Scattering of electromagnetic beams from rough surfaces

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In this paper a formalism, which leads to the exact solution of the scattering of beams of finite cross section from an arbitrary rough surface, is presented. With use of the Green theorem, a rigorous integral equation is obtained for the case where the wavelength of the incident radiation is comparable to the dimensions of the surface roughness (resonance region). Furthermore, a new explicit solution for the amplitude of the scattered field is introduced, which reduces to known expressions when the rough surface tends to a smooth surface and the beam is replaced by a plane wave. The explicit solution is applied to the particular case of gratings. Additionally, reciprocity relations for thick slit apertures in a rough-surface screen are obtained. These results are expected to be especially useful for calculating the electromagnetic field enhancement (*s* polarization) near rough surfaces and for the scattering of light atoms by nonperfect periodic hard surfaces.

I. INTRODUCTION

Diffraction by hard or perfectly conducting rough surfaces[1] has attracted considerable attention in recent years. For instance, in acoustics these hard surfaces are very interesting because they represent a realistic situation (perfectly soft[2,3] or perfectly rigid[4] surfaces).

In optics, several theories have been proposed for the scattering of electromagnetic waves by perfectly conducting rough surfaces: approximate theories[5–8] for shallow surfaces and rigorous theories[6–9] for arbitrary profiles. In the latter case, due to computer size limitations, the length of the modulated region must not exceed some wavelengths ($\sim 10\lambda$). The phenomenon of "short coupling range" in the resonance region (where the wavelength and the roughness dimension have the same order of magnitude) has been shown.[6,9] This phenomenon allows us to make a rigorous computation of the field scattered from a modulated region of arbitrary width. Besides, problems of inverse diffraction have been solved[10,11] (that of finding the surface profile from the diffraction pattern) showing the limit of resolution in the resonance region. Grating theories[12] have been compared extensively with experiments but scarcely for the case of nonperiodic surfaces.[13] The reader can find reviews of diffraction by rough surfaces in Van den Berg,[14] Baltes and Huiser,[15] Maystre,[16] Mata and Halevi,[17] and Maradudin.[18]

On the other hand, during the last few years in solid state physics, great interest has grown regarding the relationship between Raman scattering and surface polaritons. This relationship is a very important one in the utilization of surface-polariton Raman scattering as a probe of the characteristics of surfaces and interfaces.[19,20] Ushioda[21] experimentally found that the surface roughness increased the Raman-scattering intensity relative to that scattered by a smooth surface. He also noted that, due to the fact that the incident wave was a beam of finite cross section, the intensity varied from spot to spot on a given sample. In other words, the Raman-scattering intensity of surface polaritons depended on that part of the surface that the incident laser beam struck.

Reinish and Neviere[22,23] suggested a qualitative explanation of part of Ushioda's results. They used a linear theory for the excitation of surface polaritons along a grating, when the incident field was a plane wave. The existence of an optimal groove depth of the grating, for which the surface-plasmon contribution to surface-enhanced Raman scattering is the strongest, was shown numerically in Refs. 22–26. Reinish and Neviere recognized that such a theory could not be used for quantitative comparison between their results and the corresponding ones by Ushioda, since this would require a nonlinear theory with a rough random surface and a beam of finite cross section. Later, they treated the problem of incident plane waves on a grating ruled on a nonlinear medium[27–29] of arbitrary periodic profile. They found the important result[27] that the dependence of the surface polariton intensity on the groove depth, of the nonlinear calculation, was very similar to that found in the case of linear excitation.

Recently, considerable interest has been placed on the study of fields near irregularities, as a way of getting an estimate for the expected surface-enhanced Raman scattering (SERS). From a theoretical point of view it was found that the ratio $G = |E/E_0|^2$ (where E is the electric field near the surface and E_0 is the electric incident field) depends on the material used[30] and that this ratio for gratings is greater than that of smooth surfaces.[25,26] The field enhancement of several particular configurations has been theoretically analyzed: hemispherical bump,[30] square-wave grating,[31] bigrating sinusoidal,[32] and gratings of sawtooth profiles.[25,26]

Contrary to the case of gratings, Raether[33] showed theoretically that the roughness could reduce the value of G. He studied a system with two interfaces (quartz-silver-vacuum), using an expression derived for the attenuated total reflection (ATR) configuration and based on the effective dielectric function $\epsilon(\omega)$ of silver, Raether found a field enhancement ~ 50 for the smooth surface and ~ 30 on the rough surface with RMS height ~ 15 Å, at $\lambda = 5000$ Å. In other words, from the work of Raether it is found that the enhancement can decrease with roughness.

Although *s*-polarized surface polaritons are not known to exist (experimentally and theoretically) in nonmagnetic materials,[34] it is interesting to investigate if field enhancement is present with this polarization. The existence of this resonance could have importance for the enhancement of Raman scattering. Hessel and Oliner[35] predicted (using an analogy with closed waveguides) that for certain values h of the groove depth, resonances can be created in *s* polarization. Garcia and Maradudin[36] studied a sinusoidal grating but found no significant field enhancement (less than a factor of 4). Recently, in solid-state physics,[31,37] infinitely conducting gratings have received attention because it was found theoretically that a silver grating[31,37,38] gives practically the same results as for a perfectly conducting grating for all values of h. Wirgin and Maradudin[37] analyzed theoretically the particular case of an infinitely conducting lamellar grating. They showed that in the central groove the electric field is enhanced monotonically with the groove depth at certain resonance wavelengths. This same perfectly conducting lamellar grating has been studied by Andrewatha,[39] who also obtained resonances.

In conclusion, the Ushioda-Raether results suggest that, regarding surface-enhanced Raman scattering, it is interesting to include beams of finite cross section in the study of scattering by rough surfaces. In addition, the following questions could be raised.

(a) How does the field enhancement depend on the part of the surface that the incident laser beam strikes?

(b) Are the valleys on a rough surface more important for field enhancement than the tips as Raether[33] suggested?

(c) When is the field enhancement decreased by roughness? To our knowledge no study (for *s*- or *p*-polarized waves) has been carried out in these directions.

This is the first paper in a series dedicated to the study of arbitrary rough surfaces illuminated by beams of finite cross section. A rigorous integral formalism for the problem of the scattering of electromagnetic radiation (*s* polarization) from a nonperiodic rough surface is presented.[40] The details of the asperities are supposed to be of the order of the wavelength (λ) of the incident radiation, i.e., in the so-called resonant region. This formalism generalizes that of Wirgin and Maradudin[37] (an incident plane wave on a lamellar grating). As was mentioned above Raether[33] showed that roughness reduces the field enhancement compared to a smooth surface for $\lambda = 5000$ Å and $h = 15$ Å (h is the rms height): $h/\lambda \ll 1$. Therefore this suggests our considering shallow nonperiodic rough surfaces, for which we find a new explicit solution for the amplitude of the scattered field. With this explicit solution and the Rayleigh hypothesis,[16,17] it will then be possible to determine the electric field near the rough surface. In the next paper,[41] with the theory presented here, we will try to answer numerically the questions raised

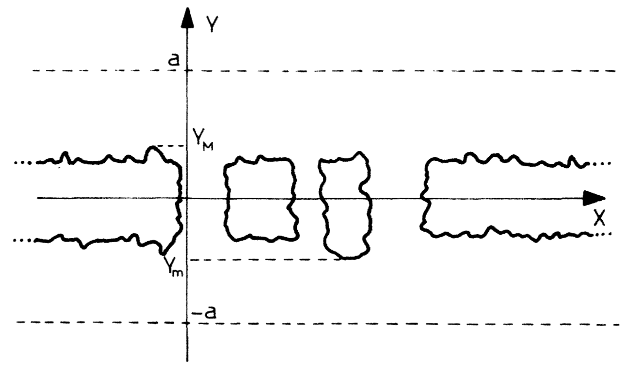

FIG. 1. The systems studied in this paper, namely, a finite number of infinitely long slits in a rough perfectly conducting thick screen.

above. In addition, we will deal with the *p* polarization.

In Sec. II, we discuss the field diffracted by a finite number of infinitely long slits in a rough-thick screen (see Fig. 1). Following Wirgin and Maradudin,[37] we assume a perfectly conducting screen, but differing from them, we have a rough surface and a beam of finite cross section. The thick slit has been studied in optics for a long time,[42] but to our knowledge, this is the first time where screen roughness is treated. In solid-state physics, we know of only one paper[43] dedicated to surface wave attenuation on a slit in a thick smooth screen. In this section, we obtain some reciprocity relations. In Sec. III, we present the case of a rough surface without the slits. We propose a new integral equation, obtained rigorously, for the scattering of beams of finite cross section from arbitrary rough surfaces (for the case where the wavelength of the incident radiation is comparable to the dimensions of the surface roughness). We get a new explicit solution, based on the Kirchhoff approximation (KA), which reduces to known expressions when the rough surface tends to a plane mirror and the beam is replaced by a plane wave. The approximate solution is applied to the particular case of gratings. A recent review paper on KA was presented by Wirgin in Ref. 44.

The results of this paper could be interesting in the scattering of light atoms from a crystal. This scattering plays an important role in studying the chemistry and crystallography of surfaces, because the atomic beams do not penetrate the top crystal layer. The surface is assumed to be a hard wall. The comparison between theory and experiment shows us that this model is able to describe a real situation.[45,46] Two-dimensional periodic surfaces,[47–49] the one-dimensional corrugation[50–53] consisting of a periodic distribution of atomic steps separated by close-packed terraces (occurring when a crystal is cut at an angle), and surfaces with attractive potential[45,54,55] have been studied. Only recently has the problem of a nonperfect periodic hard surface (empty sites, surface steps, and adsorbed atoms) been treated by several authors.[52,56,57] Regarding these last cases our theory can be applied to obtain some qualitative results.

II. ROUGH THICK SCREEN

A. Formulation of the problem

We study the electromagnetic field diffracted by a finite number of infinitely long slits in a rough, perfectly conducting, thick screen (Fig. 1). The screen is placed in the vacuum and the position of a point in space is given by its Cartesian coordinates X, Y, and Z. Our system is invariant under translation in the Z direction. We distinguish three regions, denoted as region I ($Z>a$), region II ($-a\le Z\le a$), and region III ($Z<-a$), shown in Fig. 1. The slits are illuminated by a beam of finite cross section, independent of the Z coordinate, with the wavelength $\lambda=2\pi/k$ ($k=\omega/c$). The complex representation of field quantities is used; the complex time factor $\exp(-i\omega t)$ is omitted from now on.

Let us consider an s-polarized wave, i.e., E_Z is the only component of the electric field and must be null at the interfaces. The total field E must satisfy the Helmholtz equation

$$\nabla^2 E+k^2E=0 \; . \tag{1}$$

Let Y_M and Y_m be the maximum and minimum of the system, respectively (see Fig. 1). We assume that the total field E can be Fourier analyzed as a function of X ($Y>Y_M$ or $Y<Y_m$):

$$E(X,Y)=\int_{-\infty}^{\infty}\hat{E}(\alpha',Y)e^{i\alpha' X}d\alpha' \; . \tag{2}$$

B. The Cadilhac-Maystre lemma

In 1980 Cadilhac[58] proposed an important lemma valid for gratings which, later, was extended to rough surfaces by Maystre.[5] This Cadilhac-Maystre lemma (C-M lemma) has permitted the obtaining of reciprocity relations and analytical expressions for the diffracted field from arbitrary rough surfaces.[5,58] The theoretical point of view in this paper is based on an application of this lemma to the system we are discussing here.

Let $U(X,Y)$ and $V(X,Y)$ be two bounded solutions (for large Y) of the Helmholtz equation, defined in region II and satisfying the conditions under which Green's theorem of unbounded domain is valid. We can represent U and V in a plane-wave expansion[58] as

$$U(X,Y)=\int_{-\infty}^{\infty}U_h^-(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' + \int_{-\infty}^{\infty}U_h^+(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha' \; , \tag{3}$$

$$V(X,Y)=\int_{-\infty}^{\infty}V_h^-(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' + \int_{-\infty}^{\infty}V_h^+(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha' \; , \quad \text{if } a\ge Y>Y_M \tag{4}$$

$$U(X,Y)=\int_{-\infty}^{\infty}U_b^-(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' + \int_{-\infty}^{\infty}U_b^+(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha' \; , \tag{5}$$

$$V(X,Y)=\int_{-\infty}^{\infty}V_b^-(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' + \int_{-\infty}^{\infty}V_b^+(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha' \; , \quad \text{if } -a\le Y<Y_m \; , \tag{6}$$

where $(\beta')^2=k^2-(\alpha')^2$, with β' or β'/i positive. In region II we have

$$\int (U\nabla^2 V-V\nabla^2 U)dX\,dY=0 \; . \tag{7}$$

Changing Eq. (7) by means of Green's formula, we obtain

$$\int_S\left[U\frac{dV}{dn}-V\frac{dU}{dn}\right]ds = -\int_{-\infty}^{\infty}\left[U\frac{dV}{dY}-V\frac{dU}{dY}\right]_{Y=a}dX + \int_{-\infty}^{\infty}\left[U\frac{dV}{dY}-V\frac{dU}{dY}\right]_{Y=-a}dX \; , \tag{8}$$

where s is the curvilinear coordinate on S (interface between the vacuum and the screen) and n is the inward normal to the metallic screen. After applying the Parseval-Plancherel theorem to the right-hand side of Eq. (8), the expression of the C-M lemma adapted to our system takes the form

$$\int_S\left[U\frac{dV}{dn}-V\frac{dU}{dn}\right]ds=4\pi i\int_{-\infty}^{\infty}\beta'[U_h^+(\alpha')V_h^-(-\alpha')-U_h^-(\alpha')V_h^+(-\alpha')]d\alpha' -4\pi i\int_{-\infty}^{\infty}\beta'[U_b^+(\alpha')V_b^-(-\alpha')-U_b^-(\alpha')V_b^+(-\alpha')]d\alpha' \; . \tag{9}$$

This expression relates the complex amplitudes ($U_h^\pm$, $U_b^\pm$, $V_h^\pm$, and $V_b^\pm$) and the boundary values of U and V.

In the following, we will obtain general results with physical meaning by choosing appropriate fields as U and V.

C. General relations

When the slits are illuminated by the incident field E^i which propagates downwards, the plane-wave expansions of the generated total field E are

$$E(X,Y)=\int_{-k}^{k}A(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' + \int_{-\infty}^{\infty}r(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha', \quad Y>Y_M \tag{10}$$

$$E(X,Y)=\int_{-\infty}^{\infty}t(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha', \quad Y<Y_m \tag{11}$$

where the incident beam wave E^i (incoming wave) is identified with the first integral of Eq. (10), the scattered field (outgoing and evanescent waves) with the second integral of Eq. (10), and the diffracted wave (outgoing and evanescent waves) with the right-hand side of Eq. (11).

If we let the incident beam be equal to the plane wave $\exp[i(\alpha X-\beta Y)]$, we then have

$$E(X,Y)=e^{i(\alpha X-\beta Y)}-e^{i(\alpha X+\beta Y)} + \int_{-\infty}^{\infty} R(\alpha')e^{i(\alpha' X+\beta' Y)}d\alpha', \quad Y>Y_M \tag{12}$$

$$E(X,Y)=\int_{-\infty}^{\infty} T(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha', \quad Y<Y_m \tag{13}$$

where we write the specular incident (reflected) wave explicitly. By comparison of Eqs. (10) and (11) and (12) and (13), we obtain three relations that can be used to go from beam expressions to plane-wave expressions:

$$A(\alpha')=\delta(\alpha'-\alpha)\ , \tag{14a}$$

$$r(\alpha')=-\delta(\alpha'-\alpha)+R(\alpha')\ , \tag{14b}$$

$$t(\alpha')=T(\alpha')\ . \tag{14c}$$

III. ENERGY CONSERVATION

Let $U(X,Y)$ be the total field E previously defined by Eqs. (10) and (11). Identifying terms in Eqs. (3) and (5) with Eqs. (10) and (11), we have

$$U_h^-(\alpha')=\begin{cases} A(\alpha'), & \alpha'\in J \\ 0, & \alpha'\notin J, \end{cases} \tag{15a}$$

$$U_h^+(\alpha')=r(\alpha')\ , \tag{15b}$$

$$U_b^+(\alpha')=0\ , \tag{15c}$$

$$U_b^-(\alpha')=t(\alpha')\ , \tag{15d}$$

where $J=[-k,k]$. Now, let the slits be illuminated by a second incident field E''^{i} with amplitude A'' also propagating downwards. We choose the complex conjugate of the total field E'' generated by E''^{i} as $V(X,Y)$. In this case,

$$V_h^-(\alpha')=\begin{cases} r''^{*}(-\alpha'), & \alpha'\in J \\ 0, & \alpha'\notin J \end{cases} \tag{16a}$$

$$V_h^+(\alpha')=\begin{cases} A''^{*}(-\alpha'), & \alpha'\in J \\ r''^{*}(-\alpha'), & \alpha'\notin J \end{cases} \tag{16b}$$

$$V_b^-(\alpha')=\begin{cases} 0, & \alpha'\in J \\ t''^{*}(-\alpha'), & \alpha'\notin J \end{cases} \tag{16c}$$

$$V_b^+(\alpha')=\begin{cases} t''^{*}(-\alpha'), & \alpha'\in J \\ 0, & \alpha'\notin J. \end{cases} \tag{16d}$$

After applying the C-M lemma [Eq. (9)] to the functions U and V, the left-hand side results in zero and we are left with the general relation

$$\langle r(\alpha'),r''(\alpha')\rangle+\langle t(\alpha'),t''(\alpha')\rangle=\langle A(\alpha'),A''(\alpha')\rangle, \tag{17}$$

with the notation

$$\langle f(\alpha'),g(\alpha')\rangle=\int_{-k}^{k}\beta' f(\alpha')g^{*}(\alpha')d\alpha'\ . \tag{18}$$

It is important to notice that the evanescent waves are not involved in this relation.

When we apply the relation we have just found to the particular case where $A(\alpha')=A''(\alpha')$, i.e., they represent the same incident field, we obtain the classical theorem for the conservation of energy for a beam wave:

$$\int_{-k}^{k}\beta'\,|r(\alpha')|^2 d\alpha'+\int_{-k}^{k}\beta'\,|t(\alpha')|^2 d\alpha' = \int_{-k}^{k}\beta'\,|A(\alpha')|^2 d\alpha' \tag{19}$$

and using the beam-plane wave transformation relations [Eqs. (14)], we obtain for an incident plane wave the following equation:

$$\langle T(\alpha'),T(\alpha')\rangle+\langle R(\alpha'),R(\alpha')\rangle-2\beta\,\mathrm{Re}[R(\alpha)]=0\ . \tag{20}$$

IV. RECIPROCITY RELATIONS

A. For reflection

We had previously set E and E'' as the total fields generated by incident beam waves (propagating downwards) with amplitudes A and A'', respectively. Now we will take $U=E$ and $V=E''$ (previously, we had treated the case where $U=E$ and $V=E''^{*}$). In this case the C-M lemma reduces to the general reciprocity relation for reflection:

$$\langle r(\alpha'),A''^{*}(-\alpha')\rangle=\langle r''(-\alpha'),A^{*}(\alpha')\rangle\ . \tag{21}$$

Now, if the incident fields are plane waves with amplitudes

$$A(\alpha')=\delta(\alpha'-\alpha) \tag{22a}$$

and

$$A''(\alpha')=\delta(\alpha'-\alpha'')\ , \tag{22b}$$

then, we get

$$\beta''R(-\alpha'')=\beta R''(-\alpha)\ . \tag{23}$$

Under this simple form, the physical interpretation is clear. We illustrate this final result in Fig. (2) with $\alpha=k\sin\theta$ and $\alpha''=k\sin\theta''$.

B. For transmission

$U(X,Y)$ continues to be the field E, but $V(X,Y)$ will be the total field E'' generated by an incident beam wave E''^{i}, propagating upwards with amplitude A''. The C-M lemma then gives the general reciprocity relation for transmission,

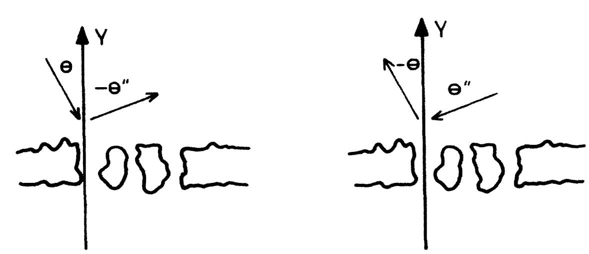

FIG. 2. Reciprocity relation for reflection.

$$\langle t''(-\alpha'), A^*(\alpha') \rangle = \langle t(-\alpha'), A''^*(\alpha') \rangle \ , \qquad (24)$$

and for incident plane waves [Eqs. (22a) and (22b)],

$$\beta T''(-\alpha) = \beta'' T(-\alpha'') \ . \qquad (25)$$

In Fig. 3, we illustrate this result. A closely related relation, an aperture in a smooth screen, was obtained by Levine and Schwinger.[59]

It must be emphasized that the reciprocity relations, Eqs. (23) and (25), are valid even if the system (Fig. 1) is not symmetrical with respect to the Y axis.

V. SURFACE CURRENT

To obtain a relation between the surface current J_s and the scattered amplitude $r(-\alpha'')$, we take $V(X,Y)$ as a downward incident field $\exp[i(\alpha''X - \beta''Y)]$ and $U(X,Y)$, again, as the total field E [Eqs. (10) and (11)]. For the amplitudes of V we get

$$V_h^-(\alpha') = V_b^-(\alpha') = \delta(\alpha' - \alpha'') \qquad (26)$$

and

$$V_h^+(\alpha') = V_b^+(\alpha') = 0 \ . \qquad (27)$$

Then, after applying the C-M lemma, we obtain the scattered amplitude as

$$r(-\alpha'') = \frac{\omega\mu_0}{4\pi\beta''} \int_S J_s e^{i(\alpha''X - \beta''Y)} ds \ . \qquad (28)$$

Similarly a relationship is obtained between J_s and the transmitted amplitude $t(-\alpha'')$, when we take $V(X,Y)$ as an upward incident field $\exp[i(\alpha''X + \beta''Y)]$ and $U(X,Y)$ as E:

$$t(-\alpha'') = \frac{\omega\mu_0}{4\pi\beta''} \int_S J_s e^{i(\alpha''X + \beta''Y)} ds + A(-\alpha'') \ . \qquad (29)$$

These expressions [Eqs. (28) and (29)] relate the amplitudes r and t to the surface current J_s. It is not surprising to see that r and t can be derived from the surface current since J_s actually generates the diffracted and scattered fields.

VI. ROUGH SURFACES

The purpose of this section is to find solutions for the scattering of beams of finite cross section by rough surfaces and to study the particular case of diffraction gratings. A rigorous integral equation is obtained for the case where the wavelength of the incident radiation is comparable to the dimensions of the surface roughness (resonance region). We show that the Kirchhoff approximation leads to a very simple formula which gives precise numerical results for shallow surfaces. The approach we follow is to make the slits disappear, hence our system becomes a rough surface (Fig. 4). Then, we can apply the results of Sec. II to rough surfaces, as long as we impose the condition that the transmission amplitudes t and t'' become equal to zero.

A. Rigorous integral equation

If $t(-\alpha'')=0$ in Eq. (29) we have that

$$A(-\alpha'') = -\frac{\omega\mu_0}{4\pi\beta''} \int_S J_s e^{i(\alpha''X + \beta''Y)} ds \ . \qquad (30)$$

This integral equation, with the unknown J_s, is the main result of this paper and is valid for an arbitrary surface height. We notice the simple and nonsingular Kernel. Other integral equations (derived by using the Green theorem) for the scattering of an incident plane wave have been reported in the literature.[6,9] They contain a singular Kernel which complicates their study.

The problem is to determine J_s when the amplitude A of the incident beam and the rough surface are known. For instance, the incident wave might be a Gaussian beam[42] or have another spatial structure.[60] The numerical solution of Eq. (30) and answers to the questions raised in the introduction to this paper will be the subject of a future report.

We are mainly interested in the scattering of an incident beam whose intersection with rough surfaces is finite. In this case, J_s is zero at sufficiently large distances from the border of this intersection and, because of this, the integral [Eq. (30)] will have a finite domain of integration and this simplifies its numerical treatment. To find the scattering field, we have to solve this integral equation and put the result in Eq. (28). To ensure the accuracy and reliability of the final numerical solution, we could perform checks on the energy conservation [Eq. (19) with

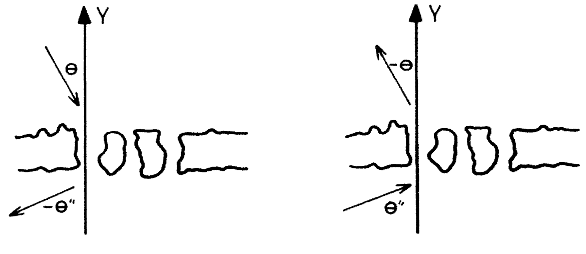

FIG. 3. Reciprocity relation for transmission.

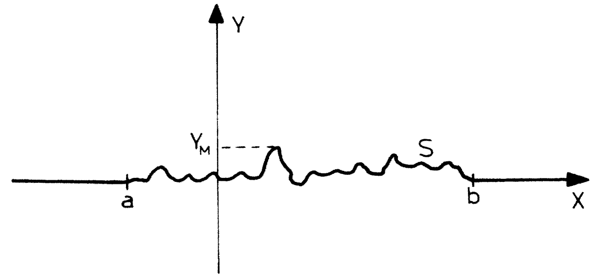

FIG. 4. The rough perfectly conducting surface.

$t=0$] and reciprocity relation for reflection [Eq. (21)]. However, we must remember that these checks are necessary but must never be considered as sufficient.

If the incident beam wave is the plane wave $\exp[i(\alpha X-\beta Y)]$, we obtain the following result from Eq. (30):

$$\delta(\alpha''+\alpha)=-\frac{\omega\mu_0}{4\pi\beta''}\int_S J_s e^{i(\alpha'' X+\beta'' Y)}ds \ ; \qquad (31)$$

this is the expression for the extinction theorem. The result is the same as the one obtained by Rogers[61] in 1984 and this agreement gives us confidence in our integral equation.

B. Kirchhoff approximation (rough surfaces)

Approximate theories have been proposed to avoid difficulties in a rigorous treatment for the scattering of waves from rough surfaces, see Fig. 4. The best known and most often used is the Kirchhoff approximation, also known as the physical-optics and Beckmann approximation.[6,44] This method assumes that, at any point on the surface S, the total field E and the incident field E^i are related by

$$\frac{dE}{dn}=2\frac{dE^i}{dn} \ . \qquad (32)$$

The important practical consequence of this approximation is that it avoids the difficulty of calculating the superficial current J_s from an integral equation [see Eq. (30)], and enables the determination of the scattering field with simple analytical expressions. To the author's knowledge, the KA has only been studied when the incident field is a plane wave. In this section, the KA is applied to beams of finite cross section.

After subtracting Eq. (29) from (28), with $t(-\alpha'')=0$, we find that the domain of integration is reduced to the interval $[a,b]$ (modulated region, see Fig. 4), simplifying the numerical calculation. Substituting Eq. (32) in this result we have

$$r(-\alpha'')=\frac{i}{2\pi\beta''}\int_a^b \left(e^{i(\alpha'' X-\beta'' Y)}-e^{i(\alpha'' X+\beta'' Y)}\right)\times\frac{dE^i}{dn}ds-A(-\alpha'') \ , \qquad (33)$$

where n is the inward normal to the metallic screen.

On the other hand, the incident beam is represented by

$$E^i(X,Y)=\int_{-k}^{k} A(\alpha')e^{i(\alpha' X-\beta' Y)}d\alpha' \ , \qquad (34)$$

so that we get

$$\frac{dE^i}{dn}(X,Y)=\int_{-k}^{k} iA(\alpha')\frac{(\alpha'\dot f+\beta')}{(1+\dot f^{\,2})^{1/2}}e^{i(\alpha' X-\beta' Y)}d\alpha' \ , \qquad (35)$$

where f is the rough profile and $\dot f=df/dx$.

If we combine Eqs. (33) and (35), changing the order of integration and realizing integration by parts, we obtain

$$r(-\alpha'')=\int_{-k}^{k} A(\alpha')I(\alpha',-\alpha'')d\alpha'-A(-\alpha'') \ , \qquad (36)$$

where

$$I(\alpha',-\alpha'')=\int_a^b e^{i(\alpha''+\alpha')X}\left[\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta'+\beta'')}+\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta''-\beta')}+e^{-i(\beta'+\beta'')f}\left[-\frac{\beta'}{2\pi\beta''}-\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta'+\beta'')}\right]+e^{i(\beta''-\beta')f}\left[\frac{\beta'}{2\pi\beta''}-\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta''-\beta')}\right]\right]dx \ . \qquad (37)$$

This result, expressed in the form of a simple integral, gives a new explicit solution for the amplitude of the scattered field. We notice that, in Eq. (37), the integrad has no pole when $\beta''=\beta'$. This expression has been obtained directly from the KA without any further approximation. If we assume that there is no corrugation present, i.e., $f(X)=0$, then the right-hand side of Eq. (37) disappears and, by Eq. (36) we reproduce the expected solution for a flat surface.

The explicit solutions [Eqs. (36) and (37)] are expected to be useful in order to understand the result that roughness can reduce the field enhancement. Raether[33] showed experimentally this result for $h/\lambda=0.003$, i.e., *for shallow surfaces.*

Next, for the particular case of plane waves, it will be shown that the new formalism gives accurate results for $h/\lambda<0.1$ (far from Raether's ratio$=0.003$). We assume that the height (h) of the surface roughness $f(X)$ is small. Then, from Eq. (36), we can deduce the scattering field to the lowest order in h. The calculation can also be readily generalized to higher orders in h.

The exponential functions in Eq. (37) can be approximated as follows:

$$e^{\pm i(\beta''\mp\beta')f(X)}\cong 1\pm i(\beta''\mp\beta')f(X) \ . \qquad (38)$$

We are assuming that $|\beta' f(X)|\ll 1$. In practical terms this means that the maximum height (h) of roughness should be much smaller than the wavelength λ:

$$h\ll\lambda \ . \qquad (39)$$

Therefore, from Eqs. (37) and (38), we obtain

$$I(\alpha',-\alpha'')=\frac{i\beta'}{\pi}\int_a^b f(X)e^{i(\alpha''+\alpha')X}dX \ . \qquad (40)$$

The Eqs. (36) and (40) are the expressions of the lowest order in $f(X)$ in the KA. We see that $I(\alpha',-\alpha'')$ is proportional to the Fourier transform of $f(X)$.

If the incident beam wave is the plane wave $e^{i(\alpha X-\beta Y)}$, we get, from Eqs. (36) and (40), the scattered field $R(\alpha'')$:

$$R(\alpha'')=\frac{i\beta}{\pi}\int_a^b f(X)e^{i(\alpha-\alpha'')X}dX\ . \tag{41}$$

This equation was also obtained by Maystre[5] *et al.*, not by using the KA but, by using a rigorous treatment. They compared their numerical results with calculations performed using rigorous integral theories. Such comparison showed that the simple equation for $R(\alpha'')$ gives results accurate for $h/\lambda<0.1$ (see Fig. 7 in Ref. 5). We, then, expect that our more general equation [Eqs. (36) and (37)] will give good numerical results for slightly rougher surfaces (far from Raether's ratio$=0.003$).

In conclusion, we have shown that the KA is capable of yielding accurate results, at least to first order in roughness. We have also applied the KA to the case of p-polarized waves following the same scheme as above and have obtained good results to first order in roughness.[62] This does not imply that the application of KA always leads to good results. For instance, if we substitute Eq. (32) directly in Eq. (28) and use the following relation:

$$\int_S E^i\frac{d}{dn}e^{i(\alpha''X-\beta''Y)}ds=\int_S e^{i(\alpha''X-\beta''Y)}\frac{dE^i}{dn}ds \tag{42}$$

we obtain a new expression for $r(-\alpha'')$ in the s-polarization case. And, if we treat the p polarization (for a perfectly conducting rough surface) similarly to the s-polarization case, we can show that the new expressions do not depend on the polarization (see Ref. 5). Hence, this procedure fails even for very shallow surfaces.

C. Kirchhoff approximation (periodic surfaces)

The expression for $I(\alpha',-\alpha'')$, Eq. (37), has the form

$$I(\alpha',-\alpha'')=\int_{-\infty}^{\infty}e^{i(\alpha''+\alpha')X}\phi(\alpha',\alpha'',X)dX\ , \tag{43}$$

where ϕ is a periodic function, with the period being equal to the groove spacing d of the grating. After the variable change $X'=-nd+X$, we obtain

$$\begin{aligned}I(\alpha',-\alpha'')&=\sum_{n=-\infty}^{\infty}\int_{nd}^{(n+1)d}e^{i(\alpha''+\alpha')X}\phi(\alpha',\alpha'',X)dX\\&=\left[\int_0^d e^{i(\alpha''+\alpha')X}\phi(\alpha',\alpha'',X)dX\right]\sum_{n=-\infty}^{\infty}e^{i(\alpha''+\alpha')nd}\end{aligned}$$

then

$$I(\alpha',-\alpha'')=\left[\int_0^d e^{i(\alpha''+\alpha')X}\phi(\alpha',\alpha'',X)\,dX\right]\frac{2\pi}{d}\sum_{n=-\infty}^{\infty}\delta\left[\alpha''+\alpha'-\frac{2\pi}{d}n\right]. \tag{44}$$

If we substitute Eq. (44) in Eq. (36), we finally obtain

$$r(-\alpha'')=\frac{2\pi}{d}\sum_{n=-\infty}^{\infty}A\left[-\frac{2\pi n}{d}-\alpha''\right]\int_0^d e^{-i(2\pi n/d)X}\phi(-2\pi n/d-\alpha'',\alpha'',X)dX-A(-\alpha'')\ , \tag{45}$$

where

$$\begin{aligned}\phi(\alpha',\alpha'',X)=&\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta'+\beta'')}+\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta''-\beta')}+e^{-i(\beta'+\beta'')f(X)}\left[-\frac{\beta'}{2\pi\beta''}-\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta'+\beta'')}\right]\\&+e^{i(\beta''-\beta')f(X)}\left[\frac{\beta'}{2\pi\beta''}-\frac{\alpha'(\alpha''+\alpha')}{2\pi\beta''(\beta''-\beta')}\right].\end{aligned} \tag{46}$$

The above expression for $r(-\alpha'')$ will be useful in the analysis of the scattering of a Gaussian beam by a grating (in the resonance region). A scalar study of this problem was carried out by Bar-Isaac and Hardy.[63] It is interesting to investigate if some of the results of the scalar study are also applicable in the resonance region. Our last expression for $r(-\alpha'')$ provides a means of investigating that. Work in this direction is in progress in our group. In the lowest order in $f(X)$, Eqs. (45) and (46) can be reduced to

$$\begin{aligned}r(-\alpha'')=&\frac{2i}{d}\sum_{n=-\infty}^{\infty}A\left[-\frac{2\pi n}{d}-\alpha''\right]\\&\times\beta\int_0^d e^{\frac{-i2\pi nX}{d}}f(X)dX\\&-A(-\alpha'')\ ,\end{aligned} \tag{47}$$

where β is evaluated in $-2\pi n/d-\alpha''$.

Maystre[5] *et al.* have studied the particular case of an incident plane wave on a grating, and their results agreed with a rigorous integral theory. When we apply our expression, Eq. (47), to the particular case of incident plane waves, we find that Eq. (47) is reduced exactly to the expression obtained by Maystre [see Eq. (28) in Ref. 5].

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