Resonant Wood’s anomaly diffraction condition in dielectric and plasmonic grating structures

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The general features of the light scattering resulting in the so-called resonant Wood’s anomalies in the reflection and transmission spectra are described using the effective parameters of a quasi-guided mode. The expression determining the spectral angular dependence of Wood’s anomaly in the case of plasmonic grating structures is given and compared to the analogous expression for dielectric grating structures. Comparison of the resonant Wood’s anomalies (RWA) with the surface plasmon-polariton resonances (SPPRs) is discussed as well.

INTRODUCTION

In the recent years in condensed-matter physics much attention has been focused on the study of the strong optical effects arising at the exterior surfaces of microstructures, in particular, of the optical resonances, which are due to the periodicity of a grating structure and can be essentially modified by intrinsic material excitations, e.g., such as plasmons [1] and [2]. As a result, these resonances lead to a high intensity of scattered light around a resonant frequency, which in some cases can be approximately determined by the corresponding diffraction condition. The well-known examples of surface optical resonances are the resonant Wood’s anomaly [3–5] and surface plasmon-polariton resonance [6–9], that manifest themselves in the optical spectra as sharp peaks whose position and height depend on the spatial configuration of the structure and the dielectric function of the constituent materials. The origin of RWA is associated with the formation of a quasi-guided mode in the near-surface layer [10].

Usually, in the case of two- and three-dimensional periodic structures it is impossible to derive explicit analytical solutions suitable for analysis and one has to resort to methods based on using effective parameters. The approach using the effective parameters of a quasi-guided mode, which allows one to formulate the diffraction condition for RWA appearing in optical spectra of dielectric grating structures (DGSs), is shortly described in [11]. In this diffraction condition a single scattering vector is taken into account explicitly, while the rest of the scattering is included in the effective parameters of a quasi-guided mode. In the present paper we generalize this theory to the grating structures containing metallic components with permittivity described by the Drude-Lorentz model and take into account the frequency dispersion of the transverse component of the wave vector in a waveguide layer.

Plasmonic grating structures (PGSs) in the simplest case are two- or three-layer structures with a periodic arrangement of metal components in the outside layer (I), or with a metallic layer from a side of the substrate (II), or combining the both types together (III). In this paper we consider PGS of the types I and III, in which case we give the expression for the positions of Wood’s anomaly peaks and the corresponding dispersion relation.

I. GENERAL DIFFRACTION CONDITION

Using the theory developed in [11], we write the diffraction condition for RWA as \( k + \mathbf{G} = k’ \), where \( \mathbf{G} \) is a reciprocal lattice vector and \( k’ \) is the wave vector of the wave propagating in a surface layer of the structure and corresponding to a quasi-guided mode ("quasi" because of wave scattering to the outside). The magnitude of \( k’ \) is \( k’ = |k’| = \omega \sqrt{\varepsilon}/c \), where \( \omega \) is the light frequency, and \( \varepsilon \) is the effective dielectric function of the surface layer.

The wave vector \( \mathbf{k} \) can be represented as \( \mathbf{k} = k|| + k_z \), where \( k|| = k_0 \sin \theta, k_0 = \omega/c. \) By combining these equations one gets

\[
k_0^2(\varepsilon - \sin^2 \theta) - 2k_0G \sin \theta \cos \varphi - G^2 - k_z^2 = 0, \tag{1}
\]

where \( \varphi \) is the angle between vectors \( k|| \) and \( \mathbf{G} \), and \( \theta \) is the outgoing angle of the light with respect to the normal to the surface. For a light wave propagating in the surface layer the transverse component \( k_z \) can be taken constant, as it occurs in typical waveguides. From Eq. (1) one gets

\[
\sin \theta = \frac{G}{k_0} \left( \pm \sqrt{k_0^2 \varepsilon - k_z^2 - \frac{G^2}{2} - \sin^2 \varphi \cos \varphi} \right) \tag{2}
\]

It must satisfy the inequality \( 0 < \sin \theta < 1 \), while the expression under the square root sign be nonnegative. Formally, there are two solutions for \( \sin \theta \) and, as the analysis shows, there are two cases: i) one solution of Eq. (2), with the plus sign before the square root, if \( -k_0(k_0 + 2G \cos \varphi) < k_z^2 + G^2 - k_0^2 \varepsilon < 0 \) (which is possible for any sign of \( \cos \varphi \)), or if \( k_0^2 \varepsilon = k_z^2 + G^2 \), then \( -k_0 < 2G \cos \varphi < 0 \); and ii) two solutions of Eq. (2) (both signs before the radical), if \( \sqrt{k_z^2 + G^2 - k_0^2 \varepsilon} \leq G |\cos \varphi|, k_z^2 + G^2 > k_0^2 \varepsilon \), \( \cos \varphi < 0 \).

The diffraction condition for RWA corresponding to the same quasi-guided mode but to different scattering vectors, \( G_1 \neq G_2 \), satisfy the equations

\[
|k_1 + G_1| = |k_2 + G_2| = \frac{\omega}{c} \sqrt{\varepsilon}, \quad |k_{1z}| = |k_{2z}|, \tag{3}
\]
and, consequently, two Eqs. (1) with the same values of \( \bar{\varepsilon} \) and \([k_z]\). However, Eqs. (1) and (3) define not only the condition for escape of the light wave from the grating structure at the angle \( \theta \), but also may give the condition at which the incident (at the angle \( \theta_0 \)) light wave is scattered to produce a quasi-guided mode. In particular, Eq. (3) is fulfilled in the case of the same scattering vector, \( \mathbf{G}_1 = \mathbf{G}_2 = \mathbf{G} \) (i.e. \( G_1 = G_2, \cos \varphi_1 = \cos \varphi_2 \)). From Eqs. (2) and (3) for incident and reflected waves we infer that the resonant Wood’s anomaly may arise at the diffraction angle \( \theta \neq \theta_0 \), that is realized in experiment \([11]\) and numerical calculations \([12]\). (The case \( \theta \neq \theta_0 \) satisfying either item ii) or Eq. (3) at \( \mathbf{G}_1 \neq \mathbf{G}_2 \) can hardly be realized, because the intensity of the specularly scattered wave.)

Thus, the effective dielectric function of the waveguide structure as well. By substituting \( \bar{\varepsilon} \) into Eq. (1), we get the expression for the Wood’s anomaly spectral peak position

\[
\lambda_W = \frac{2\pi}{G} \sqrt{(\sin \theta \cos \varphi)^2 + (b - \sin^2 \theta)(1 + a) - \sin \theta \cos \varphi},
\]

where \( a = (k_z/G)^2 + \omega_p^2/(Gc)^2 \) and \( b = \varepsilon_0 \ (b > 1) \).

Equation (4) has the same form as the analogous expression in the case of DGSs \([11]\), but where the parameter \( a \) defines a different quantity. If to set \( \omega_p = 0 \), the dependence of \( \bar{\varepsilon} \) on the frequency \( \omega \) vanishes, hence \( \bar{\varepsilon} = n_{eff}^2 \) (where \( n_{eff} \) is the effective refractive index independent of \( \omega \)) and \( a = (k_z/G)^2 \) as it is in the case of a purely dielectric structure. On the whole, Eq. (4) for \( \lambda_W(\theta) \) at different values of \( a \) and \( b \) is an almost linear function of \( \theta \) with a small curvature and with the angle of slope, \( \partial \lambda_W/\partial \theta \), depending on a relation between the values of \( a \), \( b \) and \( \cos \varphi \).

For a light wave propagating in the surface layer the transverse component \( k_z \) can be taken approximately constant, as it occurs in rectangular dielectric waveguides, however, as the surface layer is not spatially homogeneous, one should take into account the frequency dispersion of the \( k_z \) component. Since in the case of PGS a correction to the dielectric function (associated with the value of \( \varepsilon_0 \)) is taken to be constant (in zero order in \( \omega \)), in a decomposition of \( k_z^2 \) we restrict ourselves to the quadratic order in \( \varepsilon_0 \), that is \( k_z^2 = \alpha + \beta k_0 + \gamma k_0^2 \) (which in particular corresponds to the linear approximation \( |k_z| = |k_z(0)| + k_0 \delta \)), where \( \alpha, \beta, \gamma, \delta \) are some constants. Substituting the above expression for \( k_z^2 \) into Eq. (1), we obtain

\[
k_0^2(\varepsilon - \sin^2 \theta) - k_0(\beta + 2G \sin \theta \cos \varphi) - C = 0,
\]

where \( \varepsilon = \varepsilon_0 - \gamma \) and \( C = (\omega_p/c)^2 + G^2 + \alpha \) (so that, \( \varepsilon > 1 \), and \( C > 0 \)). Hence, after simple transformations, one gets the following expression:

\[
\lambda_W = \frac{\pi}{C} \sqrt{\beta + 2G \sin \theta \cos \varphi}^2 + 4(\varepsilon - \sin^2 \theta)C
\]

\[
- \frac{\pi}{C}(\beta + 2G \sin \theta \cos \varphi),
\]

This expression is a generalization of Eq. (4), which also gives an almost linear spectral angular dependence \( \lambda_W(\theta) \). In particular, such dependencies were experimentally obtained for hybrid opaline photonic crystals \([11]\): these are well described by Eq. (4) derived from Eq. (1) in which the effective dielectric function, \( \bar{\varepsilon} \), and the transverse wave-vector component, \( k_z \), are set to constant values. It may signify that the frequency dispersion of these quantities for such structures (and possibly for other dielectric structures) is rather small. Since PGSs are characterized with a larger number of parameters and commonly yield richer spectra than analogous dielectric structures, the former look more likely to give the spectral angular dependencies different from those described by Eq. (4), and Eq. (6) should be used instead.

It is convenient to introduce the following notation: \( \eta_0 = G_x(\sqrt{\beta^2 + 4\varepsilon(C - G^2)} - \beta)/[2(G_x^2 - C)] \), where \( G_x = G \cos \varphi \). From the analysis of Eq. (6) one can obtain the following conditions for the cases of increasing and decreasing \( \lambda_W \) with an increase in \( \theta \):

a) \( \partial \lambda_W/\partial \theta > 0 \) if simultaneously \( \cos \varphi < 0 \) and \( 0 < \sin \theta < \eta_0 \);

b) \( \partial \lambda_W/\partial \theta < 0 \) if simultaneously \( \cos \varphi < 0 \) and \( \eta_0 < \sin \theta < 1 \), and also if \( \cos \varphi > 0 \);

c) \( \partial \lambda_W/\partial \theta = 0 \) if simultaneously \( \cos \varphi < 0 \) and \( \eta_0 < \sin \theta < 1 \), and also if \( \cos \varphi > 0 \);

\( \theta = \arcsin \eta_0 \).

A considerable simplification of the expression for \( \lambda_W \) suitable for making rough estimates in the case of 1D geometry of scattering (\( \cos \varphi = 1 \)) can be made by setting in Eq. (6) \( \alpha = \beta = 0 \) (\( |k_z| = \sqrt{\varepsilon_0} \)). Hence, one gets

II. SPECTRAL ANGULAR DEPENDENCIES AND DISPERSION RELATION

Let us turn to the study of the resonant Wood’s anomalies in the reflection and transmission spectra for PGSs. We write the dielectric function of the metal components of the structure, e.g., of parallel metal strips on the surface of a dielectric plate as

\[
\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma \omega} + \chi_1(\omega) + i\chi_2(\omega).
\]

Here \( \omega_p \) is the plasma frequency with which the metal components are characterized, \( \gamma \) is the damping constant, and \( \chi = \chi_1 + i\chi_2 \) is a contribution in susceptibility due to interband electronic transitions \([13]\). In the simplest approximation one can take \( \chi_1 \) to be constant and neglect the imaginary part \( \chi_2 \) (far from the resonance frequency of the metal). It is also possible to neglect \( \gamma \), that can be partly justified by the fact that incident radiation supports a quasi-guided mode and therefore to some extent compensates for the energy losses caused by absorption. Thus, the effective dielectric function of the waveguide surface layer has the form \( \bar{\varepsilon} = \varepsilon_0 - (\omega_p/\omega)^2 \), where \( \varepsilon_0 \) takes into account the dielectric material of the grating structure as well. By substituting \( \bar{\varepsilon} \) into Eq. (1), we get the expression for the Wood’s anomaly spectral peak position

\[
\lambda_W = \frac{2\pi}{G} \sqrt{(\sin \theta \cos \varphi)^2 + (b - \sin^2 \theta)(1 + a) - \sin \theta \cos \varphi},
\]

where \( a = (k_z/G)^2 + \omega_p^2/(Gc)^2 \) and \( b = \varepsilon_0 \ (b > 1) \).

Equation (4) has the same form as the analogous expression in the case of DGSs \([11]\), but where the parameter \( a \) defines a different quantity. If to set \( \omega_p = 0 \), the dependence of \( \bar{\varepsilon} \) on the frequency \( \omega \) vanishes, hence \( \bar{\varepsilon} = n_{eff}^2 \) (where \( n_{eff} \) is the effective refractive index independent of \( \omega \)) and \( a = (k_z/G)^2 \) as it is in the case of a purely dielectric structure. On the whole, Eq. (4) for
\( \lambda_W(\theta) = (2\pi/G)(\hat{n} \pm \sin \theta) \), where \( \hat{n} = \sqrt{\varepsilon - \kappa} \) in the case of a DGS and \( \hat{n} = \sqrt{\varepsilon_0 - \kappa} \) for a PGS; the plus sign corresponds to \( \varphi = 180^0 \), and the minus sign to \( \varphi = 0 \).

Usually instead of the function \( \lambda_W(\theta) \) one numerically calculates the in-plane dispersion relation \( \omega(k_{||}) \), which in the framework of this approach can be obtained by solving Eq. (5) for \( k_0 \):

\[
k_0(k_{||}) = \beta + \sqrt{\beta^2 + 4(\varepsilon_0 - \gamma)(g(k_{||}) + p + \alpha)} \frac{2(\varepsilon_0 - \gamma)}{2(\varepsilon_0 - \gamma)}, \tag{7}
\]

where \( p = (\omega_c/e)^2 \) and \( g(k_{||}) = k_{||}^2 + 2k_{||}G \cos \varphi + G^2 \).

Here we will illustrate the application of Eqs. (6) and (7) to several sets of parameters \( a = (\alpha + p)/G^2 \) and \( b = \varepsilon_0 - \gamma \) used to describe the spectral angular dependencies of RWA in optical spectra of different grating structures periodic in one dimension. Figure 1 shows these dependencies in the zero diffraction order, \( \theta = \theta_0 \), when the scattering vector \( \mathbf{G} \) \((G = 2\pi/d, l = 1) \) lies in the incidence plane \((\varphi = 0 \text{ or } \varphi = \pi)\), and Fig. 2 shows the corresponding dispersion curves \( \omega(k_{||}) \). As is seen from Fig. 1, the Wood’s anomalies can be apparent in a rather wide wavelength range limited to \( \lambda_{\text{max}} = d(1 + \sqrt{\varepsilon_m}) \), where \( d \) is the period of the structure and \( \varepsilon_m \) is the maximum value of the dielectric constant. An important feature of RWA is the sign of the derivative \( \partial \lambda_W/\partial \theta \). In many experimental spectra \( \partial \lambda_W/\partial \theta > 0 \), which is possible only in the case of the backward scattering of light \((\cos \varphi < 0)\) for the diffraction angles \( \theta < \arcsin \sqrt{b/a} \). In dielectric grating structures the parameter \( a = (k_z/G)^2 \propto (nd/\lambda)^2 \) is typically of the order of 1 or less, while the parameter \( b = n_{ef}^2 \) is greater than 2, therefore the last inequality is satisfied for the whole range of angles \( \theta \). Typical spectral angular dependencies, \( \lambda_W(\theta) \), observed in optical spectra [11] are some increasing concave functions of \( \theta \), that is \( \partial \lambda_W/\partial \theta > 0 \), \( \partial^2 \lambda_W/\partial \theta^2 < 0 \), see also curves 1-3 and 6 in Fig. 1. Actually, as follows from the analysis of Eq. (4), in the case of backscattering of light at the condition \( b > a \) the second derivative of \( \lambda_W(\theta) \) remains negative up to quite large values of \( \theta \).

Equation (4) allows one to determine the peak positions of RWA corresponding to a quasi-guided mode characterized by only two parameters, \( a \) and \( b \), therefore we now use it instead of Eq. (6). The peaks corresponding to different modes can greatly differ in intensity so that in the frequency range of interest a single quasi-guided mode can dominate over the other ones. At the same time, one can expect a series of lines of the RWA peaks, which give almost parallel curves \( \lambda_W(\theta) \). This situation can be realized if for any angle \( \theta \) the derivative \( \partial \lambda_W/\partial \theta \approx \text{const} \) at a constant value of the parameter \( a \), but at different values of \( b \). In the simplest case, where \(|\cos \varphi| = 1\), this condition is satisfied if \( b(1 + a)/(a \sin^2 \theta) - 1 \gg a \); it is satisfactorily fulfilled in a wide range of the angles \( \theta \) and parameters \( a \) and \( b \).

As an example, Fig. 3 shows two sets of spectral angular dependencies plotted for two different values of the \( a \) parameter \((a = 0.1 \text{ and } 1)\), while the \( b \) parameter varies in a wide range (from 5 to 20).

### Figure 1

The spectral angular dependencies calculated by Eq. (6) for different quasi-guided modes of the Wood’s anomalies, with the following parameters \((l = 1, \beta = 0)\): \( a_1 = 0.1, b_1 = 3, \varphi_1 = \pi; a_2 = 5, b_2 = 20, \varphi_2 = \pi; a_3 = 2, b_3 = 20, \varphi_3 = \pi; a_4 = 0.2, b_4 = 10, \varphi_4 = 0; a_5 = 0.3, b_5 = 20, \varphi_5 = 0; a_6 = 0.1, b_6 = 20, \varphi_6 = \pi.\)

### Figure 2

Dispersion curves plotted by using Eq. (7) for the same parameters as in Fig. 1.

### Figure 3

The resonant Wood’s anomalies in PGSs should be distinguished from the surface plasmon-polariton reso-
The surface plasmon-polaritons:

\[ k_0^2 = \frac{p/2 + g(k_{||}) (\varepsilon_2 + 1)/(2\varepsilon_2) + \sqrt{(p/2)^2 + g(k_{||})^2 (\varepsilon_2 + 1)^2/(2\varepsilon_2)^2 + pg(k_{||}) (\varepsilon_2 - 1)/(2\varepsilon_2)}}{\varepsilon} \]

The analysis of the dispersion relations made by means of Eqs. (7) and (9) enables us to distinguish between RWA and SPPR. Though both expressions give almost straight lines \(k_0(k_{||})\), their slope and position can be quite different (the latter can be seen from the corresponding values of \(k_0\) at \(\theta = 0\)).

IV. DISCUSSION (CONNECTION TO THE SCATTERING MATRIX)

The theory presented in this paper is based on Eq. (1), which is applied to dielectric and plasmonic grating structures. Therefore it may be useful to provide some additional explanation on this point. Let us consider the scattering matrix \((2 \times 2)\) for a single plane layer with the refractive index \(n = \sqrt{\varepsilon}\), which for simplicity can be taken real (in the absence of absorption) \([12]\). The elements of the matrix \(S\) can be written in terms of the amplitude reflection and transmission coefficients, \(r\) and \(t\), for an incident plane wave. It is well-known that the equation \(det(S^{-1}) = (r^2 - t^2)^{-1} = 0\) determines the eigenfrequencies \(\Omega = \Omega' + i\Omega''\) and eigenvalues \(k_z = k'_z + i k''_z\) of the \(z\)-component of the wave vector inside the layer.

Hence, using the expressions for \(r\) and \(t\), one can show that \(1 - r_{21} r_{23} e^{2i k_z d} = 0\), where \(r_{21}\) and \(r_{23}\) are the coefficients of reflection from two interfaces and \(d\) is the layer thickness. In the case of a guided mode the light wave experiences total internal reflection from the interfaces, so that \(|r_{21}| = |r_{23}| = 1\) and, consequently, \(k_z\) is real. The magnitude \(k\) of the wave vector of light propagating in the layer satisfies the equation

\[ k^2 = (\omega n/c)^2 = k'_z + k''_z \]

Due to the conservation of the tangential component \(k_{||}\) it can be represented as \(k_{||} = k_0 \sin \theta_0\), where \(k_0 = \omega/c\) is the magnitude of the wave vector in vacuum, when a plane monochromatic wave of the frequency \(\omega\) falls onto the layer–vacuum interface from vacuum at an angle \(\theta_0\) (and reflects at the angle \(\theta = \theta_0\)); since \(k''_z = 0\), from Eq. (10) one gets \(\omega = \Omega'\). Because of the periodicity of the structure the wave corresponding to a guided mode is scattered and goes outside the layer. This is taken into account by the replacement of \(k_{||}\) in Eq. (10) by \(k_{||} + \mathbf{G}\), that eventually leads to Eq. (1).

V. CONCLUSION

In conclusion, we theoretically studied some peculiarities of the diffraction condition for the resonant Wood’s anomaly obtained in the approximation of a single scattering vector and by using the effective parameters of a
quasi-guided mode. The expression for location of the spectral peaks in the reflection and transmission spectra of plasmonic grating structures is given; if the dispersion of the transverse component of the wave vector in the waveguide layer can be ignored, this expression is converted to the analogous one for dielectric grating structures as the plasma frequency tends to zero. This approach can be useful in analyzing spectral angular dependencies obtained from the reflection and transmission spectra demonstrating the resonant Wood’s anomaly and surface plasmon-polariton resonance. In practice, the difference between these two types of resonances can be established by simulating the experimental data by numerical calculation with a subsequent model calculation performed for the same parameters by neglecting the absorption in the grating structure and then by fitting the obtained points to Eqs. (6-9).

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