Reflection of electromagnetic waves from a surface with a low relief

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A low relief on the interface between two dielectrics is shown to be equivalent, in terms of electromagnetic wave reflection, to a homogeneous but anisotropic thin film between the dielectrics. "Low" here means that the heights in the relief are small in comparison with the wavelength. The permittivity tensor of a film of this sort is calculated by solving the electrostatic problem of the effective permittivity of a layer which contains irregularities and which is bracketed by two homogeneous half-spaces. For an elongated periodic 2*D* relief, one component of the effective permittivity tensor can be calculated immediately, while the others satisfy symmetry relations of a type found previously {A. M. Dykhne, Zh. Eksp. Teor. Fiz. **59**, 110 (1970) [Sov. Phys. JETP **32**, 63 (1971)]}. All components of this tensor can be calculated analytically in the cases of "gently sloping" and "steep" irregularities, while they can be calculated numerically for a relief with plane faces and arbitrary slopes. The results found here can be used to extract information on the structure of a low relief from experiments on long-wavelength reflection of light.

FORMULATION OF THE PROBLEM; REDUCTION TO AN EQUIVALENT PROBLEM

We examine the reflection of waves from an interface between two media in the case in which the length scales of the surface relief are considerably shorter than the wavelength of the incident radiation. Problems of this type can arise in a variety of situations. The characteristics of the reflected light are sensitive to the surface relief even if the length scales of this relief are considerably shorter than the wavelength.

Consider a periodic relief. The procedure of solving this problem is analogous to going over from microscopic to macroscopic Maxwell's equations in a medium. The details of the particular structure of the relief do not affect the characteristics of the reflected radiation, i.e., its amplitude, polarization, and phase. The reflection is only influenced by a certain limited amount of information about the relief. Only this limited amount can be extracted through interpretation of the corresponding experiments.

Spatially nonuniform fields which are directly associated with the relief (in particular, which depend on the shape of the relief) vary over distances comparable to the length scales of the relief, its period and its height. Since these distances are much shorter than the wavelength, the quasistatic approximation is sufficient for calculating the "microfields." In that approximation, however, the fields satisfy the Laplace equation, and their spatially varying part is known to fall off exponentially with distance from the interface. The minimum rate of this decay is comparable to the reciprocal dimensions of the relief. Only spatially uniform fields "survive" outside a narrow surface layer.

The wave zone begins at distances from the surface which are comparable to the wavelength, where the microfields have decayed and thus cannot participate in producing the scattered radiation fields.

The presence of the relief and its shape affect the scattering only through these average fields, which are the link between the shape of the relief and its reflection characteristics. Some physical arguments which have been developed, which look fairly convincing,[1] lead to the following mathematical formulation of the problem of reflection from a rough interface.

We introduce regions I, II, and III (Fig. 1) in such a way that the thickness of layer II, H, is much larger than the period l and height h of the irregularities but much smaller than the wavelength λ of the incident radiation. We place no restriction on the relation between the period and height of the irregularities. It is thus sufficient to solve the static problem in layer II. When the fields are joined at (and near) the boundaries of layer II, only spatial averages of the fields inside this layer survive.

The spatial averages satisfy the relation

$$\langle \mathbf{D} \rangle_{\mathrm{II}} = \hat{\varepsilon}^{\mathrm{eff}} \langle \mathbf{E} \rangle_{\mathrm{II}}, \tag{1}$$

as has been known since Maxwell's time. The tensor $\hat{\varepsilon}^{\mathrm{eff}}$ here is a local tensor, in accordance with the approximation $\max(l,h)/\lambda \ll 1$. The results reported below are derived in zeroth order in this parameter.

To solve the external problem (in regions I and III), we can thus replace layer II by an equivalent layer of a homogeneous but generally anisotropic dielectric of thickness H. Clearly, the choice of H $(l,h \ll H \ll \lambda)$ should have no effect on physically observable results. The inequality $h \ll H$, used in justifying the introduction of an effective anisotropic layer, is actually not a necessary condition. The layer could be any layer which includes all the irregularities of the relief, of height h, for example, as shown in Fig. 1.

The problem is actually one of calculating the effective permittivity tensor of film II, of thickness H. This film, however, contains three layers—*a*, *b*, and *c*—which are connected electrically in parallel if $\langle \mathbf{E} \rangle$ lies in the xy plane or in series if $\langle \mathbf{E} \rangle$ is directed along the z axis (along the normal to the surface). It is thus sufficient to calculate the effective permittivity tensor of film *b*. Films *a* and *c* can be incorporated in regions I and III, respectively. The result does not depend explicitly on the thicknesses of these films. Relation (1) holds for any relief whose characteristic dimensions are short in comparison with the wavelength.

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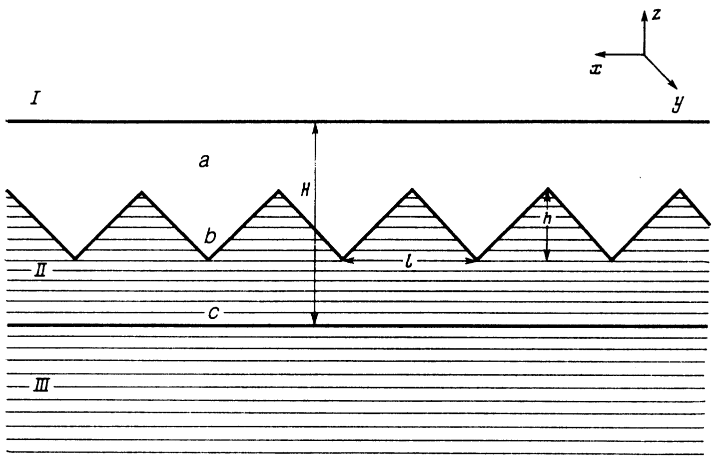

FIG. 1.

Relation (1) has no small parameter in the static approximation, and finding $\hat{\varepsilon}^{\text{eff}}$ for the general case is a difficult problem. In this paper we consider periodic, elongated, 2D reliefs. The problem can be solved analytically in the cases of "gently sloping" and "steep" irregularities; in the intermediate region it can be solved numerically. For certain types of relief, described below, the components of the tensor $\hat{\varepsilon}^{\text{eff}}$ satisfy symmetry relations of the type found in Ref. 1.

Some other published papers (e.g., Refs. 2–5), in which the dielectric characteristics of a layer with a roughness have been calculated, are not sufficiently systematic, in our opinion.

TWO-DIMENSIONAL RELIEFS; SYMMETRY RELATION

In calculating the components of the tensor $\hat{\varepsilon}^{\text{eff}}$, we use the condition of a quasistatic electromagnetic field. The vectors **E** and **D** satisfy the equations

$$\text{rot}\,\mathbf{E}=0, \quad \text{div}\,\mathbf{D}=0 \tag{2}$$

in region II and are related by

$$\mathbf{D}=\varepsilon(x,\ z)\mathbf{E}. \tag{3}$$

The permittivity $\varepsilon(x,z)$ is written as follows:

$$\varepsilon(x,\ z)=\varepsilon_1\theta(z-f(x))+\varepsilon_2\theta(f(x)-z). \tag{4}$$

Here $f(x)$ is a periodic function, which characterizes the surface relief, and

$$\theta(t)=\begin{cases}1, & t>0\\ 0, & t<0\end{cases}.$$

We assume that the field **E** is directed along the y axis. From the equation curl $\mathbf{E}=0$ we then find $\partial E_y/\partial x=\partial E_y/\partial z=0$. Taking an average of (3) over the area of one period, we find

$$\langle D_y\rangle=\langle\varepsilon(x,\ z)E_y\rangle=\langle\varepsilon(x,\ z)\rangle E_y.$$

According to definition (1) we thus have

$$\varepsilon_{yy}^{\text{eff}}=\langle\varepsilon(x,z)\rangle=\varepsilon_1\left(1-\frac{S}{S_0}\right)+\varepsilon_2\frac{S}{S_0}, \tag{5}$$

where

$$S_0=lh, \quad S=\int_0^l f(x)\,dx.$$

Expression (5) is valid for an arbitrary function $f(x)$. For the function $f(x)$ shown in Fig. 1 we have $\varepsilon_{yy}^{\text{eff}}=(\varepsilon_1+\varepsilon_2)/2$.

The other components of the tensor $\hat{\varepsilon}^{\text{eff}}$ can be found only by solving the corresponding electrostatic problem. Nevertheless, we can assert that these other components satisfy a symmetry relation of the type in Ref. 1. We will go through arguments like those carried out in Ref. 1 for the conductivity of a two-phase 2D medium. We denote by **e** and **d** the projections of the field and the electric displacement onto the xz plane, so we have $\mathbf{d}=\varepsilon(x,z)\mathbf{e}$.

We introduce the new vectors $\mathbf{e}'$ and $\mathbf{d}'$:

$$\mathbf{e}'=[\mathbf{n}_y\mathbf{d}]/(\varepsilon_1\varepsilon_2)^{1/2}, \tag{6}$$

$$\mathbf{d}'=[\mathbf{n}_y\mathbf{e}](\varepsilon_1\varepsilon_2)^{1/2}, \tag{7}$$

where $\mathbf{n}_y$ is the normal to the xz plane. Using (6) and (7), we can find the relationship between $\mathbf{d}'$ and $\mathbf{e}'$:

$$\mathbf{d}'=\varepsilon'(x,\ z)\mathbf{e}', \quad \varepsilon'(x,\ z)=\varepsilon_1\varepsilon_2/\varepsilon(x,\ z),$$

or

$$\varepsilon'(x,\ z)=\varepsilon_2\theta(z-f(x))+\varepsilon_1\theta(f(x)-z). \tag{8}$$

It is easy to show that if **e** and **d** satisfy Eqs. (2), then $\mathbf{e}'$ and $\mathbf{d}'$ will also satisfy these equations. For example,

$$\text{rot}\,\mathbf{e}'=\{\mathbf{n}_y\,\text{div}\,\mathbf{d}-(\mathbf{n}_y\nabla)\mathbf{d}\}/(\varepsilon_1\varepsilon_2)^{1/2}=0.$$

Averaging (6) and (7) over the period, we find relations among $\langle\mathbf{e}\rangle$, $\langle\mathbf{d}\rangle$, $\langle\mathbf{e}'\rangle$, $\langle\mathbf{d}'\rangle$:

$$\begin{aligned}\langle\mathbf{e}'\rangle&=[\mathbf{n}_y\langle\mathbf{d}\rangle]/(\varepsilon_1\varepsilon_2)^{1/2},\\ \langle\mathbf{d}'\rangle&=[\mathbf{n}_y\langle\mathbf{e}\rangle](\varepsilon_1\varepsilon_2)^{1/2}.\end{aligned} \tag{9}$$

According to the definition (1)

$$\langle\mathbf{d}\rangle=\hat{\varepsilon}^{\text{eff}}\langle\mathbf{e}\rangle, \quad \langle\mathbf{d}'\rangle=\hat{\varepsilon}'^{\text{eff}}\langle\mathbf{e}'\rangle. \tag{10}$$

If the $f(x)$ curve has a center of symmetry, the system of vectors $\mathbf{e}'$, $\mathbf{d}'$ and the original system of vectors differ from each other only by a rotation through an angle π in the xz plane, by virtue of (4) and (8). The quantities $\hat{\varepsilon}^{\rm eff}$ and $\hat{\varepsilon}'^{\rm eff}$ must therefore be the same. In this case, substituting (10) into (9), we find the relationship which we have been seeking among the components of the effective permittivity tensor:

$$(\varepsilon_{xx}^{\rm eff}\varepsilon_{zz}^{\rm eff}-\varepsilon_{xz}^{\rm eff}\varepsilon_{zx}^{\rm eff}-\varepsilon_1\varepsilon_2)^2+\varepsilon_1\varepsilon_2(\varepsilon_{xz}^{\rm eff}-\varepsilon_{zx}^{\rm eff})^2=0. \quad (11)$$

From this relationship we find

$$\varepsilon_{xz}^{\rm eff}=\varepsilon_{zx}^{\rm eff},\quad \varepsilon_{xx}^{\rm eff}\varepsilon_{zz}^{\rm eff}-\varepsilon_{zx}^{\rm eff})^2=\varepsilon_1\varepsilon_2. \quad (12)$$

If the function $f(x)$ has not only a center of symmetry but also a symmetry plane, the off-diagonal components of the tensor $\varepsilon^{\rm eff}$ vanish: $\varepsilon_{xz}^{\rm eff}=\varepsilon_{zx}^{\rm eff}=0$. The relationship (11) then becomes

$$\varepsilon_{xx}^{\rm eff}\varepsilon_{zz}^{\rm eff}=\varepsilon_1\varepsilon_2, \quad (13)$$

and it is sufficient to find one of the two unknowns $\varepsilon_{xx}^{\rm eff}$, $\varepsilon_{zz}^{\rm eff}$.

PARTICULAR CASES

a) Gently sloping irregularities: $h\ll l$. In this case we can use perturbation theory. As a zeroth approximation we use the potential in the absence of a corrugation of the interface; i.e., we use $f(x)=$ const. Problems for calculating the fields associated with the relief are formulated in Appendix II. The potentials φ and Ψ determined there can be written in the form

$$\varphi_{\rm I,II}=\begin{cases} z-\gamma\sum_n f_n\exp(ik_nx-|k_n|z), & z>f(x)\\ (\varepsilon_1/\varepsilon_2)\left[z+\gamma\sum_n f_n\exp(ik_nx+|k_n|z)\right], & z<f(x)\end{cases}, \quad (14)$$

$$\Psi_{\rm I,II}=\begin{cases} z+\gamma\sum_n f_n\exp(ik_nx-|k_n|z), & z>f(x)\\ (\varepsilon_2/\varepsilon_1)\left[z-\gamma\sum_n f_n\exp(ik_nx+|k_n|z)\right], & z<f(x)\end{cases} \quad (15)$$

Here

$$f_n=\frac{1}{l}\int_{-l/2}^{l/2}f(x)\exp(ik_nx)\,dx,\qquad k_n=\frac{2\pi n}{l},\qquad \gamma=\frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2+\varepsilon_1}.$$

The width of layer II is specified to be: $H=2\max(f_{\max},|f_{\min}|)$. The xy plane is chosen in such a way that the condition

$$\overline{f(x)}=\frac{1}{l}\int_0^l f(x)\,dx=0$$

holds. It can be shown that only the diagonal components of the tensor $\hat{\varepsilon}^{\rm eff}$ are nonzero to first order in the parameter h/l:

$$\varepsilon_{zz}^{\rm eff}=\frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\left(1+\frac{4\gamma^2}{H}\sum_n|f_n|^2k_n\right),$$
$$\varepsilon_{xx}^{\rm eff}=\frac{\varepsilon_1+\varepsilon_2}{2}\left(1-\frac{4\gamma^2}{H}\sum_n|f_n|^2k_n\right). \quad (16)$$

The expressions

$$\varepsilon_{xx}{}^0=\frac{\varepsilon_1+\varepsilon_2}{2},\qquad \varepsilon_{zz}{}^0=\frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}$$

correspond to a smooth boundary if we consider an imaginary film of thickness $H\ll\lambda$ with a permittivity

$$\varepsilon(z)=\begin{cases}\varepsilon_1, & 0\leqslant z\leqslant H/2\\ \varepsilon_2, & -H/2\leqslant z\leqslant 0\end{cases}.$$

The presence of this film results in a change in only a common phase of the amplitude reflection coefficients, which are defined to within a phase factor. It is easy to see that the symmetry relation (13) holds for an arbitrary function $f(x)$ to first order in the parameter h/l.

In the case (Fig. 1)

$$f(x)=\begin{cases}\dfrac{2h}{l}\left(x+\dfrac{l}{4}\right), & -\dfrac{l}{2}\leqslant x\leqslant 0\\ \dfrac{2h}{l}\left(\dfrac{l}{4}-x\right), & 0\leqslant x\leqslant\dfrac{l}{2}\end{cases}, \quad (17)$$

expressions (16) become

$$\varepsilon_{zz}^{\rm eff}=\frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\left(1+\frac{32}{\pi^3}A_3\gamma^2\frac{h}{l}\right),$$
$$\varepsilon_{xx}^{\rm eff}=\frac{\varepsilon_1+\varepsilon_2}{2}\left(1-\frac{32}{\pi^3}A_3\gamma^2\frac{h}{l}\right), \quad (18)$$

where $A_3=(7/8)\zeta(3)$, and $\zeta(3)$ is the zeta function. With $f(x)=h\sin(2\pi x/l)$ we find

$$\varepsilon_{zz}^{\rm eff}=\frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\left(1+\pi\gamma^2\frac{h}{l}\right).$$
$$\varepsilon_{xx}^{\rm eff}=\frac{\varepsilon_1+\varepsilon_2}{2}\left(1-\pi\gamma^2\frac{h}{l}\right).$$

We can go over to gently sloping but otherwise random irregularities in (16) by making the substitution

$$\sum_n|f_n|^2k_n\to\sigma^2\int_0^\infty W(k)k\,dk.$$

Here $W(k)$ is the Fourier transform of the correlation function, and σ is the standard deviation of the random function $f(x)$. The reflection coefficients found with the help of these expressions are the same as the results of Refs. 6 and 7 for 2*D* irregularities.

b) Steep irregularities: $h\gg l$. In analyzing steep irregularities, we draw on the analogy between the conductivity and the permittivity, which allows us to transform from current problems to electrostatic problems.

We partition the irregularity region of height h into layers of thickness d (Fig. 2) in such a way that the conditions $l\ll d\ll h$ hold. The inequality $d\ll h$ allows us to ignore the slope of the interface with respect to the z axis in evaluating the components of $\varepsilon^{\rm eff}$ of one of the layers, while the inequality $l \ll d$ allows us to treat the set of irregularities in a layer of thickness d as a plane–layer medium. In the x direction, the layers are connected in series, while in the z direction they are connected in parallel. As a result we find

$$\varepsilon_{zz}^{\text{eff}}(z) = \langle \varepsilon^{-1}(x,z) \rangle_d^{-1}, \qquad \varepsilon_{xx}^{\text{eff}}(z) = \langle \varepsilon(x,z) \rangle_d. \tag{19}$$

We thus find the problem of a layer which is nonuniform in the z direction. When an average is taken over z, the layers of thickness d are connected in parallel in the x direction, while they are connected in series in the z direction. We finally find

$$\varepsilon_{zz}^{\text{eff}} = \frac{1}{h}\int_0^h dz \left\{ \frac{1}{l}\int_0^l \left[\frac{1}{\varepsilon_1}\theta(z-f(x)) + \frac{1}{\varepsilon_2}\theta(f(x)-z) \right] dx \right\}^{-1}, \tag{20}$$

$$(\varepsilon_{xx}^{\text{eff}})^{-1} = \frac{1}{h}\int_0^h dz \left\{ \frac{1}{l}\int_0^l [\varepsilon_1\theta(z-f(x)) + \varepsilon_2\theta(f(x)-z)]\,dx \right\}^{-1}.$$

As examples we consider triangular irregularities describable by (17) and also trench irregularities[2]

$$f(x) = \begin{cases} 0, & 0 \leqslant x \leqslant a \\ h, & a \leqslant x \leqslant l \end{cases}.$$

In the first of these cases we have

$$\varepsilon_{zz}^{\text{eff}} = \frac{\varepsilon_1\varepsilon_2}{\varepsilon_2-\varepsilon_1}\ln\frac{\varepsilon_2}{\varepsilon_1}, \qquad \varepsilon_{xx}^{\text{eff}} = (\varepsilon_2-\varepsilon_1)\ln^{-1}\frac{\varepsilon_2}{\varepsilon_1}, \tag{21}$$

and (13) holds. In the second case we have

$$\varepsilon_{zz}^{\text{eff}} = \frac{\varepsilon_1\varepsilon_2 l}{a\varepsilon_2 + (l-a)\varepsilon_1}, \qquad \varepsilon_{xx}^{\text{eff}} = \frac{\varepsilon_2(l-a)+\varepsilon_1 a}{l}. \tag{22}$$

In this case, (13) holds only for $a = l/2$, i.e., only if the irregularities are symmetric.

RELIEFS WITH PLANE FACES; RESULTS OF A NUMERICAL CALCULATION

a) Symmetric irregularities. A detailed study has been made of the particular case of a toothed relief (Fig. 1), with a profile described by (17), as an example. By varying the height h at a given period, we can make the switch from gently sloping irregularities to steep ones.

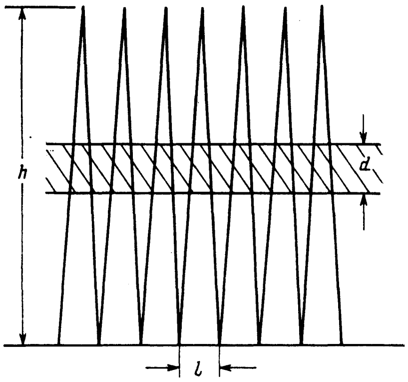

FIG. 2.

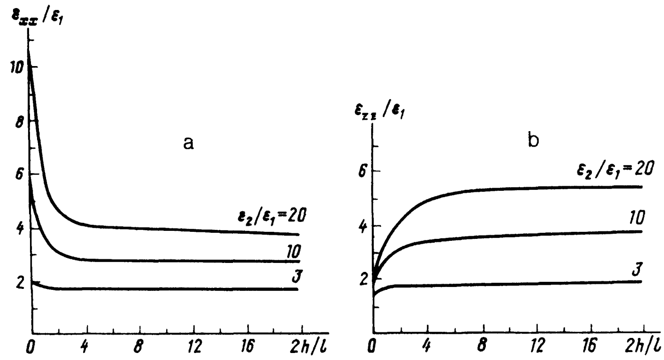

FIG. 3.

Figure 3 shows the results of numerical calculations of the quantities $\varepsilon_{zz}^{\text{eff}}/\varepsilon_1$, and $\varepsilon_{xx}^{\text{eff}}/\varepsilon_1$ as functions of the parameter $2h/l$ for three values of the ratio $\varepsilon_2/\varepsilon_1$: 3, 10, and 20. All the calculated results agree well with the asymptotic values found from (18) and (21) in the cases $2h/l \ll 1$ and $2h/l \gg 1$. Relation (13) is satisfied to within 10^{-3}. Problems for a numerical calculation of the components of the tensor $\hat{\varepsilon}^{\text{eff}}$ are formulated in Appendix II.

Although the weights of the fractions ε_1 and ε_2 are always identical for this type of relief, these curves show that as the ratio $\varepsilon_2/\varepsilon_1$ increases the dependence of $\varepsilon_{zz}^{\text{eff}}$ and $\varepsilon_{xx}^{\text{eff}}$ on the steepness of the relief becomes progressively stronger. With increasing steepness, the value of $\varepsilon_{zz}^{\text{eff}}$ increases, while that of $\varepsilon_{xx}^{\text{eff}}$ decreases. The relative change in these components in the transition from gently sloping teeth to steep teeth is on the order of $(\varepsilon_2/\varepsilon_1)\ln^{-1}(\varepsilon_2/\varepsilon_1)$ for $\varepsilon_{zz}^{\text{eff}}$ and on the order of $(\varepsilon_1/\varepsilon_2)\ln(\varepsilon_2/\varepsilon_1)$ for $\varepsilon_{xx}^{\text{eff}}$ $(\varepsilon_2/\varepsilon_1 \gg 1)$.

This result can be understood qualitatively as follows. In the case of a steep relief, the regions with ε_1 and ε_2 are connected in parallel electrically if the field $\mathbf{E}$ is directed along the z axis, or in series if this field is instead along the x axis. As a result, under the condition $\varepsilon_2 \gg \varepsilon_1$ we have $\varepsilon_{xx} \sim \varepsilon_1$ and $\varepsilon_{zz} \sim \varepsilon_2$ in the leading order. In the case of gently sloping irregularities, we instead have $\varepsilon_{xx} \sim \varepsilon_2$ and $\varepsilon_{zz} \sim \varepsilon_1$.

b) Asymmetric irregularities. If $f(x)$ has only a center of symmetry (no symmetry plane) the tensor $\hat{\varepsilon}^{\text{eff}}$ is nondiagonal: $\varepsilon_{xz} = \varepsilon_{zx} \neq 0$. Figure 4 shows an example of a corrugated surface of this sort:

$$f(x) = \begin{cases} x \operatorname{tg}\alpha, & 0 \leqslant x \leqslant l\cos^2\alpha \\ (l-x)\operatorname{ctg}\alpha, & l\cos^2\alpha \leqslant x \leqslant l \end{cases} \qquad \beta = \pi/2 - \alpha.$$

Figure 5 shows plots of the components of the tensor $\hat{\varepsilon}^{\text{eff}}$ versus the angle α for the values $\varepsilon_2/\varepsilon_1 = 10$ and 16. Relations (12) are satisfied to within the error of these calculations.

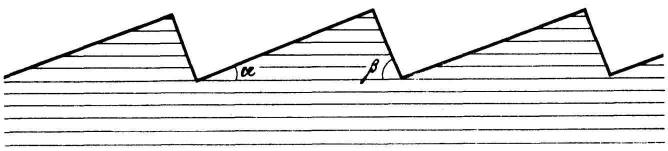

FIG. 4.

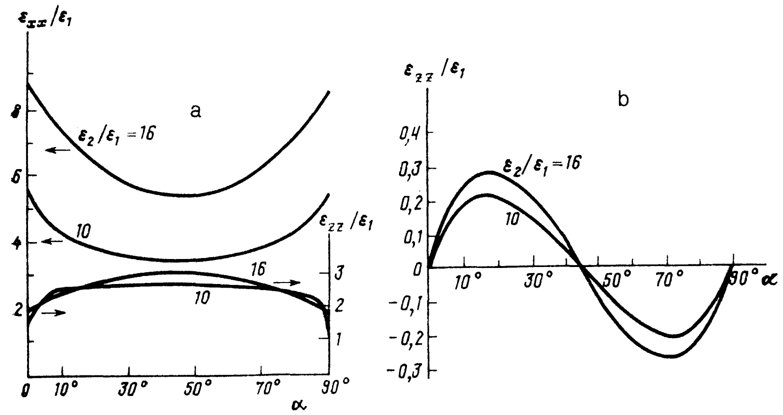

FIG. 5.

The appearance of a component $\varepsilon_{xz}^{\mathrm{eff}}$ can be demonstrated in the example of steep symmetric irregularities (Fig. 2) inclined in such a way that the bisector of the vertex angle makes an angle $\gamma_0 \ll 1$ with the normal to the surface. For triangular irregularities (17), Eqs. (21) determine the components of the tensor $\hat{\varepsilon}_0^{\mathrm{eff}}$ in the coordinate system ξ, η of the irregularity. When we go over to the coordinate system x, z, we find that the effective permittivity tensor becomes

$$\hat{\varepsilon}^{\mathrm{eff}} = \hat{T}\,\hat{\varepsilon}_0^{\mathrm{eff}}\,\hat{T}^{-1},$$

where

$$T=\begin{pmatrix} \cos\gamma_0 & \sin\gamma_0 \\ -\sin\gamma_0 & \cos\gamma_0 \end{pmatrix}$$

is a rotation matrix for a rotation through an angle γ_0. Under the condition $\gamma_0 \ll 1$ we find

$$\varepsilon_{xx} \approx \varepsilon_{\xi\xi} + o(\gamma_0^2),$$
$$\varepsilon_{zz} \approx \varepsilon_{\eta\eta} + o(\gamma_0^2),$$
$$\varepsilon_{xz} \approx (\varepsilon_{\xi\xi} - \varepsilon_{\eta\eta})\gamma_0.$$

REFLECTION FROM AN ANISOTROPIC FILM; SUMMARY OF RESULTS

Let us consider the reflection of a monochromatic plane electromagnetic wave from a system consisting of a semi-infinite homogeneous medium on which there is a plane-parallel anisotropic layer of thickness $h \ll \lambda$. The permittivity of the medium is ε. The permittivity tensor of the film is specified to be

$$\hat{\varepsilon}_1 = \begin{pmatrix} \varepsilon_{xx} & 0 & \varepsilon_{xz} \\ 0 & \varepsilon_{yy} & 0 \\ \varepsilon_{xz} & 0 & \varepsilon_{zz} \end{pmatrix}.$$

The incident and reflected waves propagate in vacuum. The reflection coefficients of this system are

$$R_{pp} = R_p^0 + \frac{2ik_1 h}{(\varepsilon k_1 + k_2)^2}\Big\{k_2^2 \varkappa \cos^2\varphi + k_2^2(\varepsilon_{yy}-1)\sin^2\varphi - \varepsilon^2 k_0^2\Big(1-\frac{1}{\varepsilon_{zz}}\Big)\sin^2\vartheta_0\Big\}.$$

$$R_{ss} = R_s^0 - \frac{2ik_1 k_0^2 h}{(k_1+k_2)^2}\{\varkappa \sin^2\varphi + (\varepsilon_{yy}-1)\cos^2\varphi\},$$

$$R_{ps,sp} = \frac{2ik_0 k_1 h \sin\varphi}{(\varepsilon k_1 + k_2)(k_1+k_2)}\Big\{\mp k_2(\varkappa - \varepsilon_{yy}+1)\cos\varphi + \varepsilon k_0 \frac{\varepsilon_{xz}}{\varepsilon_{zz}}\sin\vartheta_0\Big\}. \qquad (23)$$

Here $k_0 = 2\pi/\lambda$, ϑ_0 is the angle of incidence of the wave, φ is the angle between the plane of incidence of the wave and the xz plane, $\varkappa = \varepsilon_{xx} - 1 - \varepsilon_{xz}^2/\varepsilon_{zz}$, $k_1 = k_0 \cos\vartheta_0$, $k_2 = k_0(\varepsilon - \sin^2\vartheta_0)^{1/2}$, and R_p^0 and R_s^0 are the reflection coefficients in the absence of the layer.

Pchelyakov *et al.*[9] used reflection ellipsometry at $T \approx 750$ °C to study a Si(111) surface cleaved at an angle of 8°. They observed a reversible transition from an ordered system of steps with a height equal to twice the interplanar distance, on the one hand, to an ordered system of steps with a height equal to one interplanar distance, on the other. The terrace size in the first case was ~8 lattice constants, while it was ~4 in the second. The jump in the ellipsometric parameter found experimentally was $\delta\Delta \sim 30'$. The permittivity of Si under the experimental conditions was of order 16.

Although the equation describing the local relationship between **D** and **E** for irregularities with sizes comparable to the lattice constant is, strictly speaking, not valid, the substitution of the calculated components of the tensor $\hat{\varepsilon}^{\mathrm{eff}}$ into (23) (Fig. 5, $\varepsilon_2/\varepsilon_1 = 16$) does lead to an effect of the correct sign and to a jump $\delta\Delta \sim 10.5'$ in the ellipsometric parameter. In this calculation, it was noted that the components of the tensor $\hat{\varepsilon}^{\mathrm{eff}}$ are conserved in the course of a change of this sort in the irregularities. Since the azimuthal angle of φ was not fixed in Ref. 9, our own calculation corresponds to the case $\varphi = 0$.

CONCLUSION

A method has been developed for calculating the components of the effective permittivity tensor $\hat{\varepsilon}^{\mathrm{eff}}$ of a homogeneous but anisotropic thin film which is equivalent (in terms of reflection properties) to a rough surface with characteristic dimensions small in comparison with λ.

To calculate the tensor $\hat{\varepsilon}^{\rm eff}$ it is sufficient to solve the Laplace equation for any relief, of arbitrary complexity, through the use of the known conditions at the interface between the media and through the use of the periodicity of the unknown fields.

The components of $\hat{\varepsilon}^{\rm eff}$ have been calculated analytically for the case of gently sloping and steep irregularities. In the gently sloping case, a transition to random irregularities was made, and a comparison was made with other studies in the literature.

To follow the changes in the components of the tensor $\hat{\varepsilon}^{\rm eff}$ in the transition from gently sloping to steep irregularities, we considered the example of a toothed relief. A numerical calculation yielded results in agreement with the asymptotic values and demonstrated that the geometry of the irregularities is important.

For symmetric reliefs, an exact relation between the components of the tensor $\hat{\varepsilon}^{\rm eff}$ has been derived.

A numerical calculation has been carried out for the components of $\hat{\varepsilon}^{\rm eff}$ for asymmetric irregularities of the step type, for comparison with an experiment by reflection ellipsometry. An agreement was found in order of magnitude and in terms of the sign of the effect.

In all the cases considered, the diagonal components of the tensor $\varepsilon^{\rm eff}$ satisfy the known inequalities

$$\frac{2\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\leqslant \varepsilon_{zz}^{\rm eff},\quad \varepsilon_{xx}^{\rm eff},\quad \varepsilon_{yy}^{\rm eff}\leqslant\frac{\varepsilon_1+\varepsilon_2}{2}.$$

The error level of these calculations is, in order of magnitude, $\max(h,l)/\lambda \ll 1$. All the results on the tensor $\hat{\varepsilon}^{\rm eff}$ are given in the zeroth order in this parameter.

APPENDIX I

The wave equation in a medium with a dielectric constant described by (4) which has an interface $z=f(x)$ is

$$\Delta\mathbf{E}-\text{grad div }\mathbf{E}+k_0^2\varepsilon(z)\mathbf{E}=-k_0^2[\varepsilon(x,z)-\varepsilon(z)]\mathbf{E}, \tag{I.1}$$

where $k_0=\omega/c$, and $\varepsilon_0(z)=\varepsilon_1\theta(z)+\varepsilon_2\theta(-z)$. Using the well-known Green's function $\hat{G}$ of the operator on the left, we go over to an integral equation:

$$\mathbf{E}(x,y,z)=-k_0^2\iiint[\varepsilon(x,z)-\varepsilon_0(z)]\hat{G}(x-x',y-y',z,z')\times\mathbf{E}(x',y',z')dV'+\mathbf{\Phi}(x,y,z). \tag{I.2}$$

The integration here is over the volume between the surface $z=f(x)$ and the xy plane;

$$\mathbf{\Phi}(x,y,z)=\mathbf{\Phi}(z)\exp[i(k_{0x}x+k_{0y}y)]$$

is the solution of homogeneous Eq. (I.2).

Introducing the new function

$$\mathbf{E}'(x,z)=\mathbf{E}(x,y,z)\exp[-i(k_{0x}x+k_{0y}y)],$$

using the k representation of the Green's function $\hat{G}$, and using the relation

$$\int\mathbf{E}'(x',z')\exp[+i(k_x-k_{0x})x']dx'=\frac{2\pi}{l}\int_0^l\mathbf{E}'(x',z')\exp[i(k_x-k_{0x})x']\times\sum_n\delta(k_x-k_{0x}-k_n),$$

we finally find, after an integration over y,

$$\mathbf{E}'(x,z)=-\frac{k_0^2(\varepsilon_2-\varepsilon_1)}{l}\Big\{\iint_\Delta\hat{G}(k_{0x},k_{0y},z,z')\mathbf{E}'(x',z')dS'+\sum_n{}'\exp(-ik_nx)\iint_\Delta\hat{G}(k_{0x}+k_n,k_{0y},z,z')\times\mathbf{E}'(x',z')\exp(ik_nx')dS'\Big\}+\mathbf{\Phi}(z),\quad n\neq0. \tag{I.3}$$

The Δ here means that the integration is carried out over the area of one irregularity in the xz plane.

Since $l\ll\lambda$ (or $k_n\gg k_0$), we see that the field $\mathbf{E}_g'$ in the far zone, $z\gg\lambda$, is determined only by the term with $n=0$ which has been singled out in Eq. (4). The terms with $n\neq0$ determine the fields which are directly related to the relief and which fall off exponentially with distance from the boundary. For $z\gg z'\sim h$, we have

$$\hat{G}(k_{0x}+k_n,k_{0y},z,z')\sim\exp[iq_n(z\pm z')]\sim\exp[-|k_n|(z\pm z')],$$

since $q_n=[k_0^2-k_{0y}^2-(k_{0x}+k_n)^2]^{1/2}\approx i|k_n|$. We finally find

$$\mathbf{E}_g'(x,z)=-\frac{k_0^2(\varepsilon_2-\varepsilon_1)}{l}\hat{G}(k_{0x},k_{0y},z,0)\times\iint_\Delta\mathbf{E}'(x',z')dS'+\mathbf{\Phi}(z). \tag{I.4}$$

The Green's function $\hat{G}$ in this expression has been taken through the integral sign at the point $z'=0$, since we have

$$\hat{G}(k_{0x},k_{0y},z,z')\approx\exp[ik_{0z}(z\pm z')]\sim\exp(ik_{0z}z)[1+o(h/\lambda)],\quad k_{0z}=(k_0^2-k_{0x}^2-k_{0y}^2)^{1/2}.$$

We wish to stress that within $[\max(h,l)]/\lambda$ expression (I.4) is valid for irregularities of an arbitrary type, provided that their characteristic dimensions are small in comparison with the incident wavelength.

A roughness of any type can be described in two equivalent physical models: as elevations on a half-space or as depressions in a half-space. Expression (I.4), written for the elevation model, can also be written for the depression model. In this case, $\mathbf{E}_g'$ determines the fields between the irregularities. In the discussion below we use a combination of these expressions. This approach corresponds to taking an average over the layer (or over the period, in the case of regular irregularities).

The generalization of (I.4) to the case of $3D$ periodic irregularities is obvious: The integral over the area of the irregularity should be replaced by an integral over the volume of the irregularity, divided by the period in the y direction.

APPENDIX II

In the $2D$ case under consideration here, the relationship between $\langle \mathbf{D} \rangle$ and $\langle \mathbf{E} \rangle$ is

$$\langle D_x \rangle = \varepsilon_{zz}^{\text{eff}} \langle E_x \rangle + \varepsilon_{xx}^{\text{eff}} \langle E_z \rangle, \qquad \text{(II.1)}$$
$$\langle D_z \rangle = \varepsilon_{zx}^{\text{eff}} \langle E_x \rangle + \varepsilon_{xz}^{\text{eff}} \langle E_z \rangle.$$

To calculate the components of the tensor $\hat{\varepsilon}^{\text{eff}}$, we need to solve two electrostatic problems. This system should be placed in a uniform electric field, directed along the z axis in one case and along the x axis in the second.

1. In the first case, we solve the problem of finding the electrostatic potential φ such that $\mathbf{E} = -\operatorname{grad} \varphi$. In each of regions I and II (with ε_1 and ε_2), the potential φ satisfies the Laplace equation

$$\frac{\partial^2 \varphi_{\text{I,II}}}{\partial x^2} + \frac{\partial^2 \varphi_{\text{I,II}}}{\partial z^2} = 0, \qquad \text{(II.2)}$$

the periodicity conditions

$$\varphi(0, z) = \varphi(l, z), \quad \left.\frac{\partial \varphi}{\partial x}\right|_{x=0} = \left.\frac{\partial \varphi}{\partial x}\right|_{x=l}, \qquad \text{(II.3)}$$

and boundary conditions on the line $z = f(x)$,

$$\varphi_{\text{I}} = \varphi_{\text{II}}, \quad \varepsilon_1 \frac{\partial \varphi_{\text{I}}}{\partial N} = \varepsilon_2 \frac{\partial \varphi_{\text{II}}}{\partial N}, \qquad \text{(II.4)}$$

where N is the normal to the interface. In addition, we have $\varphi(x, +\infty) = U_1$, $\varphi(x, -\infty) = U_2$. It can be shown that the x component of the average field vanishes by virtue of conditions (II.3) and (II.4):

$$\langle E_x \rangle = \iint \frac{\partial \varphi}{\partial x} dS = 0. \qquad \text{(II.5)}$$

The integration is carried out over the area of a rectangle of height h and length l. From Eqs. (II.1) we then find

$$\varepsilon_{zz}^{\text{eff}} = \frac{\langle D_z \rangle}{\langle E_z \rangle} = \iint \varepsilon(x, z) \frac{\partial \varphi}{\partial z} dS \Big/ \iint \frac{\partial \varphi}{\partial z} dS, \qquad \text{(II.6)}$$
$$\varepsilon_{xz}^{\text{eff}} = \frac{\langle D_x \rangle}{\langle E_z \rangle} = \iint \varepsilon(x, z) \frac{\partial \varphi}{\partial x} dS \Big/ \iint \frac{\partial \varphi}{\partial z} dS.$$

For symmetric irregularities, since the function $f(x)$ and the potential $\varphi(x,z)$ are even, we have $\langle D_x \rangle = 0$ in addition to condition (II.5). It thus follows that we have $\varepsilon_{xz}^{\text{eff}} = 0$.

2. In the second case we find the vector potential $\mathbf{A} = \Psi(x,z)\mathbf{e}_y$ (Ref. 10) such that

$$\mathbf{D} = -\operatorname{rot} \mathbf{A}, \quad D_x = \frac{\partial \Psi}{\partial z}, \quad D_z = -\frac{\partial \Psi}{\partial x}.$$

The function Ψ also satisfies the Laplace equation (II.2) and the periodicity conditions (II.3). The boundary conditions on the line $z = f(x)$ are

$$\Psi_{\text{I}} = \Psi_{\text{II}}, \quad \frac{1}{\varepsilon_1} \frac{\partial \Psi_{\text{I}}}{\partial N} = \frac{1}{\varepsilon_2} \frac{\partial \Psi_{\text{II}}}{\partial N}. \qquad \text{(II.7)}$$

In addition, we have

$$\Psi(x, +\infty) = V_1, \quad \Psi(x, -\infty) = V_2.$$

By virtue of the periodicity conditions and the equality of the potentials on the line $z = f(x)$, we can write

$$\langle D_z \rangle = \iint \frac{\partial \Psi}{\partial x} dS = 0, \qquad \text{(II.8)}$$

and from Eqs. (II.1) we find

$$\varepsilon_{xx}^{\text{eff}} = \frac{\langle D_x \rangle}{\langle E_x \rangle} - \varepsilon_{zx}^{\text{eff}} \frac{\langle E_z \rangle}{\langle E_x \rangle} = \iint \frac{\partial \Psi}{\partial z} dS \Big/ \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial z} dS$$
$$+ \varepsilon_{zz}^{\text{eff}} \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial x} dS \Big/ \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial z} dS,$$
$$\varepsilon_{xz}^{\text{eff}} = -\varepsilon_{xz}^{\text{eff}} \frac{\langle E_z \rangle}{\langle E_x \rangle}$$
$$= \varepsilon_{zz}^{\text{эфф}} \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial x} dS \Big/ \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial z} dS, \qquad \text{(II.9)}$$

where $\varepsilon_{zz}^{\text{eff}}$ and $\varepsilon_{xz}^{\text{eff}}$ are given by (II.6). If the irregularities are symmetric, the equality $\langle E_z \rangle = 0$ holds along with condition (II.8). We then have $\varepsilon_{zx}^{\text{eff}} = 0$ and

$$\varepsilon_{xx}^{\text{eff}} = \frac{\langle D_x \rangle}{\langle E_x \rangle} = \iint \frac{\partial \Psi}{\partial z} dS \Big/ \iint \frac{1}{\varepsilon(x, z)} \frac{\partial \Psi}{\partial z} dS. \qquad \text{(II.10)}$$

In the case of symmetric irregularities, the periodicity conditions in (II.3) can be replaced by

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x=0} = \left.\frac{\partial \varphi}{\partial x}\right|_{x=l/2} = 0, \quad \left.\frac{\partial \Psi}{\partial x}\right|_{x=0} = \left.\frac{\partial \Psi}{\partial x}\right|_{x=l/2} = 0,$$

and we can examine the x interval $0 \leqslant x \leqslant l/2$.

Equations (II.6) and (II.9) can be used for $2D$ reliefs which are periodic and otherwise arbitrary; it is not necessary that relations (12) hold.

[1] Formal calculations which confirm these arguments are given in Appendix I for readers who prefer a formal derivation to a physical level of rigor.

[2] In a recent paper[8] (submitted for publication half a year after the present paper), Aspnes takes up a corresponding problem: calculating the change in the reflection coefficient associated with the presence of a low relief at an interface between two media for the case of a normally incident wave. The first-order effect is proportional to the surface integral of the local potential. That approach is successful in solving the problem only for a relief of a certain shape, for which the local potential can be determined from auxiliary considerations. The reflection coefficients calculated in the present paper, for two types of relief—steep trench irregularities and gently sloping sinusoidal irregularities—are completely the same as the results of Ref. 8.

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