \alpha_0 \vec{e}_z, \\ \vec{e}_0^- &= [\vec{e}_y, \vec{k}_0]/k = -\beta_0 \vec{e}_x - \alpha_0 \vec{e}_z. \end{aligned} \quad (18)$$

According to Eq. (10) the specular reflected wave polarization amplitudes may be presented in the matrix form

$$E_0^\sigma = \sum_{\sigma'=\pm 1} R_0^{\sigma\sigma'} E^{\sigma'} \quad (19)$$

with transformation coefficients (TC):

$$\begin{aligned} R_0^{++} &= -1 + 2\beta_0 \kappa^2 \mu^2 \sin^2(\varphi) / D + O(\xi), \\ R_0^{+-} &= -R_0^{-+} = \kappa^2 \mu^2 \sin(2\varphi) / D, \\ R_0^{--} &= 1 - 2\kappa^2 \mu^2 \cos^2(\varphi) / (\beta_0 D) + O(\xi). \end{aligned} \quad (20)$$

The terms ± 1 in R_0^{--} , R_0^{++} correspond to Fresnel reflection coefficients in $|\xi| \ll \beta_0$ limit.

Nondiagonal components R_0^{-+} and R_0^{+-} of the matrix describe polarization conversion effect. Let us emphasize the equality $R_0^{-+} = -R_0^{+-}$. It presents a direct corollary of reciprocity theorem formulated in the work¹⁶ for gratings with arbitrary symmetric profile, see Ref. 17. The above presented explicit expressions demonstrate this property for the case of resonance diffraction at (co) sinusoidal grating. Note here that from results of Ref. 1 it follows that antisymmetry $R_0^{-+} = -R_0^{+-}$ takes place in the main approximation for grating of arbitrary profile. It is caused by the fact that the resonance wave amplitude is proportional to the resonance Fourier amplitude ζ_r of the grating. In turn, specular reflection coefficients contain terms proportional to $|\zeta_r|^2$. Other grating Fourier amplitudes ζ_n influence only the resonance shift and broadening that depend on the $|\zeta_n|^2$. Therefore, these terms are invariant under the grating reflections and the equality $R_0^{-+} = -R_0^{+-}$ holds as approximate one.

Let us examine some general properties of the coefficients $R_0^{\sigma\sigma'}$. They depend on parameters of the incident wave (namely, the angle of incidence θ and wavelength λ), grating orientation φ , period d and grooves depth $h=2a$, and also on the surface impedance ξ : $R_0^{\sigma\sigma'} = R_0^{\sigma\sigma'}(\kappa, \varphi, \nu, \theta, \xi)$, where $\nu \equiv \kappa\mu = ga/2$. Note, that separate dependence on the wavelength takes place only if we take into account dispersion, i.e., $\xi = \xi(\lambda)$. If dispersion is negligible, then all TC depend on the wavelength and grating period through the combination $\kappa = \lambda/d$ only.

Numerators in TC are quadratic in the small dimensionless parameter $\kappa\mu = \nu$ and if the denominator D is of the order of unity (i.e., we are far away from the resonance) then diagonal TC $R_0^{\sigma\sigma}$ are close to Fresnel values and nondiagonal ones are small. As a consequence TC strongly depend on the values of propagating constants β_r , that allows to examine their dependence on the parameters in two steps: (a) fast dependence on parameters determining β_r (neglecting slow dependence on these parameters in other terms), that allows to determine the position of the resonance peculiarities and (b) examine the resonance values of TC as (slow) functions of other parameters.

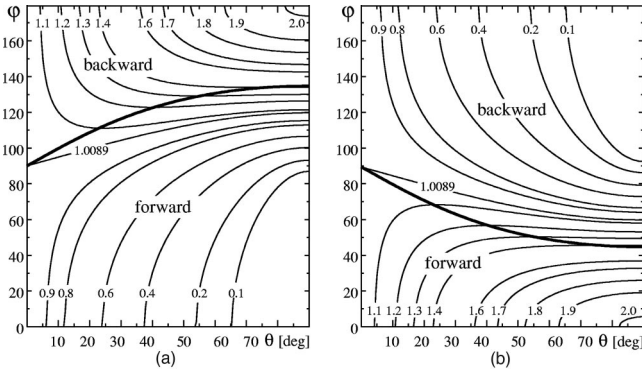


FIG. 3. Resonance curves [Eq. (21)] for the different κ in the subregion $0 \leq \theta \leq \pi/2$, $0 \leq \varphi \leq \pi$ in the +1st (a), and -1st, (b), resonance. Bold lines correspond to the minimal/maximal values of the azimuthal angle $\varphi_{min}(\kappa)$ for +1/-1 resonance, $K \leq \kappa \leq \sqrt{K^2 + 1}$.

A. TC fast (resonance) dependence

Let us first examine the fast dependence for some fixed grating depth. If φ is not close to $\pm \pi/2$ value then TC extremes correspond to the single resonance. As it follows from the representation (20) the specular TC extremes correspond to the minimum values of the denominator D modulus, i.e., to the minimum values of $|\tilde{\beta}_r|$ [and to the maximum values of the corresponding resonance wave amplitude E_{rz} , see Eq. (7) or (12)]. Taking into account that the real part of $\tilde{\beta}_r$ is positively defined, but the imaginary one changes sign, it may be found that TC achieve its extremes at the point

$$\beta_r'' = -\xi'' + (\vec{\alpha}_r \vec{\kappa})^2 \mu^2 / \beta_{2r}'' > 0, \quad \beta_r' = 0. \quad (21)$$

The relation (21) defines the resonance surface in φ , θ , κ space, see Fig. 3. The surface depends on the grating grooves depth through dimensionless parameter $\mu = ka/2$, but this dependence is weak [quadratic in μ^2 term in Eq. (21) corresponds to nonlinear in the grating amplitude shift of the resonance caused by scattering of resonance wave in the second-order ($2r$) wave]. Neglecting this small term we can represent condition (21) in the simplified explicit form

$$\varphi = \pm \varphi(r\kappa, \theta),$$

$$\varphi(r\kappa, \theta) \equiv \arccos[(\cos^2 \theta - r^2 \kappa^2 + \xi''^2) / (2r\kappa \sin \theta)] \quad (22)$$

that is convenient for comparison with the experimental data. Two signs in Eq. (22) correspond to the reflective symmetry (about the incidence plane) orientations of the grating. The two corresponding resonance waves \vec{E}_r (with the same r value) are propagating symmetrically to the incidence plane also. Figure 4 shows the resonance curves, [Eq. (22)], for $r = 1$ (solid line) and $r = -1$ (dashed line) order resonance. As it is obvious, for a fixed angle of incidence it is possible up to four resonance waves, that correspond both to the different grating orientation and diffraction order. If the incident angle $\theta < \theta_{min} \equiv \arcsin|K - \kappa|$, $K = \sqrt{1 + \xi''^2}$, then the resonance is impossible. In the $\kappa \leq K$ case, the two curves [Eq. (22)] corresponding to the opposite sign diffraction orders, intersect at

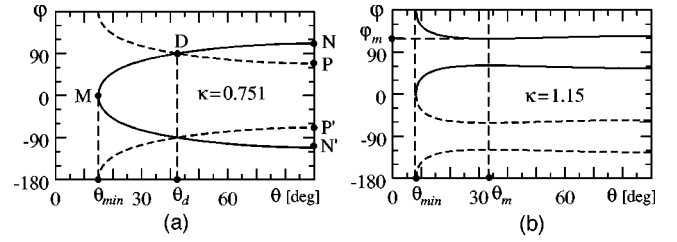


FIG. 4. Resonance curves for $r = 1$ (solid line) and $r = -1$ (dashed line) order resonance for $\kappa = 0.751$ (a), and $\kappa = 1.15$ (b).

the points $\varphi = \pm \pi/2$, $\theta = \theta_d(\kappa) \equiv \arcsin \sqrt{K^2 - \kappa^2}$ (point D and symmetrical one, see Fig. 4). In this particular case of the grating grooves being parallel to the plane of incidence (degenerated resonance), one obtains the double ± 1 resonance, the different signs resonances merge and arise simultaneously.

Note here that besides the double resonance in the degenerated geometry in the first orders $r = \pm 1$, there may exist (for some combinations of parameters) other double resonances as well. Namely, double resonance of the type $(m, -n)$ with $m, n = 1, 2, \dots$ (diffracted waves with numbers m and $-n$ are close to SEW, i.e., β_m, β_{-n} are small simultaneously) occurs if (1) degenerated case: $n = m$ and $\varphi \approx \pi/2$,

$$\theta \approx \theta_{mm}(\kappa) \equiv \arcsin \sqrt{K^2 - m^2 \kappa^2}, \quad |\xi''| \leq m \kappa \leq K;$$

(2) nondegenerated case: $n \neq m$ and

$$\theta \approx \theta_{mn}(\kappa) \equiv \arcsin \sqrt{K^2 - mn \kappa^2},$$

$$\varphi \approx \varphi_{mn}(\kappa) \equiv \arccos \left[\frac{(m-n)\kappa}{2\sqrt{K^2 - mn \kappa^2}} \right],$$

that may take place for $|\xi''|/\sqrt{mn} \leq \kappa \leq 2K/(m+n)$, $4mn \geq (m-n)^2 \xi''^2$.

Note the above-mentioned inequalities are not rigorous, that is caused by two facts: first of all, the resonance surface position was treated with neglecting of the μ^2 term, and second, we neglected the resonance width (in terms of the variable β_r'' it is of the order of $\delta \beta_r'' = \xi' + (\vec{\alpha}_r \vec{\kappa})^2 \mu^2 / \beta_0$).¹⁸

For the harmonic grating double resonance for $mn \geq 2$ case are relatively weak, and will be discussed for periodic grating of general profile in forthcoming papers.

Proceeding with the first-order resonance, we see that it is possible if $K - 1 \leq \kappa \leq 1 + K$, $K \approx 1 + \xi''^2/2$. From the both possible cases $r = \pm 1$, it is sufficient to examine the case $r = 1$, one may receive the $r = -1$ case by transformation $\varphi \rightarrow \pi - \varphi$, see Fig. 3 and detailed analysis of the symmetry properties in Sec. III B. Here exist three distinct cases in accordance with the grating period value. The first one corresponds to the large enough grating periods $\kappa \leq K$. In the case the resonance grating azimuth $\varphi(\kappa, \theta)$ changes monotonically starting from zero value for $\theta = \theta_{min}(\kappa)$ (point M in Fig. 4) up to $\varphi_{max}(\kappa) \approx \pi - \arccos(\kappa/2)$ for $\theta = \pi/2$ (point N in Fig. 4), passing the point $\varphi = \pi/2$ at $\theta = \theta_d(\kappa)$ (point D). For $r = -1$ the resonance grating azimuth, is monotonically decreasing function with the minimal value, $\varphi_{min}(-\kappa)$,

$\varphi_{min}(-\kappa) \equiv \varphi(-\kappa, \pi/2) \approx \arccos(\kappa/2)$, see point P in Fig. 4. The resonance wave propagates “forward,” i.e., the value of α_{rx} is positive. Hereafter, we restrict ourselves with the positive φ values, the negative φ case strictly follows from the reflective symmetry of the resonance curves relative to the $\varphi=0$ axis.

The second case corresponds to the subset of gratings with intermediate period, $K < \kappa < \sqrt{K^2+1} \approx \sqrt{2}$. In this case $\varphi(\kappa, \theta)$ is nonmonotonic function of θ . In the subregion $[\theta_{min}(\kappa), \theta_m(\kappa)]$, where $\theta_m(\kappa) \equiv \arcsin \sqrt{\kappa^2 - K^2}$, $\varphi(\kappa, \theta)$ decreases monotonically from π to $\varphi_m(\kappa) \equiv \pi - \arccos \sqrt{1 - K^2/\kappa^2}$, and in the subregion $(\theta_m(\kappa), \pi/2)$ increases up to $\pi - \arccos(\kappa/2)$, see Figs. 3 and 4. The curve corresponding to the φ minimal values for various κ is defined by the parametric representation $\theta = \theta_m(\kappa)$, $\varphi = \varphi_m(\kappa)$, or in the explicit form

$$\cos \varphi = -\sin \theta / \sqrt{K^2 + \sin^2 \theta}, \quad (23)$$

and is shown in Fig. 3(a) by the bold line. The points of this curve separate regions of the resonance curves corresponding to the “forward” ($\alpha_{1x} > 0$ for $\theta > \theta_m$) or “backward” ($\alpha_{1x} < 0$ for $\theta < \theta_m$) propagation of the resonance wave.

The third case corresponds to the grating with $\kappa > \sqrt{K^2+1}$. Here $\varphi(\kappa, \theta)$ is monotonically decreasing function of θ , changing from π to $\pi - \arccos(\kappa/2)$. The resonance wave propagates “backward.”

The $\kappa \approx K$ region is the special one, because for this values of κ resonance occurs close to normal incidence, and thus both first-order diffracted waves with $r = \pm 1$ are close to the resonance simultaneously. Double resonance for close to normal incidence also presents the case of “degenerated” resonance.

Let us underline that “backward” or “forward” propagation of the resonance wave is independent on the resonance order sign, depending only on the grating period and the angle of incidence.

As one can see from the relations (22), the resonance surface possesses symmetries, connected first, with equivalent grating positions relative to the incidence plane, and second, with transition between the two resonances that differ only by the sign of diffraction order. It is obvious that these geometric symmetries lead to some symmetry properties of all diffracted wave amplitudes and TC [see, for instance, Eq. (12) for resonance waves].

B. Symmetry properties

Zero-order TC's, [Eq. (20)], do not change under transformation $\varphi \rightarrow \varphi + \pi$. This transformation corresponds to the π rotation of the grating and in the case of (co) sinusoidal grating the latter is invariant under the transformation (the grooves are mirror symmetric). Other transformations $\varphi \rightarrow \pi - \varphi$ and $\varphi \rightarrow -\varphi$ do not change the diagonal TC's $R_0^{\sigma\sigma}$ and change the sign of the nondiagonal ones, or (taking into account $R_0^{+-} = -R_0^{-+}$ identity) transform $R_0^{-+} \leftrightarrow R_0^{+-}$. These simple transformation properties lead to definite observable symmetry in intensity and phase of the reflected waves.

Let us introduce short notation for operators of mirror reflection in the plane of incidence \hat{G}_y and in the perpendicular plane \hat{G}_x acting on a vector (a, b, c) according to $\hat{G}_y(a, b, c) = (a, -b, c)$, $\hat{G}_x(a, b, c) = (-a, b, c)$ and on the angle φ as $\hat{G}_y \varphi = -\varphi$, $\hat{G}_x \varphi = \pi - \varphi$. Thus, the operator \hat{G}_y transforms resonance to the symmetric one about the plane of incidence without changing resonance order r . On the contrary, operator \hat{G}_x transforms $r = n$ resonance, occurring at the angle $\varphi(r\kappa, \theta)$, to $r' = \bar{n} = -r$ resonance at the angle $\varphi(-r\kappa, \theta) = \pi - \varphi(r\kappa, \theta)$. Both transformations, \hat{G}_y and \hat{G}_x , convert the initial resonance wave to another resonance one, propagating in the mirror symmetric direction relative to the incidence plane. But if in the first case the symmetric resonances correspond to the same grating Fourier amplitude, for instance, ζ_r , in the second case symmetry transformation will change sign of the corresponding grating harmonic number from r to \bar{r} . The TC symmetry properties may be written in the form

$$\hat{G}_t R_0^{\sigma\sigma'}(\varphi) \equiv R_0^{\sigma\sigma'}(\hat{G}_t \varphi) = \sigma\sigma' R_0^{\sigma\sigma'}(\varphi), \quad t = x, y. \quad (24)$$

These transformations do not act on the incident wave field. Therefore, for specular reflected wave amplitudes one obtains from Eq. (19)

$$\hat{G}_t E_0^\sigma(\varphi) \equiv E_0^\sigma(\hat{G}_t \varphi) = \sigma \sum_{\sigma'} \sigma' R_0^{\sigma\sigma'}(\varphi) E^{\sigma'}. \quad (25)$$

In the case of s - (or p -) incident wave polarization the intensity of the specular reflected wave $I_0 = \beta_0 |\vec{E}_0|^2 \equiv \beta_0 \sum_{\sigma} |E_0^\sigma|^2$ is invariant under this transformation. But for arbitrary polarization of the incident wave it is not so, the specularly reflected wave intensity changes under above-mentioned transformations. These changes may be compensated by some transformations of the incident wave. Namely, for this it is necessary to change polarization of the incident wave into the “reflected” one. The latter means that we have to change the two-dimensional vector (\vec{E}^+, \vec{E}^-) by $(-\vec{E}^+, \vec{E}^-)$ or by $(\vec{E}^+, -\vec{E}^-)$, that is equivalent to reflection of the vector \vec{E} in the xOz plane or the plane parallel to the wave vector \vec{k} and perpendicular to the plane of incidence, respectfully. Denoting these transformations, acting on polarization amplitudes, as \hat{L}^+ and \hat{L}^- :

$$\hat{L}^{\sigma'} E^\sigma = \sigma\sigma' E^\sigma, \quad (26)$$

we may present the result of composed transformations in the form

$$\begin{aligned} (\hat{L}^{\sigma''} \hat{G}_t) E_0^\sigma(\varphi) &\equiv \sum_{\sigma'} R_0^{\sigma\sigma'}(\hat{G}_t \varphi) \hat{L}^{\sigma''} E^{\sigma'} \\ &= \sigma\sigma'' \sum_{\sigma'} R_0^{\sigma\sigma'}(\varphi) E^{\sigma'} = \sigma\sigma'' E_0^\sigma(\varphi), \\ &t = x, y. \end{aligned} \quad (27)$$

From these relations it follows that composed transformations $\hat{L}\hat{G}$ change only the sign of some (*s*- or *p*-) polarization amplitude of the reflected wave and therefore does not change its intensity.

Note that this symmetry property is proved here for the special case of (co) sinusoidal grating. The last possesses additional symmetry, namely, its grooves relief is mirror symmetric. So here the question arises: what symmetry properties will remain for the asymmetric grating? Postponing the detailed answer to the forthcoming paper, we emphasize here that for the transformation $\hat{L}^\sigma\hat{G}_y$ the invariance is exact and for the other one, $\hat{L}^\sigma\hat{G}_x$, it is in any case valid in the main approximation.

Noteworthy that symmetry properties discussed in this section are additional to $R_0^{-+} = -R_0^{+-}$ condition related to the reciprocity.

C. Polarization of specular reflected wave

Let us continue investigating the single resonance case. According to Eqs. (16)–(20) the specular reflected wave amplitude may be presented in the transparent and convenient form

$$\vec{E}_0 = \vec{E}_0^L + \vec{E}_0^F. \quad (28)$$

Here the first term presents the linearly polarized wave (for any polarization of the incident wave!),

$$\vec{E}_0^L = \mathcal{L}(\theta, \mu, \vec{\kappa}, \vec{E})(\vec{e}_0^- \beta_0 \sin \varphi + \vec{e}_0^+ \cos \varphi). \quad (29)$$

The second term is equal to the field reflected by the flat boundary with the reflection coefficient $\mathcal{F}(\theta, \mu, \vec{\kappa})$

$$\vec{E}_0^F = \mathcal{F}(\theta, \mu, \vec{\kappa})\vec{E}_{0,flat}, \quad \vec{E}_{0,flat} = \vec{e}_0^- E^- - \vec{e}_0^+ E^+. \quad (30)$$

The coefficients \mathcal{L} , \mathcal{F} are (in general) complex functions of the parameters of the diffraction problem,

$$\mathcal{L} = 2\kappa\mu^2(\beta_0 D)^{-1}[\vec{E}, \vec{\kappa}]_z, \quad \mathcal{F} = 1 - 2\mu^2 A(\beta_0 D)^{-1},$$

$$A = \beta_0^2 \kappa^2 + (\vec{\alpha}_0 \vec{\kappa})^2. \quad (31)$$

In the resonance vicinity the specular reflected wave is elliptic polarized for arbitrary polarization of the incident wave (including linear polarization). It is due to the fact that transformation coefficients $R_0^{\sigma\sigma'}$ are complex numbers. The ellipticity level may be high in contrast with the case of a flat boundary.¹⁹ The phase and amplitude of the reflected wave undergoes rapid resonance changes with a variation in the angle of incidence, wavelength, period and grating orientation in the resonance surface vicinity (dependence on the grating depth, in general, is slow). Immediately on the resonance surface the TC's $R_0^{\sigma\sigma'}$ become real, and polarization types (linear, elliptical) of the reflected and incident wave coincide, but polarization parameters are different. However, in the particular case of the grating with the optimal depth, Eq. (14), the specular reflected wave is linearly polarized in any case.²⁰

Specifically, in the single resonance case for the grating with $\mu = \mu_{opt} \equiv \sqrt{\beta_0 \xi' / A}$, the resonance value of \mathcal{F} becomes zero, that causes the linear polarization of the reflected wave for any polarization of the incident wave,

$$\vec{E}_{0,res}(a_{opt}) = [(\vec{\alpha}_0 \vec{\kappa})\vec{e}_0^+ + (k[\vec{\alpha}_0 \vec{\kappa}]/k)\vec{e}_0^-] \times [\vec{E}_t, \vec{\kappa}]_z / [\alpha_0(\vec{\alpha}_1 \vec{\kappa})^2]. \quad (32)$$

Under these conditions the polarization of the incident wave affects the amplitude of the reflected wave only, but does not affect its polarization. The polarization of the reflected wave is determined by geometrical parameters only.

Realization of this regime requires that the resonance condition, defined by Eq. (22), along with $\mu = \mu_{opt}$, should hold. These two equations involve four parameters, namely, θ , φ , κ , $N = \kappa\mu/\sqrt{\xi'} = \pi a/(\sqrt{\xi'}d)$. Here, any two parameters may be defined as functions of the two remaining. The results of examination of the system presented may be summarized as follows. For a given values of the two parameters chosen, there may exist one or two solutions, or no one at all. For instance, assigning wavelength and grating parameters (i.e., κ and N are specified) one arrives at a conclusion that for small grating depth,

$$N < N_0(\kappa) \equiv \frac{2\kappa}{1+\kappa^2} \quad \text{or} \quad a < 2d\sqrt{\xi'}\kappa[\pi(1+\kappa^2)]^{-1}, \quad (33)$$

solution does exist for any κ and is unique. For deeper gratings, $N \geq N_0(\kappa)$, the results differ for the short- ($\kappa > \sqrt{3}$) and long-period gratings ($\kappa < \sqrt{3}$). In the first case there are no solutions, and in the second one there are two or none solutions for $N^2 < 3\sqrt{3}/(4\kappa)$ and $N^2 > 3\sqrt{3}/(4\kappa)$, respectively.

Let us consider some special cases.

(1) If the incident wave is linearly polarized with $\vec{E}_t \parallel \vec{\kappa}$, then the diffraction under resonance conditions, [Eq. (21)], at the grating with optimal depth, [Eq. (14)], leads to the total suppression of specular reflection,

$$\vec{E}_0(a_{opt}) = 0 \quad \text{for} \quad \vec{E}_t \parallel \vec{\kappa}, \quad \beta_1'' = -\xi'' + \beta_0 \xi' / \beta_2''. \quad (34)$$

This result was first obtained in the simplest geometry case in Ref. 21 and observed experimentally in Ref. 22.

(2) In the case of arbitrary polarization of the incident wave any special polarization component (in particular, *s* or *p*) of the specular reflected wave can be totally suppressed. It follows from Eq. (32) that suppression of *s* (or *p*) component takes place if the ort \vec{e}_0^+ (or \vec{e}_0^-) multiplier vanishes. That occurs at the appropriate grating orientation and amplitude. For instance, if $\vec{\kappa} \parallel \vec{\alpha}_0$ ($\varphi = 0, \pi$) then

$$\vec{E}_0(a) = -E^+ \vec{e}_0^+ - \frac{\mu^2 - \mu_{opt}^2}{\mu^2 + \mu_{opt}^2} E^- \vec{e}_0^-, \quad \mu_{opt} = \sqrt{\beta_0 \xi'} / \kappa. \quad (35)$$

For other grating orientation, $\vec{\kappa} \perp \vec{\alpha}_0$ ($\varphi = \pm \pi/2$) that corresponds to the degenerated $(1, -1)$ resonance, one obtains the expression similar to the previous one,

$$\vec{E}_0(a) = \frac{\mu^2 - \tilde{\mu}_{opt}^2}{\mu^2 + \tilde{\mu}_{opt}^2} E^+ \vec{e}^+ + E^- \vec{e}_0^-, \quad \tilde{\mu}_{opt} = \kappa^{-3/2} \sqrt{\xi'/2}. \quad (36)$$

It follows from Eq. (20) that in these particular cases the conversion coefficients $R_0^{\sigma\bar{\sigma}}$ vanish, i.e. polarization conversion vanishes due to the symmetry. One of the polarization components (s in the first case and p in the second one) does not “feel” the grating and cannot be suppressed: the corresponding TC’s are equal to ∓ 1 (or Fresnel values R_s, R_p for more precise calculations). On the contrary, the second polarization component vanishes for the grating with $\mu = \mu_{opt}$ or $\mu = \tilde{\mu}_{opt}$, respectively. Passing through the zero value the corresponding component undergoes π phase jump.

(3) One can produce the specular reflected wave with linear polarization for any polarization of the incident one using the grating with appropriate properties. Supposing reflected wave to be linearly polarized we can introduce unit vector $\vec{m} = m_s \vec{e}^+ + m_p \vec{e}_0^-$ being perpendicular both to the wave vector \vec{k}_0 and \vec{E}_0 (Fig. 1). Condition $\vec{E}_0 \vec{m} = 0$ is fulfilled for the grating orientation angle $\varphi = \varphi_0$,

$$\tan \varphi_0 = -m_s / (\beta_0 m_p). \quad (37)$$

It is obvious that the last condition corresponds to the vector \vec{m} projection onto $z=0$ plane being parallel to the $\vec{\kappa}$, $\vec{m}_t \parallel \vec{\kappa}$. In this case the specular wave amplitude is as follows:

$$\vec{E}_0 = \left(\frac{[\vec{m} \vec{k}_0]}{k} \right) \left(\frac{[\vec{E} \vec{m}]_z}{\beta_0} \right), \quad \vec{m}_t \parallel \vec{\kappa}. \quad (38)$$

For the particular case with \vec{E}_t being parallel to \vec{m}_t (for linear polarization of the incident wave), we obtain $\vec{E}_0 = 0$, that coincides with the second point due to $\vec{\kappa} \parallel \vec{m}_t \parallel \vec{E}_t$.

Here a question arises, if it is possible to find the grating parameters (κ, N) and geometry of the resonance diffraction (θ, φ) allowing one to make the specular reflected wave being polarized under the condition $\vec{E}_0 \vec{m} = 0$ for the arbitrary vector \vec{m} , i.e., for the arbitrary value of $M = m_s / m_p$? Besides above-formulated conditions, here we have to consider Eq. (37) as the additional restriction on the angles θ and φ for a given M value. Consider, for instance, the case with a fixed grating period and wavelength (or fixed $\kappa = \lambda/d$). Then, for the case of long-period grating $\kappa < 1$, there are two sets of convenient parameters ($\theta_1, \varphi_1, \mu_1$ and $\theta_2, \varphi_2, \mu_2$) for arbitrary M value, $\cos \theta_1 < \kappa < \cos \theta_2$, $\cos \varphi_1 < 0$, $\cos \varphi_2 > 0$, $M \tan \varphi_{1,2} < 0$. For a short-period grating $\kappa > 1$, there exists a pair of convenient gratings only for sufficiently small values of $|M|$, $|M| < M_0(\kappa)$, and there are no gratings if $|M|$ exceeds the critical value $M_0(\kappa)$. We do not present a rather complicated expression for $M_0(\kappa)$, noting only that it presents the decreasing function that vanishes at $\kappa \rightarrow 2$.²³

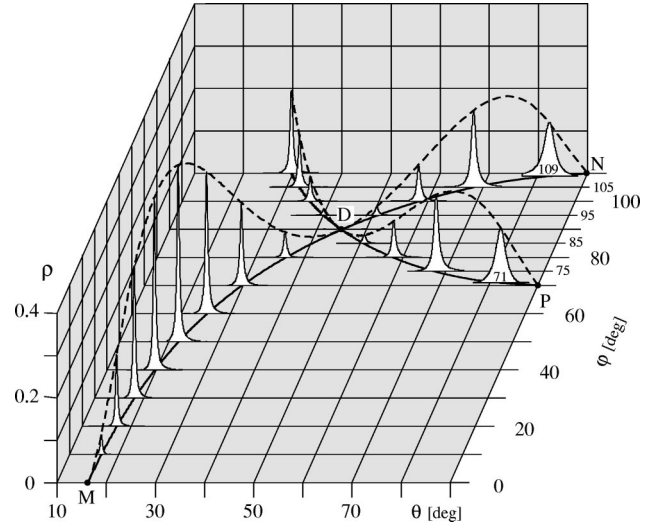


FIG. 5. PCE dependence on the angle of incidence for different azimuthal angles φ . Here and in the following figures the parameters ε, λ , and d coincide with ones of the experimental work.³ In the $0 \leq \theta \leq 45^\circ$, $0 \leq \varphi \leq 90^\circ$ region the theoretical curves are very close to the experimental data. Underline the mirror symmetry relative to the $\varphi = 90^\circ$ plane. The characteristic points M, D, P , and N are the same as in Fig. 4.

Thus, the harmonic diffraction grating under resonance conditions may serve as a polarization and/or amplitude transformation element. This element is fully described in terms of the transformation matrix with real elements. Of special interest is the strong resonance effect of the polarization conversion. In the following section, we examine it in details and make comparison with experimental data.

IV. POLARIZATION CONVERSION

Let us examine the polarization conversion effect in details, comparing results with the experimental ones in Ref. 3. It is described by nondiagonal transformation matrix elements $R_0^{+-} = -R_0^{-+}$. Let us introduce the quantity

$$\rho \equiv |R_0^{-+}|^2 \quad (39)$$

that presents PCE. For the fixed grating parameters (period d and depth $h = 2a$) and wavelength λ the ρ depends on the angle of incidence θ and the grating azimuthal angle φ . Figure 5 shows the $\rho(\theta, \varphi)$ dependence for the parameters of the experiment³ (the Ag grating, $\lambda = 0.6328 \mu\text{m}$, $\varepsilon = -16 + 0.71i$, $\xi = 0.005 - 0.25i$, $d = 0.8425 \mu\text{m}$, $\kappa = 0.751$). As one can see the ρ value becomes negligible away from the resonance, that is caused by small grating depth, $\mu \ll 1$. But nearby the resonance curves [Eq. (22) (bold lines)] ρ increases up to the values of the order of unity.

Let us examine ρ variation along the curves that correspond to the resonance in ± 1 st diffraction order (Fig. 4) for some definite grating (period and depth are constant). By means of the approximate resonance condition (22), one may eliminate the angle of incidence and represent $\rho = \rho_{res}(\varphi)$ in the form

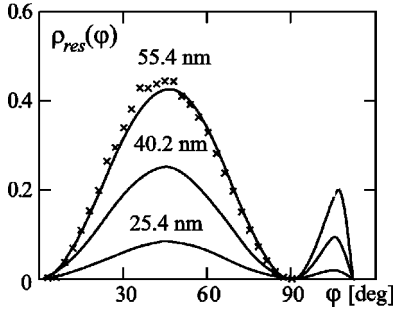


FIG. 6. Dependence of PCE on the azimuthal angle φ along the resonance curve, Eq. (22) for different grating depth. The crests correspond to the experimental data (Ref. 3) for $h = 55.4$ nm.

$$\rho_{res}(\varphi) = \nu^4 [\xi' + B(\varphi)\nu^2]^{-2} \sin^2 2\varphi, \quad r=1, \quad \nu \equiv \pi a/d, \quad (40)$$

$$B(\varphi) = \frac{(\kappa \sin^2 \varphi \pm Q \cos \varphi)^2}{[-\xi'^2 - \kappa^2 \cos 2\varphi \pm 2\kappa Q \cos \varphi]^{1/2}},$$

$$Q = [1 + \xi'^2 - \kappa^2 \sin^2 \varphi]^{1/2}. \quad (41)$$

Here upper sign (+) corresponds to the forward resonance wave propagation, opposite (lower) sign corresponds to the backward propagation. Remember that the lower case is possible only for the grating with period satisfying the condition $K < \kappa < 2K$.

Equation (40) corresponds to the single +1st diffraction order resonance and presents approximate magnitude of PCE at the corresponding resonance curve (22) [for -1st resonance one has to replace $B(\varphi)$ in Eq. (40) by $B(\pi - \varphi)$].

In the vicinity of the double (degenerate) resonance points, $\varphi = \pm \pi/2$, $\theta = \theta_d$, the both first-order resonances $r = \pm 1$ are to be taken into account simultaneously. In these cases approximate proportionality of PCE to the $\sin^2 2\varphi$ holds true with some more complicated coefficient (it differs from the multiplier $\nu^4 [\xi' + B(\varphi)\nu^2]^{-2}$ values by a factor of 2).

Thus, we obtain the explicit analytical expression for the resonance value of the PCE dependence on the grating depth, orientation, and period. These results allow us to understand the physical meaning and role of all parameters influencing the effect. They are in a very good accordance with the experimental data, cf. Ref. 3 (in spite of moderate smallness of the surface impedance value, $|\xi| \approx 0.25$).

The dependence $\rho_{res}(\varphi)$ for the parameters of the experiment, (Ref. 3), is presented in Fig. 6. In $0 \leq \varphi \leq \pi/2$ region the $\rho_{res}(\varphi)$ does not differ essentially from the reference function $\rho_m \sin^2 2\varphi$, where ρ_m denotes maximum value of $\rho_{res}(\varphi)$ (Fig. 6). This property follows strictly from the representation of $\rho_{res}(\varphi)$, if one takes into account that $B(\varphi)$ [Eq. (41)], is a slow function in the region $0 \leq \varphi \leq \pi/2$ and moreover, enters denominator of the expression (40) with a small multiplier ν^2 . Note that $B(\varphi)$ diverges for a specific value of the resonance azimuthal angle $\varphi = \varphi_{max}(\kappa) > \pi/2$, corresponding to the grazing incidence, see Eq. (41) and figure of $B(\varphi)$ in Ref. 24. As function of the grating depth the PCE increases monotonically with depth increasing that is illustrated by Fig. 7.

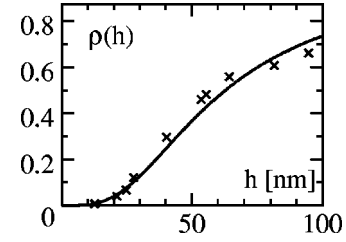


FIG. 7. Dependence of the maximal values of the PCE [Eq. (40)] ($\varphi = \pi/4$) on the grating depth. The crests correspond to the experimental data.³

Equation (40) describes saturation for $\nu \gg \sqrt{\xi'}$. The dependence obtained is in excellent agreement with the experimental results of Ref. 3 without any fitting of parameters. The only divergence is that the calculated resonance width is smaller than the experimental one. This obstacle may be caused as by the rather large surface impedance value for Ag at wavelength $0.63 \mu\text{m}$, $|\xi| \approx 0.25$, and also by the difference of the impedance real part from the value $\xi' = 0.005$.²⁵ Note that the resonance width in the main approximation is proportional to $\xi' + f_1 \nu^2$ with coefficient f_1 of the order of unity. In general, it is represented as a series in ν^2 with coefficients f_n of the order of unity. Thus, for $\nu^2 \ll \xi'$ the resonance width is stipulated by strict light absorption, the nonlinear in the grating depth broadening becomes essential for $\nu^2 \geq \xi'$.

V. SUMMARY

In this work, the opportunities of the developed modified perturbation theory for investigation of the resonance diffraction at high reflecting surface are demonstrated. The approach presented enables one to derive explicit analytical expressions for the complex amplitudes of diffracted waves and carry out the comprehensive investigation of their dependence on the parameters of the problem. The results of calculations even in the lowest-order approximation are in a very good accordance with the experimental data; small discrepancies are within the uncertainty bounds of the data. Besides the antisymmetry of the TC matrix, following from the reciprocity theorem, we have found the additional symmetry properties that were not discussed earlier and are essential for the experimental data analysis. Detailed investigation of the polarization transformation effect (including the polarization conversion) is presented. In particular, the parameters of the resonance diffraction that allow one to produce the linearly polarized specular reflected wave and to control its polarization direction in a wide range, are presented.

On the basis of the results obtained the effective calculations may be performed in order to build the unique gratings with the predetermined parameters. The results may be used also in solving such problems as measurement, both the grating and the medium parameters with high accuracy.

ACKNOWLEDGMENT

Authors are highly indebted to N. A. Balakhonova for her kind assistance in numerical calculations and illustrations.

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- ¹⁴The problem may be solved analytically for rather general form of the relief grating and for the case of grating formed by modulation of the medium dielectric properties and for combined grating as well, see Refs. 1,2.
- ¹⁵Other double resonances may exist also. We neglect them in Eqs. (7)–(10) by two reasons. First, for the harmonic grating they are weak. Second, for $\kappa > \tilde{\kappa} \approx 2/3$ [that is the case of experiment (Ref. 3)] all double resonances, except the ± 1 st ones, do not arise.
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- ¹⁹Note that Fresnel coefficients $R_s = (\beta_0 \xi - 1)/(\beta_0 \xi + 1) \approx -1$ and $R_p = (\beta_0 - \xi)/(\beta_0 + \xi) \approx 1$ are almost real for $\beta_0 \gg |\xi|$, $|\xi| \ll 1$. So for the case of a flat boundary the induced ellipticity of the reflected wave is small.
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