Diffraction of light from a rough surface with an arbitrary "deep" profile: interaction of diffracted beams, anomalous absorption, and maximum attainable local fields

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We develop an analytic theory of the diffraction of light from a rough surface with an arbitrary "deep" profile. The crucial factor enabling one to go from an infinite set of equations for the amplitudes of the diffracted waves to a finite, analytically solvable system is the separation of resonant waves. The effectiveness of the proposed procedure is demonstrated by examples dealing with the suppression of specular reflection, the calculation of the maximum attainable local fields near the surface, and anomalous absorption of light by the surface. For these problems, our method makes it possible for the first time to trace in detail the effects of anharmonicity and of the depth of the surface relief. We discuss new possibilities for controlling the reflection and absorption of light by a rough surface. The approach we have developed seems promising in the theory of light scattering from a statistically rough surface, and in nonlinear surface optics.

1. INTRODUCTION

The problem of the diffraction of light from a nonplanar interface first arose in the theory of reflecting diffraction gratings[1–3] and in the theory of molecular scattering of light from the surface of a liquid.[4] Modern laser optics has posed a number of new physical problems which belong essentially to this same class. Foremost among these are Raman scattering of light by molecules adsorbed on a surface,[5,6] and a variety of problems associated with nonlinear reflection from a surface.[7–10]

One unexpected circumstance was that both linear and nonlinear interactions of light waves diffracted from a surface may be strong; under suitable conditions, the pattern of linear and nonlinear reflections from a rough surface differ fundamentally from the pattern produced by a smooth surface. A classic example of this type is the famous Wood anomaly.[2] Besides the already well known surface-enhanced Raman scattering of light from a rough surface, the most recent intensive research has been directed towards the suppression of specular reflection from metals, semiconductors, and dielectrics,[11–18] anomalous absorption of light by a corrugated surface,[19–21] laser-induced development of instabilities in surface relief,[22–24] and low-threshold breakdown near a surface.[25] Other topics discussed (see also the present paper) include the possibility of effective reflection control, and obtaining at a surface strong nonlinear effects leading to optical bistability and optical chaos.[26] These are obviously problems which cannot be solved by standard perturbation methods,[27–32] since strong interactions among the diffracted waves dominate.

The diffraction of light from a nonplanar interface under conditions for which perturbation methods do not work, such a diffraction from "deep" gratings with a sinusoidal or biharmonic profile, has been investigated numerically for certain specific instances.[11–13,33] Moreover, it is obviously highly desirable to extend analytic methods beyond the limits of perturbation theory. Naturally, this is the approach which makes it possible to expose the physics of strong interactions and self-action of light waves at a surface. Along these lines, a number of analytic results for a sinusoidal grating appear in Refs. 15–17, 20, and 21. The theory discussed in Ref. 24, however, which allows for many gratings, was developed with a severe upper bound on the amplitude of the relief; this prevents consideration of the phenomenon of total suppression of specular reflection, and of questions relating to the maximum attainable local fields and to anomalous absorption of light by a surface.

In the present paper we develop an analytic theory of the diffraction of light by a surface with an arbitrary profile and with a fairly large modulation amplitude of the surface relief (making it necessary to take account of cross-scattering between the diffracted fields); this theory is valid for metals, semiconductors, and dielectrics for which $|\varepsilon|\gg 1$. That such a theory can be constructed is due to the existence (for $|\varepsilon|\gg 1$) of sharp resonances in the amplitudes of the diffracted fields. The latter circumstance enables one to go from an infinite set of equations for the amplitudes of the diffracted waves to a finite, analytically solvable system for the individual resonant waves. Simple expressions have deen derived in explicit form for the amplitudes of the diffracted fields in vacuum and in a medium. We have investigated the conditions for total suppression of specular reflection (TSSR) in the presence of many gratings, as well as the conditions for attainment of the maximum local field at a rough surface. We have determined the optimal relief for which the absorption capability A of a surface with spatially modulated relief can be much greater than that of a surface with planar relief ($A_{\rm pl} = 1$–3%), and can, under certain circumstances, approach 100%. Using as an example surface with two gratings oriented arbitrarily with respect to one another, we have investigated the conditions under which there is practically total conversion of the energy of the incident field into the energy of a wave reflected into the vacuum are propagating in a previously specified direction which differs from the direction of the specular reflection.

2. STATEMENT OF THE PROBLEM INITIAL EQUATIONS

Assume that an electromagnetic wave given by

$$\mathbf{E}_i(x, y, z, t)=\mathbf{E}_i \exp(ik_t y+ik_z z-i\omega t) + \text{c.c.},$$
$$k_t=k_0 \sin\theta, \quad k_z=k_0\cos\theta,$$

is incident from a vacuum on the surface of medium with

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dielectric constant $\varepsilon(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega) = (n + im)^2$ and magnetic permeability $\mu \equiv 1$, which fills the semi-infinite space $z \geqslant f(x,y)$; here k_t and k_z are the projections of the wave vector $\mathbf{k}_0 (k_0 = \omega/C)$ of the incident wave on the y and z axes, θ is the angle of incidence of the wave, and $f(x,y)$ is a function which describes the surface relief.

As a result of diffraction of the incident radiation by the modulated interface $z = f(x,y)$, diffraction fields arise both inside and outside the medium. The fields $\mathbf{E}(x,y,z,t) = \mathbf{E}(\omega)\exp(-i\omega t) + \text{c.c.}$ in vacuum and $\mathbf{E}'(x,y,z,t) = \mathbf{E}'(\omega)\exp(-i\omega t) + \text{c.c.}$ in the medium satisfy Maxwell's equations:

$$\begin{gathered}\text{rot}\,\mathbf{E}(\omega)=ik_0\mathbf{H}(\omega), \quad \text{rot}\,\mathbf{E}'(\omega)=ik_0\mathbf{H}'(\omega),\\ \text{rot}\,\mathbf{H}(\omega)=-ik_0\mathbf{E}(\omega), \quad \text{rot}\,\mathbf{H}'(\omega)=-ik_0\varepsilon(\omega)\mathbf{E}'(\omega), \qquad (1)\\ \text{div}\,\mathbf{E}(\omega)=0, \quad \text{div}\,[\varepsilon(\omega)\mathbf{E}'(\omega)]=0,\\ \text{div}\,\mathbf{H}(\omega)=0, \quad \text{div}\,\mathbf{H}'(\omega)=0.\end{gathered}$$

The boundary conditions, which formulate the equality of the tangential components of the electric and magnetic fields at the boundary $z = f(x,y)$ and the equality of the normal (to the surface) components of the electric and magnetic induction vectors, may be written in the form

$$\begin{gathered}\mathbf{E}(\omega)-\mathbf{n}(\mathbf{n}\mathbf{E}(\omega))=\mathbf{E}'(\omega)-\mathbf{n}(\mathbf{n}\mathbf{E}'(\omega)),\\ \mathbf{n}\mathbf{E}(\omega)=\varepsilon(\omega)\mathbf{n}\mathbf{E}'(\omega), \qquad (2)\\ \mathbf{H}(\omega)-\mathbf{n}(\mathbf{n}\mathbf{H}(\omega))=\mathbf{H}'(\omega)-\mathbf{n}(\mathbf{n}\mathbf{H}'(\omega)), \quad \mathbf{n}\mathbf{H}(\omega)=\mathbf{n}\mathbf{H}'(\omega),\end{gathered}$$

where $\mathbf{n} = (f_x\mathbf{x} + f_y\mathbf{y} - \mathbf{z})/(1 + f_x^2 + f_y^2)^{1/2}$ is the unit normal to the surface $z = f(x,y)$ and is directed into the vacuum; $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ are unit vectors along the x, y, and z axes; $f_x = \partial f(x,y)/\partial x$ and $f_y = \partial f(x,y)/\partial y$.

We represent the surface relief $f \equiv f(x,y)$ by its Fourier spectrum:

$$f=\sum_{\mathbf{g}_i}[\xi_{\mathbf{g}_i}\exp(-i\mathbf{g}_i\mathbf{r}) + \text{c.c.}], \qquad \xi_0=0, \qquad (3)$$

where ξ_{g_i} is the complex amplitude of the corresponding Fourier component of the surface relief, $\mathbf{r} = (x,y,0)$, and $\mathbf{g}_i = (g_{ix}, g_{iy}, 0)$, where for uniqueness in the specification of the gratings we assume $g_{ix} \geqslant 0$ (if $g_{ix} = 0$, then $g_{iy} < 0$). Consider the set $\{\Sigma_i p_i \mathbf{g}_i\}$ of vectors $\Sigma_i p_i \mathbf{g}_i$, where $p_i = 0, \pm 1, \ldots$. In this set we can set apart a subset $\{\mathbf{q}\}$ of mutually distinct vectors $\mathbf{q}$. We seek fields $\mathbf{E}(\omega)$ in the vacuum and $\mathbf{E}'(\omega)$ in the medium in the form

$$\mathbf{E}(\omega)=\mathbf{E}_i\exp(ik_ty+ik_zz)+\sum_{\mathbf{q}}\mathbf{E}_{\mathbf{q}}\exp[i(\mathbf{k}_t-\mathbf{q})\mathbf{r}+\Gamma_{\mathbf{q}}z], \quad (4)$$

$$\mathbf{E}'(\omega)=\sum_{\mathbf{q}}\mathbf{E}_{\mathbf{q}}'\exp[i(\mathbf{k}_t-\mathbf{q})\mathbf{r}-\gamma_{\mathbf{q}}z], \qquad (5)$$

where $\mathbf{k}_t = (0,k_t,0)$. The value $\mathbf{q} = 0$ corresponds to Fresnel waves specularly reflected into the vacuum and refracted into the medium. The expressions for the fields $\mathbf{H}(\omega)$ and $\mathbf{H}'(\omega)$ in the vacuum and the medium have exactly the same structure, and are obtained from Eqs. (4) and (5) by making the replacements $\mathbf{E}_i, \mathbf{E}_\mathbf{q}, \mathbf{E}'_\mathbf{q} \to \mathbf{H}_i, \mathbf{H}_\mathbf{q}, \mathbf{H}'_\mathbf{q}$. The amplitudes of $\mathbf{H}_i$, $\mathbf{H}_\mathbf{q}$, and $\mathbf{H}'_\mathbf{q}$ may be expressed in terms of the amplitudes of $\mathbf{E}_i$, $\mathbf{E}_\mathbf{q}$, and $\mathbf{E}'_\mathbf{q}$ via the Maxwell equations (1). Substituting Eqs. (4) and (5) into Eq. (1), we find $\Gamma_\mathbf{q}^2 = (\mathbf{k}_t - \mathbf{q})^2 - \mathbf{k}_0^2$ and $\gamma_\mathbf{q}^2 = (\mathbf{k}_t - \mathbf{q})^2 - \mathbf{k}_0^2\varepsilon$. We then have $\text{Re}\,\gamma_\mathbf{q} \geqslant 0$; $\text{Re}\,\Gamma_\mathbf{q} \geqslant 0$ if $|\mathbf{k}_t - \mathbf{q}| \geqslant k_0$; $\text{Im}\Gamma_\mathbf{q} \leqslant 0$ if $|\mathbf{k}_t - \mathbf{q}| \leqslant k_0$. In what follows, we employ the notation $\mathbf{E}_q \equiv \mathbf{E}_\mathbf{q}$, $\mathbf{E}'_q \equiv \mathbf{E}'_\mathbf{q}$, $\Gamma_q \equiv \Gamma_\mathbf{q}$, $\gamma_q \equiv \gamma_\mathbf{q}$, and $\mathbf{k}_q = (k_{qx}, k_{qy}, 0) \equiv \mathbf{k}_t - \mathbf{q}$.

3. FIELD DISTRIBUTION IN VACUUM AND IN THE MEDIUM TAKING ACCOUNT OF INTERACTIONS BETWEEN DIFFRACTED FIELDS WHEN $|\varepsilon| \gg 1$

We consider media in which $|\varepsilon| \gg 1$. Under these circumstances, when f_x^2, f_y^2, and $|f_x f_y| \ll 1$, almost all the energy of the electromagnetic field in the medium is contained in the diffracted waves $\mathbf{E}'_q$ and $\mathbf{H}'_q$ for which

$$k_q^2 \ll k_0^2|\varepsilon| \qquad (|\varepsilon|\gg 1), \qquad (6)$$

so we can assume that all $\gamma_q \approx \gamma \equiv k_0(-\varepsilon)^{1/2} = k_0(m - in)$. Equation (5) then takes the form

$$\mathbf{E}'(\omega)\approx\exp(-\gamma z)\sum_{\mathbf{q}}\mathbf{E}_q'\exp(i\mathbf{k}_q\mathbf{r}). \qquad (7)$$

We also have an analogous relation for the magnetic field in the medium.

A. The system of equations governing the field amplitudes in vacuum

The boundary conditions (2) are expressed in terms of the fields in vacuum and in the medium. We now derive approximate boundary conditions containing only the fields in vacuum. On the one hand, from the exact boundary conditions (2) with f_x^2, f_y^2, and $|f_x f_y| \ll 1$ and $|\varepsilon| \gg 1$, we find $(z = f(x,y))$

$$\begin{gathered}E_x'(\omega)\approx E_x(\omega)+f_xE_z(\omega),\; E_y'(\omega)\\ \approx E_y(\omega)+f_yE_z(\omega),\; \mathbf{H}'(\omega)=\mathbf{H}(\omega). \qquad (8)\end{gathered}$$

On the other hand, from Eq. (7) and the Maxwell equation $ik_0\mathbf{H}'(\omega) = \text{curl}\mathbf{E}'(\omega)$, bearing in mind the relation $E'_{qz} = (ik_{qx}E'_{qx} + iK_{qy}E'_{qy})/\gamma$ which follows from div $\mathbf{E}'(\omega) = 0$, we have

$$E_x'(\omega)\approx-ik_0H_y'(\omega)/\gamma, \qquad E_y'(\omega)\approx ik_0H_x'(\omega)/\gamma. \qquad (9)$$

Eliminating the fields in the medium from Eqs. (8) and (9), we arrive at a system of boundary conditions at $z = f(x,y)$ containing only the fields in vacuum:

$$\begin{gathered}E_x(\omega)+f_xE_z(\omega)=-ik_0H_y(\omega)/\gamma,\\ E_y(\omega)+f_yE_z(\omega)=ik_0H_x(\omega)/\gamma. \qquad (10)\end{gathered}$$

We now calculate the field distribution in vacuum under the conditions

$$k_0^2f^2(x,y)\ll 1, \qquad |\Gamma_qf(x,y)|^2\ll 1. \qquad (11)$$

Integrating both sides of the first inequality in (11) with respect to x and y over the region S and making use of Parseval's theorem, we obtain

$$\overline{k_0^2f^2}\equiv\lim_{S\to\infty}\frac{1}{S}\iint_S k_0^2f^2(x,y)\,dx\,dy=2k_0^2\sum_{\mathbf{g}_i}|\xi_{\mathbf{g}_i}|^2\ll 1.$$

The conditions (11) thus impose constraints on the spectrum of the surface relief and on the mean squared deviation of the relief from a plane surface.

If in Eq. (10) we express the field $\mathbf{H}(\omega)$ in terms of the field $\mathbf{E}(\omega)$ using the Maxwell equation $ik_0\mathbf{H}(\omega) = \text{curl}\,\mathbf{E}(\omega)$, we find using Eq. (4) that

$$\begin{aligned}&[(\gamma+ik_z)E_{ix}+\gamma f_x E_{iz}]\exp(ik_z f)\\ &=-\sum_{\mathbf{q}}[(\gamma+\Gamma_q)E_{qx}-(ik_{qx}-\gamma f_x)E_{qz}]\exp(-i\mathbf{qr}+\Gamma_q f),\\ &[(\gamma k_z+ik_0^2)/k_t-\gamma f_y]E_{iz}\exp(ik_z f)\\ &=\sum_{\mathbf{q}}[(\gamma+\Gamma_q)E_{qy}-(ik_{qy}-\gamma f_y)E_{qz}]\exp(-i\mathbf{qr}+\Gamma_q f).\end{aligned}\tag{12}$$

In the system (12), we expand $\exp(ik_z f)$ and $\exp(\Gamma_q f)$ in Taylor series, and by virtue of (11), we keep only the first two terms. Equating terms of equal degree, we arrive at a system of coupled equations for the amplitudes of the diffracted fields. Using this system to express the components E_{qx}, E_{qy}, and E_{qz} in terms of the amplitude of the incident field and the amplitudes of the other diffracted fields, and bearing in mind that div $\mathbf{E}(\omega) = 0$, we have for the components of the zeroth-order diffraction field $\mathbf{E}_0$

$$\begin{aligned}&E_{0x}=\frac{k_z-i\gamma}{k_z+i\gamma}E_{ix}-\sum_{\mathbf{q}}[\Gamma_q E_{qx}-ik_{qx}E_{qz}]\xi_{-\mathbf{q}},\qquad E_{0y}=\frac{k_z}{k_t}E_{0z},\\ &E_{0z}=\frac{\varepsilon k_z-i\gamma}{\varepsilon k_z+i\gamma}E_{iz}-\frac{\varepsilon k_t}{\varepsilon k_z+i\gamma}\sum_{\mathbf{q}}[\Gamma_q E_{qy}+i(k_t-k_{qy})E_{qz}]\xi_{-\mathbf{q}},\end{aligned}\tag{13}$$

and for the components of the fields $\mathbf{E}_q$ ($\mathbf{q}\neq 0$), we obtain

$$\begin{aligned}&E_{qx}=E_{qz}ik_{qx}/\gamma-i[k_z(E_{ix}-E_{0x})+k_{qx}(E_{iz}+E_{0z})]\xi_{\mathbf{q}}\\ &\quad-\sum_{\mathbf{q}'\neq 0}[\Gamma_{q'}E_{q'x}+i(k_{qx}-k_{q'x})E_{q'z}]\xi_{\mathbf{q}-\mathbf{q}'},\\ &E_{qy}=E_{qz}ik_{qy}/\gamma+i(k_0^2-k_t k_{qy})(E_{iz}+E_{0z})\xi_{\mathbf{q}}/k_t\\ &\quad-\sum_{\mathbf{q}'\neq 0}[\Gamma_{q'}E_{q'y}+i(k_{qy}-k_{q'y})E_{q'z}]\xi_{\mathbf{q}-\mathbf{q}'},\\ &E_{qz}=\frac{\varepsilon}{\varepsilon\Gamma_q+\gamma}\Big\{\Big[-k_z k_{qx}(E_{ix}-E_{0x})+\frac{k_{qy}k_0^2-k_t k_q^2}{k_t}(E_{iz}+E_{0z})\Big]\\ &\quad\times\xi_{\mathbf{q}}+\sum_{\mathbf{q}'\neq 0}[i\Gamma_{q'}\mathbf{k}_q\mathbf{E}_{q'}-\mathbf{k}_q(\mathbf{k}_q-\mathbf{k}_{q'})E_{q'z}]\xi_{\mathbf{q}-\mathbf{q}'}\Big\},\end{aligned}\tag{14}$$

where $\xi_{\mathbf{q}-\mathbf{q}'}\equiv\xi_{\mathbf{k}q'-\mathbf{k}q}=\xi_{\mathbf{g}_i}$ if $\mathbf{q}-\mathbf{q}'=\mathbf{k}_{q'}-\mathbf{k}_q=\mathbf{g}_i$; $\xi_{\mathbf{q}-\mathbf{q}'}=\xi^*_{\mathbf{g}_i}$ if $\mathbf{q}-\mathbf{q}'=-\mathbf{g}_i$; and $\xi_{\mathbf{q}-\mathbf{q}'}=0$ if $\mathbf{q}-\mathbf{q}'\neq\pm\mathbf{g}_i$. The solution of Eqs. (13) and (14) determines the amplitude of the diffracted fields in vacuum when the radiation is incident with arbitrary polarization at an arbitrary angle on a surface with arbitrary profile. The system (13), (14), which takes account of cross-scattering between the fields $\mathbf{E}_q$, $\mathbf{E}_{q'}$, for which $\mathbf{k}_\mathbf{q}-\mathbf{k}_{q'}=\pm\mathbf{g}_i$, is valid for the conditions (6), (11) and $f_x^2, f_y^2, |f_x f_y|\ll 1$.

It is not possible to obtain a general solution to the infinite-dimensional system (13), (14). Below, we develop a method for solving this system which holds both for "shallow" and "deep" relief. The possibility of constructing such a method is a consequence of the existence, for $|\varepsilon|\gg 1$, of sharp resonances in the amplitude of the diffracted waves.

B. Electromagnetic resonances and the possibility of obtaining analytic solutions for relief with a "deep" profile

For small modulation amplitudes of the relief ($|k_0|\xi_{\mathbf{g}_i}\to 0$), the system (13), (14) can be solved by perturbation methods. Since perturbation theory enables one to make sense of the approximations made below and to clearly define the concepts of "shallow" and "deep" relief, we present the basic qualitative results obtained by this method.

According to perturbation theory, we assume that, to zeroth order, the amplitude of $\mathbf{E}_0$ is given by the Fresnel equations $\mathbf{E}_0=\mathbf{E}_F$ (see (13)), and that $\mathbf{E}_{\pm\mathbf{g}_i}=0$. To first order in $k_0\xi_\mathbf{q}$, the amplitudes of the $\mathbf{E}_{\pm\mathbf{g}_i}=0$ are found by substituting $\mathbf{E}_0=\mathbf{E}_F$ into Eq. (14). To second order in $k_0\xi_\mathbf{q}$, the amplitudes of the fields $\mathbf{E}_0$, $\mathbf{E}_q$ ($\mathbf{q}\neq 0$) are obtained from Eqs. (13), (14) using the values of the $\mathbf{E}_{\pm\mathbf{g}_i}=0$ already found, etc. As a result, the expressions for the amplitudes of the diffracted fields are of the form

$$\begin{aligned}&E_0=\Big[1-\sum_{\mathbf{q}}\tilde a_q\frac{\varepsilon k_0}{\varepsilon\Gamma_q+\gamma}|k_0\xi_\mathbf{q}|^2+\dots\Big]E_\Phi,\\ &E_q=\frac{\varepsilon k_0}{\varepsilon\Gamma_q+\gamma}\Big[\tilde b_q(k_0\xi_\mathbf{q})+\sum_{\mathbf{q}'}\tilde c_{qq'}\frac{\varepsilon k_0}{\varepsilon\Gamma_{q'}+\gamma}(k_0\xi_{\mathbf{q}'})(k_0\xi_{\mathbf{q}-\mathbf{q}'})\\ &\qquad+\dots\Big]E_i,\end{aligned}\tag{15}$$

where $\tilde a_q$, $\tilde b_q$, and $\tilde c_{qq'}$ are quantities of order unity.

From (14) and (15), we find that the amplitudes of the diffracted fields are proportional to the factor

$$l_q=l_q'+il_q''\equiv\varepsilon k_0/(\varepsilon\Gamma_q+\gamma).\tag{16}$$

We now introduce the following notation ($\varepsilon^{1/2}=n+im$):

$$\tilde x_q=[(k_q^2-k_0^2)/k_0^2]^{1/2}-\beta_m,\quad \tilde y_q=[(k_0^2-k_q^2)/k_0^2]^{1/2}+\beta_n,$$
$$\beta_m=m/(m^2+n^2),\quad \beta_n=n/(m^2+n^2).$$

With this notation, the real and imaginary parts of l_q may be represented in the form

$$\begin{aligned}&l_q'=\tilde x_q/(\tilde x_q^2+\beta_n^2),\quad l_q''=\beta_n/(\tilde x_q^2+\beta_n^2),\quad\text{if}\quad k_q\geqslant k_0,\\ &l_q'=-\beta_m/(\tilde y_q^2+\beta_m^2),\quad l_q''=\tilde y_q/(\tilde y_q^2+\beta_m^2)\quad\text{if}\quad k_q\leqslant k_0.\end{aligned}$$

It is then obvious that when $|\varepsilon|\gg 1$ and $\tilde x_q=0$ (i.e., when $k_q\approx k_0$), $|l_q|=(m^2+n^2)/n\gg 1$, whereupon (14) implies that there is a pronounced increase in the amplitude of the diffracted fields $\mathbf{E}_q$, for which $k_q\approx k_0$, both in metals ($m>n$) and dielectrics ($m<n$). We will call such fields $\mathbf{E}_{qr}$ resonant, along with their associated vectors $\mathbf{k}_{gr}$, $\mathbf{q}_r$. The width of the resonance is governed by the factor β_n when $k_q>k_0$ and β_m when $k_q<k_0$. for resonant fields (see (14), (16)), we have

$$|E_{qrz}|\gg|E_{qrx}|,\quad |E_{qry}|.\tag{17}$$

We refer to the fields $\mathbf{E}_q$ with $\mathbf{q}\neq 0$, for which $k_q\neq k_0$($|\varepsilon\Gamma_q|\gg|\gamma|$), as nonresonant, along with their associated vectors $\mathbf{k}_q$, and we denote these by the symbols $\mathbf{E}_{qn}$, $\mathbf{k}_{qn}$.

We consider the relief to be "shallow" if in calculating the field amplitudes by perturbation methods (see (15)), we can stop at the terms linear in $k_0\xi_\mathbf{q}$. In the absence of resonant fields, this can be done when the conditions (11) hold; when they are present, but there is no cross-scattering between them (see (15) and (16)), we must have

$$(m^2+n^2)|k_0\xi_{\mathbf{q}_r}|^2/n\ll 1.\tag{18}$$

In the presence of both resonant fields and cross-scattering between them, the relief can be considered "shallow" if

$$(m^2+n^2)|k_0\xi_{q_r}|/n \ll 1. \quad (19)$$

When either (18) or (19) fails to hold, we refer to the relief as being "deep." Perturbation theory is then inapplicable. We now describe a method for solving the systems of (13) and (14) which is valid for both "deep" and "shallow" relief.

It is clear from (13) that when (11) holds, the presence of nonresonant gratings has no particular influence on $\mathbf{E}_0$. Significant corrections to $\mathbf{E}_0 = \mathbf{E}_F$ can only come from resonant gratings. In line with this, the summation in the expressions for $\mathbf{E}_0$ (see (13)) can be carried out over the resonant gratings exclusively. We reach a similar conclusion with regard to the other nonresonant fields. In the expressions for the resonant fields $\mathbf{E}_{qr}$ (see (14)), the sum must be taken over both the resonant fields $\mathbf{E}_{qr'}$ ($\mathbf{q}_r' \neq \mathbf{q}_r$) and the nonresonant fields $\mathbf{E}_{qn}$, since the latter can make a substantial contribution to the field $\mathbf{E}_{qr}$ through the resonant factor (16).

Let the spectrum of the surface relief contain a finite number of resonant gratings $\mathbf{g}_r$ which scatter the fields $\mathbf{E}_i$ and $\mathbf{E}_0$ into the resonant waves $\mathbf{E}_{qr}$ ($\mathbf{k}_{qr} = \mathbf{k}_t \pm \mathbf{g}_r$). Then when

$$|E_i k_{q_n} \xi_{q_n}| + \sum_{\mathbf{q}_r} |E_{q_r} k_{q_r} \xi_{\mathbf{q}_n-\mathbf{q}_r}| \gg \sum_{\mathbf{q}_n'} |E_{q_n'} k_{q_n'} \xi_{\mathbf{q}_n-\mathbf{q}_n'}|$$

we have from (14), with (11), (17), and the foregoing remarks taken into consideration, that the amplitudes $\mathbf{E}_{qn}$ of the nonresonant fields with $\mathbf{k}_{qn} = \mathbf{k}_t \pm \mathbf{g}_r$ or $\mathbf{k}_t \pm \mathbf{g}_r \pm \mathbf{g}_i$ can be represented in the form

$$E_{q_n x} = -i\Big\{[k_z(E_{ix}-E_{0x}) + k_{q_n x}(E_{iz}+E_{0z})]\xi_{q_n} + \sum_{\mathbf{q}_r}(k_{q_n x} - k_{q_r x})E_{q_r z}\xi_{\mathbf{q}_n-\mathbf{q}_r}\Big\},$$

$$E_{q_n y} = (-k_{q_n x}E_{q_n x} + i\Gamma_{q_n}E_{q_n z})/k_{q_n y},$$

$$E_{q_n z} = -\Big\{\Big[k_z k_{q_n x}(E_{ix}-E_{0x}) + \frac{k_t k_{q_n}^2 - k_{q_n y}k_0^2}{k_t}(E_{iz}+E_{0z})\Big]\xi_{q_n} + \sum_{\mathbf{q}_r}\mathbf{k}_{q_n}(\mathbf{k}_{q_n}-\mathbf{k}_{q_r})E_{q_r z}\xi_{\mathbf{q}_n-\mathbf{q}_r}\Big\}\Big/\Gamma_{q_n}, \quad (20)$$

while the component E_{qrz} of the resonant fields may be written as

$$E_{q_r z} = \frac{\varepsilon}{\varepsilon\Gamma_{q_r}+\gamma}\Big\{-\Big[k_z k_{q_r x}(E_{ix}-E_{0x}) + (k_t - k_{q_r y})(E_{iz}+E_{0z})k_0^2/k_t\Big]\xi_{q_r} + \sum_{\mathbf{q}=\mathbf{q}_n,\mathbf{q}_r'}[i\Gamma_q \mathbf{k}_{q_r}\mathbf{E}_q - \mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_q)\mathbf{E}_{qz}]\xi_{\mathbf{q}_r-\mathbf{q}}\Big\}. \quad (21)$$

The amplitudes E_{0x}, E_{0z} are then given by ($E_{0y} = k_z E_{0z}/k_t$)

$$E_{0x} = \frac{k_z - i\gamma}{k_z + i\gamma}E_{ix} - \sum_{\mathbf{q}_r} iq_x E_{qz}\xi_{-\mathbf{q}}, \quad E_{0z} = \frac{\varepsilon k_z - i\gamma}{\varepsilon k_z + i\gamma}E_{iz} - \frac{\varepsilon k_t}{\varepsilon k_z + i\gamma}\sum_{\mathbf{q}_r} iq_y E_{qz}\xi_{-\mathbf{q}}. \quad (22)$$

Substitution of (20) into (21) eliminates the nonresonant fields from the system (20)–(22). The resulting expressions are

$$E_{q_r z} = -\Big\{[k_z k_{q_r x}(E_{ix}-E_{0x}) + (k_t - k_{q_r y})(E_{iz}+E_{0z})k_0^2/k_t]\xi_{\mathbf{q}_r} + \sum_{\mathbf{q}_r'}\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_r'})E_{q_r' z}\xi_{\mathbf{q}_r-\mathbf{q}_r'}\Big\}\Big/k_0 T_{q_r}, \quad (23)$$

where

$$T_{q_r} = \frac{\Gamma_{q_r}}{k_0} + \frac{\gamma}{\varepsilon k_0} - \sum_{\mathbf{k}_{q_n}}\frac{(\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n}))^2}{k_0\Gamma_{q_n}}|\xi_{\mathbf{q}_r-\mathbf{q}_n}|^2.$$

The system (22), (23) is the foundation for further analysis. If deviations from the Fresnel equations are significant, the solution of (22), (23) completely determines the amplitudes of the fields $\mathbf{E}_0$, E_{qrz}. The dimension of this system is finite, and is related to the number of resonant fields. After the amplitudes of $\mathbf{E}_0$ and E_{qrz} are found, the amplitudes $\mathbf{E}_{qn}$ of the nonresonant fields and the components E_{qrx}, E_{qry} of the resonant fields are calculated using Eqs. (20) and (14). When the deviations from the Fresnel equations are minor (which is also possible when there are resonant gratings with large $|\xi_{\mathbf{qr}}|$), the amplitudes of the fields $\mathbf{E}$, $\mathbf{E}_{qr}$, $\mathbf{E}_{qn}$, are obtained from (13), (14) by perturbation methods, where as the zeroth-order approximation, we use the amplitudes $\mathbf{E}_0$, E_{qrz} found by solving the system (22), (23). The proposed method is analogous to the perturbation approach employed in quantum mechanics when there is degeneracy in the levels.[34]

C. The relationship between the field amplitudes in vacuum and in the medium

Assume that the field distribution in vacuum is known. We now express the field amplitudes in the medium in terms of the vacuum field amplitudes. With $|\varepsilon| \gg 1$, it follows from Eqs. (5) and (7) that the field $\mathbf{E}'(\omega)$ inside the medium is determined by the value $\mathbf{E}'(\omega)|_{z=f}$ at the boundary:

$$\mathbf{E}'(\omega) = \exp[-\gamma(z-f)]\mathbf{E}'(\omega)|_{z=f}. \quad (24)$$

If we make use of Eqs. (8) and (9) to express the field $\mathbf{E}'(\omega)|_{z=f}$ in (24) in terms of the field $\mathbf{H}(\omega)|_{z=f}$, we find that

$$E_x'(\omega) = -\exp[-\gamma(z-f)]ik_0 H_y(\omega)|_{z=f}/\gamma,$$
$$E_y'(\omega) = \exp[-\gamma(z-f)]ik_0 H_x(\omega)|_{z=f}/\gamma. \quad (25)$$

In these equations, we can express the field $\mathbf{H}(\omega)|_{z=f}$ in terms of the field $\mathbf{E}(\omega)|_{z=f}$ using $ik_0\mathbf{H}(\omega) = \operatorname{curl}\mathbf{E}(\omega)$. The expressions obtained in this way may be represented in the form

$$E_x'(\omega) = \exp[-\gamma(z-f)]\sum_{\mathbf{q}}\varphi_q\exp(i\mathbf{k}_q\mathbf{r}),$$

$$E_y'(\omega) = \exp[-\gamma(z-f)]\sum_{\mathbf{q}}\psi_q\exp(i\mathbf{k}_q\mathbf{r}), \quad (26)$$

where

$$\varphi_0 = ik_z(E_{0x}-E_{ix})/\gamma, \quad \varphi_q(\mathbf{q}\neq 0) = (ik_{qx}E_{qz} - \Gamma_q E_{qx})/\gamma,$$
$$\psi_0 = ik_0^2(E_{0z}+E_{iz})/\gamma k_t, \quad \psi_q(\mathbf{q}\neq 0) = (ik_{qy}E_{qz} - \Gamma_q E_{qy})/\gamma.$$

The equations (26), taken together with the condition div $\mathbf{E}'(\omega) = 0$, completely determine the field amplitudes in the medium if the vacuum field distribution is known.

The difficulty involved in analyzing Eqs. (22) and (23) is that one encounters such a multitude of different situations when the surface relief is arbitrary. The amplitudes of the diffracted fields depend sensitively on the angle of incidence and the polarization of the radiation, on the mutual orientation and magnitudes of the vectors $\mathbf{k}_0$ and $\mathbf{g}_i$, on the magnitudes of the amplitudes $\xi_{\mathbf{g}_i}$, and on the number of resonant fields. We next go on to discuss with specific examples some of the general features of mutual interaction between the gratings and the field distribution in vacuum.

D. Analytic expressions for the amplitudes of diffracted fields in vacuum for p-polarized incident radiation

Consider the case (which fairly well takes in the typical features of the field distribution in vacuum) in which there is one resonant field and several non-resonant ones. Let the incident radiation be p-polarized ($E_{ix} = 0$, $E_{iz} \neq 0$), and let $\mathbf{g}_r \| \mathbf{k}_t$ (see Fig. 1). Then from Eqs. (20), (22), and (23), we find ($\cos\theta \gg 1/|\varepsilon|^{1/2}$, $|\varepsilon\Gamma_{qn}| \gg |\gamma|$)

$$E_{0x}=0, \quad E_{0y}=\frac{k_z}{k_t}E_{0z},$$

$$E_{0z}=\frac{\varepsilon k_z-i\gamma}{\varepsilon k_z+i\gamma}\left\{1+\frac{2i}{\cos\theta}\frac{|g_r\xi_{g_r}|^2}{\Delta}\right\}E_{iz},$$

$$E_{q_rx}=0, \quad E_{q_ry}=i\Gamma_{q_r}E_{q_rz}/k_{q_ry}, \quad E_{q_rz}=2g_r\xi_{g_r}E_{i0}/\Delta,$$

$$E_{q_nx}=-ik_{q_nx}[(E_{iz}+E_{0z})\xi_{q_n}+E_{q_rz}\xi_{q_n-q_r}], \qquad (27)$$

$$E_{q_ny}=(-k_{q_nx}E_{q_nx}+i\Gamma_{q_n}E_{q_nz})/k_{q_ny},$$

$$E_{q_nz}=\left\{\frac{k_{q_ny}k_0^2-k_tk_{q_n}^2}{k_t}(E_{iz}+E_{0z})\xi_{q_n}-\mathbf{k}_{q_n}(\mathbf{k}_{q_n}-\mathbf{k}_{q_r})E_{q_rz}\xi_{q_n-q_r}\right\}\Big/\Gamma_{q_n},$$

where

$$E_{i0}=k_0E_{iz}/k_t, \quad \mathbf{k}_{q_r}=\mathbf{k}_t-\mathbf{g}_r,$$

$$\Delta=\frac{\Gamma_{q_r}}{k_0}+\frac{\gamma}{\varepsilon k_0}-\sum_{\mathbf{k}_{q_n}}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0\Gamma_{q_n}}|\xi_{q_r-q_n}|^2-i\frac{|g_r\xi_{g_r}|^2}{\cos\theta}, \quad \Gamma_{q_r}^2=k_{q_r}^2-k_0^2.$$

When $\mathbf{E}_{qr}$ is a surface wave ($k_{qr} > k_0$), we have ($\Delta = \mathrm{Re}\,\Delta - i\,\mathrm{Im}\,\Delta$)

$$\mathrm{Re}\,\Delta=[(\sin\theta+g_r/k_0)^2-1]^{1/2}-\frac{m}{m^2+n^2}-\sum_{k_{q_n}>k_0}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0\Gamma_{q_n}}|\xi_{q_r-q_n}|^2,$$

$$\mathrm{Im}\,\Delta=\frac{n}{m^2+n^2}+\sum_{k_{q_n}<k_0}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0|\Gamma_{q_n}|}|\xi_{q_r-q_n}|^2+|g_r\xi_{g_r}|^2/\cos\theta. \qquad (28)$$

It can be seen from Eqs. (27) and (28) that the amplitudes of the diffracted fields are nonmonotonic functions of the amplitudes $\xi_{\mathbf{g}_r}$ and $\xi_{\mathbf{g}_j}$ of the relief, and are determined by the magnitude of the resonant denominator Δ. The last term in

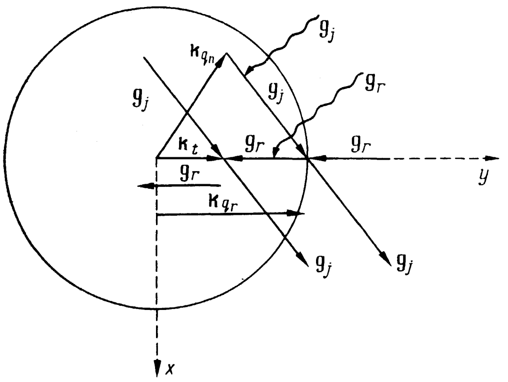

FIG. 1. Mutual orientation of the vector $\mathbf{k}_t$ of an incident field, the vector $\mathbf{g}_r$ of a resonant grating, and the vectors $\mathbf{g}_j$ ($j = 1,2,...$) of nonresonant gratings. The radius of the circle is approximately k_0. The vector $\mathbf{k}_{qr} = \mathbf{k}_t - \mathbf{g}_r$ corresponds to the resonant wave $\mathbf{E}_{qr}$; the vectors $\mathbf{k}_{qn} = \mathbf{k}_t \pm \mathbf{g}_j$, $\mathbf{k}_t - \mathbf{g}_r \pm \mathbf{g}_j$, $\mathbf{k}_t + \mathbf{g}_r$, and $\mathbf{k}_t - 2\mathbf{g}_r$ correspond to nonresonant diffracted waves $\mathbf{E}_{qn}$.

the expression for Δ results from cross-scattering between the fields $\mathbf{E}_0$ and $\mathbf{E}_{qr}$ at the grating $\mathbf{g}_r$. The third term in Δ comes from cross-scattering between the fields $\mathbf{E}_{qr}$ and $\mathbf{E}_{qn}$ at the gratings $\mathbf{g}_r$ and $\mathbf{g}_j$ (the summation in this term is to be carried out over the nonresonant waves $\mathbf{E}_{qn}$ with $\mathbf{k}_{qn} = \mathbf{k}_t - 2\mathbf{g}_r$, $\mathbf{k}_t - \mathbf{g}_r \pm \mathbf{g}_j$ (see Fig. 1)). Depending on the type of wave (a wave $\mathbf{E}_{qn}$ is a nonradiating surface wave if $k_{qn} > k_0$, with $\Gamma_{qn} > 0$; it is a radiating, detached wave if $k_{qn} < k_0$, with $\mathrm{Im}\,\Gamma_{qn} < 0$), the corresponding cross-scattering makes a contribution to the real or imaginary part of the resonant denominator Δ. It is clear from (27) that the condition $\mathrm{Re}\,\Delta = 0$ determines the maximum value of the field $\mathbf{E}_{qr}$ for given amplitudes $\xi_{\mathbf{g}_r}$, $\xi_{\mathbf{g}_j}$ of the surface gratings, and is the dispersion relation for the resonant wave $\mathbf{E}_{qr}$. For the case of an s-polarized incident wave ($E_{ix} \neq 0$, $E_{iz} = 0$) and $\mathbf{g}_r \perp \mathbf{k}_t$, it is easy to find expressions analogous to (27) from (20), (22), and (23).

4. INTERACTION OF DIFFRACTED WAVES AND WOOD'S ANOMALY

The strong dependence of the amplitudes of the diffracted fields (26), (27) on λ and θ (Wood's anomaly) shows up in a great many effects, some of which we now consider.

A. Total suppression of specular reflection

Making use of Eqs. (27) for the specular reflection coefficient $R_0 = |\mathbf{E}_0|^2/|\mathbf{E}_i|^2$, we have

$$R_0=\left|\frac{\varepsilon k_z-i\gamma}{\varepsilon k_z+i\gamma}\right|^2\left\{1-4\frac{|g_r\xi_{g_r}|^2}{\cos\theta}\left[\frac{n}{m^2+n^2}+\sum_{k_{q_n}<k_0}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0|\Gamma_{q_n}|}|\xi_{q_r-q_n}|^2\right]\Big/[(\mathrm{Re}\,\Delta)^2+(\mathrm{Im}\,\Delta)^2]\right\}, \qquad (29)$$

where $\mathrm{Re}\,\Delta$ and $\mathrm{Im}\,\Delta$ are given by (28). It is easy to see from (29) that R_0 attains its minimum value when $\mathrm{Re}\,\Delta = 0$. An analysis of Eqs. (27)–(29) shows that for nonmonochromatic relief, with nonresonant gratings present in addition to resonant ones, TSSR ($E_{0x} = E_{0y} = E_{0z} = 0$) occurs for p-polarized incident radiation ($k_{qr} > k_0$) when

$$\mathrm{Re}\,\Delta=0,$$

$$\frac{n}{m^2+n^2}+\sum_{k_{q_n}<k_0}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0|\Gamma_{q_n}|}|\xi_{\mathbf{q}_r-\mathbf{q}_n}|^2=\frac{|g_r\xi_{\mathbf{g}_r}|^2}{\cos\theta}. \quad (30)$$

$\mathbf{E}_{qr}$ then corresponds to a surface wave. For given $\mathbf{g}_j$, $\xi_{\mathbf{g}_j}$, $\mathbf{g}_r$, and k_0, Eq. (30) determines the optimum amplitude $|\xi_{\mathbf{g}_r}|$ and optimum angle of incidence θ of p-polarized radiation, as required to exhibit TSSR. When cross-scattering between the fields $\mathbf{E}_{qr}$ and $\mathbf{E}_{qn}$ is neglected, Eq. (30) is transformed into the corresponding expressions of Refs. 15–17 for sinusoidal relief. Figure 2 shows qualitatively the θ-dependence of R_0 corresponding to Eqs. (29) and (28). It can be seen from Fig. 2 that, compared with sinusoidal relief, the presence of additional gratings which scatter the field $\mathbf{E}_{qr}$ into surface waves $\mathbf{E}_{qn}$ results (for fixed $\xi_{\mathbf{g}_r}$) in a change in the optimum angle θ at which R_0 is minimized, and the presence of gratings which scatter the field $\mathbf{E}_{qr}$ into radiation fields $\mathbf{E}_{qn}$ changes θ, reduces the depth, and increases the width of the dip in $R_0(\theta)$.

A question which then arises is what types of surface relief make total suppression of specular reflection possible, and which do not. The answer is that if the shape of the src relief is specified, and only the depth h of the relief can be changed, then there exists a relation

$$\xi_{\mathbf{q}-\mathbf{q}'}=a_{\mathbf{q}-\mathbf{q}'}\xi_{\mathbf{g}_r}, \quad (31)$$

where the coefficients $a_{\mathbf{q}-\mathbf{q}'}$ are determined by the shape of the relief. With this in mind, the requisite conditions for TSSR take the form

$$\mathrm{Re}\,\Delta=[(\sin\theta+g_r/k_0)^2-1]^{1/2}-\frac{m}{m^2+n^2}-\sum_{k_{q_n}>k}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0\Gamma_{q_n}}|a_{\mathbf{q}_r-\mathbf{q}_n}|^2\times|\xi_{\mathbf{g}_r}|^2=0,$$

$$\frac{n}{m^2+n^2}=\left\{\frac{g_r^2}{\cos\theta}-\sum_{k_{q_n}<k_0}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0|\Gamma_{q_n}|}|a_{\mathbf{q}_r-\mathbf{q}_n}|^2\right\}|\xi_{\mathbf{g}_r}|^2. \quad (32)$$

Since $k_0^2 f^2 x,y)\ll 1$, as can be seen from the first equality in (32), if TSSR is possible, then it is only so in over a small range of angles $\theta\gtrsim\arcsin\{-g_r/k_0+[1+m^2/(m^2+n^2)^2]^{1/2}\}$. If there are in the spectrum of the relief gratings which scatter the field $\mathbf{E}_{qr}$ into radiation waves, such that over this range of angles the expression in curly brackets in the second equality in (32) is negative, then for the given shape of the surface relief, TSSR is impossible at any angle of incidence θ or depth h.

Using Eqs. (29) and (28), a method of determining the optical constants m and n of a material with a nonplanar surface can be developed, based on the experimentally measured location and depth of the dip in $R_0(\theta)$.

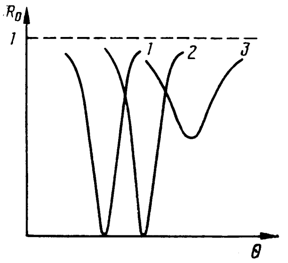

FIG. 2. θ-dependences of R_0 based on Eqs. (27)–(29) for fixed amplitude $\xi_{\mathbf{g}_r}$. Curve 1 is for sinusoidal relief with the optimum value of $\xi_{\mathbf{g}_r}$ (see condition (30)); curve 2 is for nonmonochromatic relief. The parameters of the resonant grating are the same as for curve 1, but with additional nonresonant gratings with amplitudes $\xi_{\mathbf{g}_j}$ which scatter the resonant wave $\mathbf{E}_{qr}$ into surface waves $\mathbf{E}_{qn}$. Curve 3 is for the resonant grating corresponding to curve 1, with additional nonresonant gratings which scatter the wave $\mathbf{E}_{qr}$ into radiation fields $\mathbf{E}_{qn}$.

B. Possibility of controlling the reflection of light

Let us calculate the coefficient η_{qn} for conversion of energy of the incident field $\mathbf{E}_i$ into energy of the vacuum radiation field $\mathbf{E}_{qn}$. From Eqs. (27) and (28), we find

$$\eta_{q_n}\equiv\frac{|\Gamma_{q_n}||\mathbf{E}_{q_n}|^2}{k_z|\mathbf{E}_i|^2}=4x_{q_r}y_{q_n}\Big/\left\{\left(\frac{m^2+n^2}{n}\mathrm{Re}\,\Delta\right)^2+\left(1+x_{q_r}+\sum_{k_{q_n}<k_0}y_{q_n}\right)^2\right\} \quad (33)$$

$$x_{q_r}=\frac{m^2+n^2}{n}\frac{|g_r\xi_{\mathbf{g}_r}|^2}{\cos\theta},$$

$$y_{q_n}=\frac{m^2+n^2}{n}\frac{[\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n})]^2}{k_0|\Gamma_{q_n}|}|\xi_{\mathbf{q}_r-\mathbf{q}_n}|^2.$$

Now let there be only a single radiation field $\mathbf{E}_{qn}$ (i.e., apart from the resonant grating, there is only a single nonresonant grating $\mathbf{g}_j$ in the relief spectrum, scattering the wave $\mathbf{E}_{qr}$ into the wave $\mathbf{E}_{qn}$). The simplest example of such a surface is one consisting of only two gratings, with each of the values $|\mathbf{k}_t-\mathbf{g}_r\pm\mathbf{g}_j|<k_0$ (see Figs. 1,3). Then when $\mathrm{Re}\,\Delta=0$, Eq. (33) takes the form

$$\eta_{q_n}=4x_{q_r}y_{q_n}/(1+x_{q_r}+y_{q_n})^2.$$

In order for the coefficient η_{qn} to be a maximum at fixed y_{qn}, it is necessary that $x_{qr}=1+y_{qn}$, which corresponds to the second condition in (30). Then

$$\eta_{q_n}=y_{q_n}/(1+y_{q_n}). \quad (34)$$

Equation (34) implies that $\eta_{qn}<1$, and that it tends to unity as $y_{qn}\to\infty$ (this is possible when $|\varepsilon|\gg 1$). We then have $|\mathbf{E}_{q\text{-}r}|^2\approx|\mathbf{E}_{i0}|^2(m^2+n^2)/n(1+y_{qn})$. Thus, when the conditions (30) for TSSR are met, the energy of the incident field is redistributed among the fields $\mathbf{E}_{qr}$ and $\mathbf{E}_{qn}$, and as $y_{qn}\to\infty$, it is practically entirely transformed into energy of the radiation field $\mathbf{E}_{qn}$, which propagates in a direction other than that of specular reflection (see Fig. 3).

We see from the foregoing discussion that by dynamically varying the surface relief (for example, by exciting surface acoustic waves), it is possible to control the direction of a beam reflected into the vacuum, with a high transmission coefficient for energy coming from the incident field.

When there are two gratings on the surface, with vectors $\mathbf{g}_r\|\mathbf{k}_t$ and $\mathbf{g}_j=2\mathbf{g}_r$ (see Fig. 1), there are two contributions to the non-resonant field $\mathbf{E}_{\mathbf{k}_t+\mathbf{g}_r}$: the first is due to scattering of the incident field $\mathbf{E}_i$ and the zero-order diffraction field $\mathbf{E}_0$ by the grating $\mathbf{g}_r$, and the second is due to scattering of the resonant field $\mathbf{E}_{qr}$ by the grating $2\mathbf{g}_r$. Interference

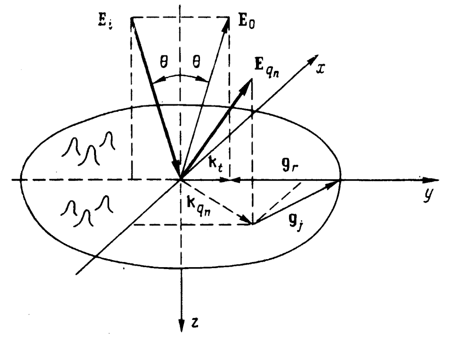

FIG. 3. Conversion of energy of the incident field $\mathbf{E}_i$ into energy of the vacuum radiation field $\mathbf{E}_{qn}$. Heavy arrows indicate the direction of propagation of the incident wave and the wave $\mathbf{E}_{qn}$. The radius of the circle is approximately k_0.

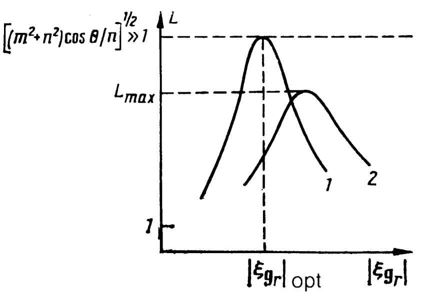

FIG. 5. Dependence of the local field-amplification factor L on $|\xi_{\mathbf{g}_r}|$ at optimum θ (see (30)) for the case of nonmonochromatic relief. 1) Relief for which nonresonant gratings do not scatter the resonant field $\mathbf{E}_{qr}$ into radiation fields; 2) the relief spectrum contains nonresonant gratings which do scatter the fields $\mathbf{E}_{qr}$ into radiation fields $\mathbf{E}_{qn}$.

between these two contributions leads to the Wood anomaly for the coefficients $\eta_{\mathbf{k}_t+\mathbf{g}_r}$. The θ-dependence of $\eta_{\mathbf{k}_t+\mathbf{g}_r}$ (see (27), (28)), as shown in Fig. 4, is qualitatively consistent with the experimental and numerical results in Ref. 33. The high sensitivity of $\eta_{\mathbf{k}_t+\mathbf{g}_r}$ to the phase and amplitude relations between harmonics of the surface relief (see Fig. 4) can be exploited to reconstruct the actual surface profile.[33]

C. Local fields near a surface with arbitrary profile

We now calculate the maximum attainable local fields near a rough surface. We define a local-field augmentation factor $L = |\mathbf{E}(\omega)|/|\mathbf{E}_i|$, where $\mathbf{E}(\omega)$ has been defined in (4). An analysis of Eqs. (27) and (28) shows that L is maximized under conditions for which $\mathbf{E}_{qr}$ is resonant ($k_{qr} \approx k_0$). Since near resonance, the amplitude $|E_{qrz}|$ of the resonant field is much greater than that of any other diffracted field (see (27), (26)), we have

$$L \approx |E_{qrz}|/|\mathbf{E}_i| = 2|g_r \xi_{\mathbf{g}r}|/[(\mathrm{Re}\,\Delta)^2 + (\mathrm{Im}\,\Delta)^2]^{1/2}. \qquad (35)$$

For fixed $\xi_{\mathbf{g}_j}$, the amplitude ratio (35) increases with increasing $|\xi_{\mathbf{g}_r}|$, reaches a maximum for some value of $|\xi_{\mathbf{g}_r}|$, and then decreases as $|\xi_{\mathbf{g}_j}|$ increases still more. It is easily seen that (35) reaches its maximum when (30) is satisfied, i.e., under conditions supporting TSSR; the maximum value

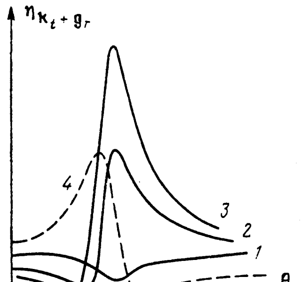

FIG. 4. Behavior of the conversion coefficient $\eta_{\mathbf{k}_t+\mathbf{g}_r}$ for energy in the incident field $\mathbf{E}_i$ into energy in the wave $\mathbf{E}_{\mathbf{k}_t+\mathbf{g}_r}$ as a function of the surface relief $z = 2\xi_{\mathbf{g}_r}\cos(g_r y) + 2\xi_{2\mathbf{g}_r}\cos(2g_r y)$, at fixed amplitude $\xi_{\mathbf{g}_r} > 0$ and for various values of $\xi_{\mathbf{g}_r}$:

1) $\xi^{(1)}_{2\mathbf{g}_r} = 0$; 2 – 4) $\xi^{(3)}_{2\mathbf{g}_r} > \xi^{(2)}_{2\mathbf{g}_r} = -\xi^{(4)}_{2\mathbf{g}_r}$.

is

$$L \approx \left(\frac{|\mathbf{E}_{q_r z}|}{|\mathbf{E}_i|}\right)_{max} = \left\{\cos\theta \Big/ \left[\frac{n}{m^2+n^2} + \sum_{k_{q_n}<k_0} \frac{(\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n}))^2}{k_0|\Gamma_{q_n}|}\,|\xi_{q_r-q_n}|^2\right]\right\}^{1/2}. \qquad (36)$$

It is clear from (36) that when $|\varepsilon| \gg 1$ (then $n/(m^2+n^2 \ll 1$ for both metals and dielectrics) and $|\xi_{\mathbf{g}_j}|$ is small, the factor $L \gg 1$. For example, when one illuminates a silvered sinusoidal grating of period $d = 1.4\,\mu$m with light having a wavelength $\lambda = 1\,\mu$m ($\varepsilon = (0.129 + i\cdot 6.83)^2$, Ref. 35), the maximum of L, according to (30) and (36), occurs at $\theta = 17.24°$ and $4|\xi_{\mathbf{g}_r}| = 0.0046\,\mu$m, and is equal to 18.6. Since $I_{SHRS}/I_{RS} \sim L^4$ (Ref. 6), where I_{SHRS} is the intensity of surface enhanced Raman scattering from molecules adsorbed on the surface, and I_{RS} is the Raman scattering intensity from the same molecules at a distance from the surface, it is to be expected that for the sinusoidal grating in under consideration, $I_{SHRS}/I_{RS} = 1.2\cdot 10^5$. A similar enhancement associated with the increase in L should also occur for other linear and nonlineaar optical effects at the surface. This is quite important for the development of spectroscopic methods for small numbers of molecules adsorbed on a rough surface. The qualitative dependence of L on $|\xi_{\mathbf{g}_r}|$ predicted by Eqs. (35) and (36) is shown in Fig. 5.

We see from Eq. (36) that compared with a sinusoidal grating, the maximum value of L decreases with increasing $|\xi_{\mathbf{g}_j}|$ and with an increasing number of gratings $\mathbf{g}_j$ scattering the field $\mathbf{E}_{qr}$ into radiation fields (see Fig. 5). If only nonresonant gratings are present in the spectrum of the relief (so that only nonresonant surface waves $\mathbf{E}_{qn}$ ($k_{qn} > k_0$) result from scattering of the field $\mathbf{E}_{qr}$), the optimum amplitude $|\xi_{\mathbf{g}_r}|$ and maximum L take on almost the same values as for a pure sinusoidal grating with $\mathbf{g} = \mathbf{g}_r$ (see Fig. 5). The minor difference between the quantities is due to the change in the optimum angle θ (see condition (30), $\mathrm{Re}\,\Delta = 0$). The fact of the decrease in the local field in the presence of an additional nonresonant grating is discussed in Ref. 20 phenomenologically.

If the shape of the surface relief is given, then in accordance with (31), (27), and (26), the maximum amplification L of the local field occurs when

$$\mathrm{Re}\,\Delta=0,\quad \frac{n}{m^2+n^2}=\left\{\sum_{k_{q_n}<k_0}\frac{(\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n}))^2}{k_0|\Gamma_{q_n}|}|a_{\mathbf{q}_r-\mathbf{q}_n}|^2+\frac{g_r^{\,2}}{\cos\theta}\right\}|\xi_{g_r}|^2 \tag{37}$$

and is equal to

$$L=\left\{\frac{m^2+n^2}{n}\cos\theta\Big/\left[1+\sum_{k_{q_n}<k_0}\frac{(\mathbf{k}_{q_r}(\mathbf{k}_{q_r}-\mathbf{k}_{q_n}))^2\cos\theta}{k_0|\Gamma_{q_n}|g_r^{\,2}}|a_{\mathbf{q}_r-\mathbf{q}_n}|^2\right]\right\}^{1/2}. \tag{38}$$

Clearly, then, the optimum θ and ξ_{g_r} (and consequently the optimum overall depth of the surface relief) and the maximum value of L are sensitive functions of the shape of the surface profile, and can differ significantly from the corresponding values for a sinusoidal profile.

It can be seen from a comparison of the second expression in (37) and the second expression in (32) that when the shape of the surface relief is fixed, the amplitude $|\xi_{g_r}|$ of a resonant grating (and thus the overall depth h of the surface relief) for which $L=L_{\max}$ is lower than the corresponding value for which $R_0=(R_0)_{\min}$. We can account for this by noting that as the depth h of the relief increases, scattering of the field $\mathbf{E}_0$ into the field $\mathbf{E}_{qr}$ dominates at first; for further increases in h, the scattering of $\mathbf{E}_{qr}$ into radiation fields $\mathbf{E}_{qn}$ becomes important, which then reduces the amplitude of the local field.

D. Anomalously high absorption of light by a rough surface

Up to this point, we have dealt with vacuum fields. We now consider whether the presence of both resonant and non-resonant gratings in the spatial Fourier spectrum of a surface has any effect on the absorption factor A of a rough surface, which is determined by the fields in the medium. We can calculate the absorption factor using the relation $A=\overline{S_z'/S_{iz}}$, where $S_z'=c\,(\mathbf{E}'\times\mathbf{H}')/4\pi$ is the z-component of the Poynting vector in the medium, S_{iz} is the z-component of the Poynting vector for the incident radiation, and $\mathbf{E}'$ is the field in the medium (see (5)). The superior bar denotes averaging over time and over x, and y. For $|\varepsilon|\gg1$, we have from (27) and (26)

$$A=\frac{4n}{(m^2+n^2)\cos\theta}\left\{1+\frac{|g_r\xi_{g_r}|^2}{(\mathrm{Re}\,\Delta)^2+(\mathrm{Im}\,\Delta)^2}\right\}, \tag{39}$$

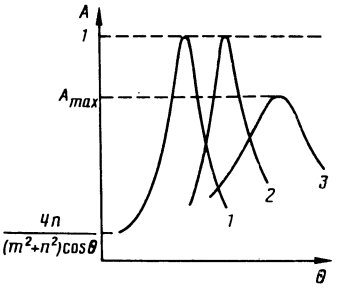

FIG. 6. Dependence of A on θ for fixed amplitude ξ_{g_r}, according to Eq. (39). Curve 1 is for sinusoidal relief with the optimum value of ξ_{g_r}; for curve 2, the surface relief is a superposition of a resonant grating (with the same parameters as for curve 1) and nonresonant gratings, which scatter the field $\mathbf{E}_{qr}$ into the surface fields $\mathbf{E}_{qn}$; for curve 3, we have supplemented a resonant grating with the same parameters as for curve 1 with nonresonant gratings which scatter the field $\mathbf{E}_{qr}$ into the radiation fields $\mathbf{E}_{qn}$.

where Re Δ and Im Δ are defined in (27), (28). The factor preceding the curly brackets in Eq. (39) represents the absorption factor ($A\ll1$) for a plane surface, with $|\varepsilon|\gg1$ and p-polarized incident radiation.[36] If the ξ_{g_j} are fixed, the optimum values of θ and $|\xi_{g_r}|$ (the optimal surface relief) will be given by (30), i.e., by the conditions required for TSSR. Then A will reach a maximum value equal to

$$A=\frac{4n}{(m^2+n^2)\cos\theta}\left\{1+\frac{L^2}{4}\right\}, \tag{40}$$

where the factor L is defined in (36). If in fact we are given the shape of the surface profile (see section 4C), the optimal relief will be defined by (37). The maximum of A is then determined by Eq. (40), in which L is given by Eq. (38). We have plotted the θ-dependence of A from (39) in Fig. 6. If the surface relief is optimal (i.e., an angle $\theta_{\rm opt}$ exists for which either (30) or (37) holds), and no fields $\mathbf{E}_{qr}$ are reradiated into the vacuum, then $A_{\max}=1$ (see Fig. 6). If there is reradiation of $\mathbf{E}_{qr}$ into vacuum radiation fields, then $A_{\max}<1$. This qualitatively distinguishes between nonmonochromatic and sinusoidal profiles. If the relief is actually not optimal, then $A_{\max}<1$ always. Such behavior of A as a function of θ is consistent with experimental research reported in Ref. 19, in which there was a fivefold enhancement of absorption in a duraluminum grating with $d=13.6\ \mu$m illuminated with radiation at a wavelength $\lambda=10.6\,\mu$m. Thus, the application of a surface profile with $\overline{f^2}\ll\lambda$ can significantly enhance absorption, up to a value of unity, by an initially highly reflecting plane surface.

5. CONCLUSION

We now wish to reemphasize the main ideas, based on an analytic solution for the diffraction of light from a rough surface having an arbitrary deep profile. For maximum clarity, we use the example of a sinusoidal grating with vector $\mathbf{g}$.

1) When $|\varepsilon|\gg1$ and $k_0^2f^2(x,y)\ll1$, the exact boundary conditions (2) can be replaced by the approximate boundary conditions (10), containing only the fields in vacuum. We thereby obtain an infinite set of linear algebraic equations in the amplitudes of the vacuum fields.

2) Since $k_0^2f^2(x,y)\ll1$, we can limit our attention in this system to fields $\mathbf{E}_q$ of low diffraction order, with $\mathbf{k}_q=\mathbf{k}_t,\mathbf{k}_t\pm\mathbf{g}$, and $\mathbf{k}_t\pm2\mathbf{g}$. This leads to a system of 15 algebraic equations, which cannot in general be solved analytically.

3) The presence of resonant fields makes it possible to eliminate nonresonant fields from this system. As a result, we arrive at a system of equations solely for the amplitudes of the zero diffraction order fields $\mathbf{E}_0$ and the E_{qrz} of the resonant fields ($|E_{qrx}|\gg|E_{qrx}|$, $|E_{qry}|$), which takes into ac-

count cross-scattering between zeroth-, and second-order diffraction fields.

4) When there is only a single resonant field $\mathbf{E}_{qr}$ ($k_{qr} \approx k_0$), the system of three linear algebraic equations for the amplitudes E_{0x}, E_{0z} ($E_{0y} = k_z E_{0z}/k_t$), and E_{qrz} permits of a simple, compact analytic solution. The technique for obtaining an analytic solution when the surface relief is comprised of many gratings is similar.

A detailed comparison of the analytic results with experimental and numerical results for a sinusoidal profile (see Refs. 16, 17, and 21), and for a profile composed of two gratings (see section 4B of the present paper, and Ref. 33), shows that both qualitative and quantitative agreement are good. The accuracy of the method improves with increasing $|\varepsilon|$. For fairly small values of $|\varepsilon|$ ($|\varepsilon| \lesssim 10$), we have qualitative agreement. In order to obtain good quantitative agreement, subsequent corrections to the field amplitudes, of order $|\varepsilon|^{-1/2}$, must be taken into account. This has been done by the authors. The equations obtained for the amplitudes of the diffracted fields are reasonably simple, but of a somewhat more involved form (compared with the analytic results in the present paper).

The approach described here enables one to formulate regular methods for the solution of new problems dealing with the diffraction of light from a surface. Among these, problems of special interest include the following.

Firstly, when considering the statistics of surface irregularities, the present approach can serve as a foundation for further development of the theory of light scattering from a rough surface with a fairly high-profile modulation amplitude, which would take resonant scattering channels into consideration.

Secondly, the nonlinear (in the profile modulation amplitude) theory of light diffraction can be used to describe the nonlinear regime in the production of periodic structures of complex form, localized cavities, protruberances, and so on, by high-power radiation at a surface.

Thirdly, effects similar to those considered here should also show up at a planar surface with spatially modulated dielectric constant $\varepsilon = \varepsilon_0 + \varepsilon_1(x,y,z)$ ($|\varepsilon| \gg 1$). When ε depends nonlinearly on the field $\mathbf{E}$, one would expect to see optical bistability effects, such as a hysteretic dependence of the reflected signal on the intensity of the signal incident at the surface. There is also a great deal of interest in the possibility of controlling the reflection and absorption properties of a surface via external radiation.

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