Determination of the normalized surface height autocorrelation function of a two-dimensional randomly rough dielectric surface by the inversion of light scattering data in p-polarization

J.B. Kryvi^a, I. Simonsen^{a,b}, and A.A. Maradudin^c

^aDepartment of Physics, NTNU Norwegian University of Sciences and Technology, NO-7491 Trondheim, Norway

^bSurface du Verre et Interfaces, UMR 125 CNRS/Saint-Gobain, F-93303 Aubervilliers, France ^cDepartment of Physics and Astronomy, University of California, Irvine, CA 92697, U.S.A.

ABSTRACT

The contribution to the mean differential reflection coefficient from the in-plane, co-polarized scattering of ppolarized light from a two-dimensional randomly rough dielectric surface is used to invert scattering data to obtain the normalized surface height autocorrelation function of the surface. Within phase perturbation theory this contribution to the mean differential reflection coefficient possesses singularities (poles) when the polar scattering angle θ_s equals $\pm \theta_B = \pm \tan^{-1} \sqrt{\varepsilon}$, where ε is the dielectric constant of the dielectric medium and θ_B is the Brewster angle. Nevertheless, we show in this paper that if the mean differential reflection coefficient is measured only in the angular range $|\theta_s| < \theta_B$, these data can be inverted to yield accurate results for the normalized surface height correlation function for weakly rough surfaces. Several parameterized forms of this correlation function, and the minimization of a cost function with respect to the parameters defining these representations, are used in the inversion scheme. This approach also yields the rms height of the surface roughness, and the dielectric constant of the scattering medium if it is not known in advance. The input data used in this minimization procedure consist of computer simulation results for surfaces defined by exponential and Gaussian surface height correlation functions, without and with the addition of multiplicative noise. The proposed inversion scheme is computationally efficient.

1. INTRODUCTION

In a recent paper by the present authors and their colleagues,¹ a method based on second-order phase perturbation theory² was presented for inverting experimental scattering data to obtain certain statistical properties of the roughness of a two-dimensional randomly rough dielectric surface. The scattering data set used in this inversion scheme was the dependence on the polar scattering angle of the contribution to the mean differential reflection coefficient from the in-plane co-polarized component of the light scattered diffusely from the surface when the latter is illuminated by s-polarized light. The statistical properties of the random surface obtained by this approach were the normalized surface height autocorrelation function, the rms height of the surface roughness, the transverse correlation length of the surface roughness, and the dielectric constant of the substrate if it is not known in advance. The determination of these parameters was quite accurate, for weakly rough surfaces.

It therefore seemed worthwhile to explore the inversion of the contribution to the mean differential reflection coefficient from the in-plane, co-polarized light of p polarization scattered from a two-dimensional randomly rough dielectric surface to obtain the normalized surface height autocorrelation function. Within phase perturbation theory this contribution to the mean differential reflection coefficient possesses poles when the polar angle of scattering θ_s equals $\pm \theta_B = \pm \tan^{-1} \sqrt{\varepsilon}$, where ε is the dielectric constant of the dielectric medium and θ_B is the Brewster angle. Nevertheless, we show in this paper that if the mean differential reflection coefficient is measured only in the angular interval $|\theta_s| < \theta_B$, these data can be inverted to yield accurate results for the normalized surface height autocorrelation function of weakly rough surfaces.

Correspondence should be addressed to A.A. Maradudin, aamaradu@uci.edu.

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The inversion is carried out by creating several parameterized forms of the surface height autocorrelation functions and minimizing a cost function with respect to the parameters defining these forms. The input scattering data used in the minimization of the cost function consist of computer simulation results obtained with the assumption of exponential and Gaussian surface height autocorrelation functions, with and without the addition of multiplicative noise. The use of a mean differential reflection coefficient generated by a known normalized surface height autocorrelation function in our inversion approach enables us to assess the quality of the reconstructions we obtain.

This approach also yields the rms height of the surface roughness, and the dielectric constant of the scattering medium if it is not known in advance. It is computationally efficient.

2. THE SYSTEM STUDIED

The physical system we study in this paper consists of vacuum in the region $x_3 > \zeta(\mathbf{x}_{\parallel})$, and a dielectric medium, whose dielectric constant is ε , in the region $x_3 < \zeta(\mathbf{x}_{\parallel})$ (Fig. 1). Here $\mathbf{x}_{\parallel} = (x_1, x_2, 0)$ is a position vector in the plane $x_3 = 0$. The surface profile function $\zeta(\mathbf{x}_{\parallel})$ is assumed to be a single-valued function of \mathbf{x}_{\parallel} that is differentiable with respect to x_1 and x_2 . It is also assumed to constitute a stationary, zero-mean, isotropic, Gaussian random process defined by

$$\left\langle \zeta(\mathbf{x}_{\parallel})\zeta(\mathbf{x}_{\parallel}')\right\rangle = \delta^2 W(|\mathbf{x}_{\parallel} - \mathbf{x}_{\parallel}'|)$$
 (1a)

$$\left\langle \zeta^2(\mathbf{x}_{\parallel}) \right\rangle = \delta^2,\tag{1b}$$

where the angle brackets denote an average over the ensemble of realizations of $\zeta(\mathbf{x}_{\parallel})$, δ is the rms height of the surface, and $W(|\mathbf{x}_{\parallel}|)$ is the normalized surface height autocorrelation function. It has the property that W(0) = 1.

We introduce the Fourier integral representation of the surface profile function

$$\zeta(\mathbf{x}_{\parallel}) = \int \frac{d^2 Q_{\parallel}}{(2\pi)^2} \hat{\zeta}(\mathbf{Q}_{\parallel}) \exp(i\mathbf{Q}_{\parallel} \cdot \mathbf{x}_{\parallel}), \tag{2}$$

where $\mathbf{Q}_{\parallel} = (Q_1, Q_2, 0)$, so that

$$\hat{\zeta}(\mathbf{Q}_{\parallel}) = \int d^2 x_{\parallel} \zeta(\mathbf{x}_{\parallel}) \exp(-i\mathbf{Q}_{\parallel} \cdot \mathbf{x}_{\parallel}).$$
(3a)

We also introduce the function

$$\hat{\zeta}^{(n)}(\mathbf{Q}_{\parallel}) = \int d^2 x_{\parallel} \zeta^n(\mathbf{x}_{\parallel}) \exp(-i\mathbf{Q}_{\parallel} \cdot \mathbf{x}_{\parallel}), \tag{3b}$$

so that $\hat{\zeta}^{(0)}(\mathbf{Q}_{\parallel}) = (2\pi)^2 \delta\left(\mathbf{Q}_{\parallel}\right)$ and $\hat{\zeta}^{(1)}(\mathbf{Q}_{\parallel}) = \hat{\zeta}(\mathbf{Q}_{\parallel})$.

The Fourier coefficient $\hat{\zeta}(\mathbf{Q}_{\parallel})$ is a zero-mean Gaussian random process defined by

$$\left\langle \hat{\zeta}(\mathbf{Q}_{\parallel})\hat{\zeta}(\mathbf{Q}_{\parallel}')\right\rangle = (2\pi)^2 \delta(\mathbf{Q}_{\parallel} + \mathbf{Q}_{\parallel}')\delta^2 g(Q_{\parallel}),\tag{4}$$

where $g(Q_{\parallel})$, the power spectrum of the surface roughness, is defined by

$$g(Q_{\parallel}) = \int d^2 x_{\parallel} W(|\mathbf{x}_{\parallel}|) \exp(-i\mathbf{Q}_{\parallel} \cdot \mathbf{x}_{\parallel}).$$
(5)

It follows from Eqs. (1) and (5) that $g(Q_{\parallel})$ is normalized to unity,

$$\int \frac{d^2 Q_{\parallel}}{(2\pi)^2} g(Q_{\parallel}) = 1.$$
(6)

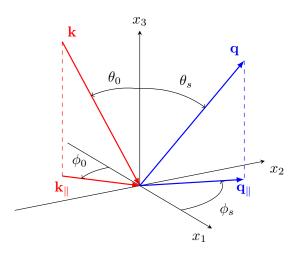


Figure 1. A schematic depiction of the scattering geometry considered in this work.

3. SCATTERING THEORY

The surface $x_3 = \zeta(\mathbf{x}_{\parallel})$ is illuminated from the vacuum by an electromagnetic field of frequency ω . The electric field in the vacuum above the surface is the sum of an incident and a scattered field, $\mathbf{E}(\mathbf{x},t) = [\mathbf{E}^{(i)}(\mathbf{x}|\omega) + \mathbf{E}^{(s)}(\mathbf{x}|\omega)] \exp(-i\omega t)$, where

$$\mathbf{E}^{(i)}(\mathbf{x}|\omega) = \left\{ -\frac{c}{\omega} \left[\hat{\mathbf{k}}_{\parallel} \alpha_0(k_{\parallel}) + \hat{\mathbf{x}}_3 k_{\parallel} \right] B_p(\mathbf{k}_{\parallel}) + \left[\hat{\mathbf{x}}_3 \times \hat{\mathbf{k}}_{\parallel} \right] B_s(\mathbf{k}_{\parallel}) \right\} \exp\left[i \{ \mathbf{k}_{\parallel} - \hat{\mathbf{x}}_3 \alpha_0(\mathbf{k}_{\parallel}) \} \cdot \mathbf{x} \right]$$
(7a)

$$\mathbf{E}^{(s)}(\mathbf{x}|\omega) = \int \frac{d^{-}q_{\parallel}}{(2\pi)^{2}} \left\{ \frac{c}{\omega} \left[\hat{\mathbf{q}}_{\parallel} \alpha_{0}(\mathbf{q}_{\parallel}) - \hat{\mathbf{x}}_{3}q_{\parallel} \right] A_{p}(\mathbf{q}_{\parallel}) + \left[\hat{\mathbf{x}}_{3} \times \hat{\mathbf{q}}_{\parallel} \right] A_{s}(\mathbf{q}_{\parallel}) \right\} \exp \left[i \{ \mathbf{q}_{\parallel} + \hat{\mathbf{x}}_{3}\alpha_{0}(q_{\parallel}) \} \cdot \mathbf{x} \right].$$
(7b)

The subscripts p and s denote the p-polarized (TM) and s-polarized (TE) components of each of these fields, respectively. A caret over a vector indicates it is a unit vector. In writing Eqs. (7) we have introduced the function $\alpha_0(q_{\parallel})$ defined by

$$\alpha_0(q_{\parallel}) = \left[\left(\frac{\omega}{c}\right)^2 - q_{\parallel}^2 \right]^{\frac{1}{2}}, \quad \operatorname{Re}\alpha_0(q_{\parallel}) > 0, \operatorname{Im}\alpha_0(q_{\parallel}) > 0.$$
(8)

Maxwell's equations imply linear relations between $A_{\alpha}(\mathbf{q}_{\parallel})$ and $B_{\beta}(\mathbf{k}_{\parallel})$, which we write in the form ($\alpha = p, s, \beta = p, s$)

$$A_{\alpha}(\mathbf{q}_{\parallel}) = \sum_{\beta} \frac{\alpha_0^{\frac{1}{2}}(q_{\parallel})}{\alpha_0^{\frac{1}{2}}(k_{\parallel})} S_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) B_{\beta}(\mathbf{k}_{\parallel}), \tag{9}$$

where $\mathbf{S}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})$ is the scattering matrix. The elements of the scattering matrix play a significant role in the present theory because the mean differential reflection coefficient is expressed in terms of them. The differential reflection coefficient $(\partial R_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})/\partial \Omega_s)$ is defined such that $[\partial R_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})/\partial \Omega_s]d\Omega_s$ is the fraction of the total time-averaged flux in an incident field of β polarization, the projection of whose wave vector on the mean scattering plane is \mathbf{k}_{\parallel} , that is scattered into a field of α polarization, the projection of whose wave vector on the mean scattering plane is \mathbf{q}_{\parallel} , within an element of solid angle $d\Omega_s$ about the scattering direction defined by the polar and azimuthal scattering angles (θ_s, ϕ_s) . It is given by³

$$\frac{\partial R_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})}{\partial \Omega_s} = \frac{1}{S} \left(\frac{\omega}{2\pi c}\right)^2 \cos\theta_s \left| S_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) \right|^2, \tag{10}$$

with (see Fig. 1)

$$\mathbf{k}_{\parallel} = -\frac{\omega}{c} \sin \theta_0 (\cos \phi_0, \sin \phi_0, 0) \tag{11a}$$

$$\mathbf{q}_{\parallel} = -\frac{\omega}{c} \sin \theta_s (\cos \phi_s, \sin \phi_s, 0), \tag{11b}$$

where (θ_0, ϕ_0) and (θ_s, ϕ_s) are the polar and azimuthal angles of incidence and scattering, respectively. S is the area of the plane $x_3 = 0$ covered by the rough surface. Since we are dealing with scattering from a randomly rough surface, it is the average of this function over the ensemble of realizations of the surface profile function that we have to calculate. The contribution to this average from the light scattered incoherently (diffusely) is

$$\left\langle \frac{\partial R_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})}{\partial \Omega_{s}} \right\rangle_{\text{incoh}} = \frac{1}{S} \left(\frac{\omega}{2\pi c} \right)^{2} \cos \theta_{s} \left[\left\langle |S_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})|^{2} \right\rangle - |\left\langle S_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) \right\rangle|^{2} \right].$$
(12)

The definition of the mean differential reflection coefficient in terms of the elements of the scattering matrix is useful. Because they satisfy the reciprocity relations⁴

$$S_{pp}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = S_{pp}(-\mathbf{k}_{\parallel}|-\mathbf{q}_{\parallel}) \tag{13a}$$

$$S_{ss}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = S_{ss}(-\mathbf{k}_{\parallel}|-\mathbf{q}_{\parallel})$$
(13b)

$$S_{ps}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = -S_{sp}(-\mathbf{k}_{\parallel}|-\mathbf{q}_{\parallel}), \tag{13c}$$

their satisfaction serves as a check on the correctness of their derivation.

It is shown in Ref. 5 that the pp element of the expression given by Eq. (12) obtained on the basis of second order phase perturbation theory can be written as

$$\left\langle \frac{\partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel})}{\partial \Omega_{s}} \right\rangle_{\text{incoh}} = 2\pi \left(\frac{\omega}{2\pi c} \right)^{2} (\varepsilon - 1)^{2} \frac{|f(q_{\parallel})f(k_{\parallel})|}{|d_{p}(q_{\parallel})d_{p}(k_{\parallel})|^{2}} \cos \theta_{s} \exp[-2M(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel})] \\ \times \sum_{n=1}^{\infty} \frac{1}{n!} \left[4\delta^{2} \left| \frac{\alpha_{0}(q_{\parallel})\alpha_{0}(k_{\parallel})}{f(q_{\parallel})f(k_{\parallel})} \right| \left| H_{p}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) \right|^{2} \right]^{n} \int_{0}^{\infty} du_{\parallel} u_{\parallel} J_{0}(|\mathbf{q}_{\parallel} - \mathbf{k}_{\parallel} | u_{\parallel}) W^{n}(u_{\parallel}), \quad (14)$$

where $J_0(z)$ is the Bessel function of the first kind and order zero. In writing this expression we have introduced the functions

$$d_p(q_{\parallel}) = \varepsilon \alpha_0(q_{\parallel}) + \alpha(q_{\parallel}) \tag{15a}$$

$$d_s(q_{\parallel}) = \alpha_0(q_{\parallel}) + \alpha(q_{\parallel}), \tag{15b}$$

where

$$\alpha(q_{\parallel}) = \left[\varepsilon \left(\frac{\omega}{c}\right)^2 - q_{\parallel}^2\right]^{\frac{1}{2}}, \quad \operatorname{Re}\alpha(q_{\parallel}) > 0 \quad \operatorname{Im}\alpha(q_{\parallel}) > 0, \tag{16}$$

and

$$f(q_{\parallel}) = \varepsilon \left(\frac{\omega}{c}\right)^2 - (\varepsilon + 1)q_{\parallel}^2.$$
(17)

The function $2M(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})$ is given by

$$2M(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = -4\delta^{2}\operatorname{Re}\left[\frac{\alpha_{0}(q_{\parallel})\alpha_{0}(k_{\parallel})}{f(q_{\parallel})f(k_{\parallel})}\right]^{\frac{1}{2}}\int\frac{d^{2}p_{\parallel}}{(2\pi)^{2}}F_{p}(\mathbf{q}_{\parallel}|\mathbf{p}_{\parallel}|\mathbf{k}_{\parallel})g(|\mathbf{p}_{\parallel}-\mathbf{k}_{\parallel}|),\tag{18}$$

where

$$F_{p}(\mathbf{q}_{\parallel}|\mathbf{p}_{\parallel}|\mathbf{k}_{\parallel}) = \frac{1}{2} \left[\alpha(q_{\parallel}) + \alpha(k_{\parallel}) \right] \left[q_{\parallel}k_{\parallel} - \alpha(q_{\parallel})\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel}\alpha(k_{\parallel}) \right] \\ + \left(\frac{\varepsilon - 1}{\varepsilon} \right) \left\{ \alpha(q_{\parallel})\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{p}}_{\parallel}\alpha(p_{\parallel})\hat{\mathbf{p}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel}\alpha(k_{\parallel}) \right. \\ \left. - \frac{\left[\varepsilon q_{\parallel}p_{\parallel} - \alpha(q_{\parallel})\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{p}}_{\parallel}\alpha(p_{\parallel}) \right] \left[\varepsilon p_{\parallel}k_{\parallel} - \alpha(p_{\parallel})\hat{\mathbf{p}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel}\alpha(k_{\parallel}) \right]}{d_{p}(p_{\parallel})} \\ \left. - \varepsilon \left(\frac{\omega}{c} \right)^{2} \frac{\alpha(q_{\parallel})[\hat{\mathbf{q}}_{\parallel} \times \hat{\mathbf{p}}_{\parallel}]_{3}[\hat{\mathbf{p}}_{\parallel} \times \hat{\mathbf{k}}_{\parallel}]_{3}\alpha(k_{\parallel})}{d_{s}(p_{\parallel})} \right\}.$$
(19)

The function $H_p(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})$ is defined by

$$H_p(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = \varepsilon q_{\parallel}k_{\parallel} - \alpha(q_{\parallel})\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel}\alpha(k_{\parallel}).$$
⁽²⁰⁾

We can rewrite the expression for $2M(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})$ in terms of $W(|\mathbf{x}_{\parallel}|)$ in the following way. We begin by writing $g(|\mathbf{q}_{\parallel} - \mathbf{k}_{\parallel})$ with the aid of Eq. (5) as

$$g(|\mathbf{q}_{\parallel} - \mathbf{k}_{\parallel}|) = \int d^{2}x_{\parallel} W(x_{\parallel}) \exp\left[-i(\mathbf{q}_{\parallel} - \mathbf{k}_{\parallel}) \cdot \mathbf{x}_{\parallel}\right]$$
$$= \sum_{m=-\infty}^{\infty} g_{m}(q_{\parallel}|k_{\parallel}) \exp\left[im(\phi_{q} - \phi_{k})\right],$$
(21a)

where

$$g_m(q_{\parallel}|k_{\parallel}) = 2\pi \int_0^\infty dx_{\parallel} x_{\parallel} W(x_{\parallel}) J_m(q_{\parallel} x_{\parallel}) J_m(k_{\parallel} x_{\parallel})$$

= $g_{-m}(q_{\parallel}|k_{\parallel}).$ (21b)

In Eq. (21) ϕ_q and ϕ_k are the azimuthal angles of the unit vectors $\hat{\mathbf{q}}_{\parallel}$ and $\hat{\mathbf{k}}_{\parallel}$, respectively, measured from the positive x_1 axis (see Fig. 1). When Eq. (21a) is substituted into Eq. (18) and the angular integrals are carried out, we obtain the result

$$2M(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = -4\delta^2 Re \left[\frac{\alpha_0(q_{\parallel})\alpha_0(k_{\parallel})}{f(q_{\parallel})f(k_{\parallel})}\right]^{\frac{1}{2}} I(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}),$$
(22)

where

$$\begin{split} I(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) &= \frac{1}{2} q_{\parallel} [\alpha(q_{\parallel}) + \alpha(k_{\parallel})] k_{\parallel} \\ &+ \frac{1}{4\pi} \int_{0}^{\infty} dp_{\parallel} p_{\parallel} \left\{ -\left(\frac{\varepsilon - 1}{\varepsilon}\right) \frac{1}{d_{p}(p_{\parallel})} \left[2\varepsilon^{2} q_{\parallel} p_{\parallel}^{2} k_{\parallel} g_{0}(p_{\parallel}|k_{\parallel}) - 2\varepsilon q_{\parallel} p_{\parallel} \alpha(p_{\parallel}) \alpha(k_{\parallel}) g_{1}(p_{\parallel}|k_{\parallel}) \right] \right\} \\ &+ \left(\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel} \right) \left[-\frac{1}{2} \alpha(q_{\parallel}) \left[\alpha(q_{\parallel}) + \alpha(k_{\parallel}) \right] \alpha(k_{\parallel}) \right. \\ &+ \frac{1}{4\pi} \int_{0}^{\infty} dp_{\parallel} p_{\parallel} \left\{ \left(\frac{\varepsilon - 1}{\varepsilon} \right) \alpha(q_{\parallel}) \alpha(p_{\parallel}) \alpha(k_{\parallel}) \left[g_{0}(p_{\parallel}|k_{\parallel}) + g_{2}(p_{\parallel}|k_{\parallel}) \right] \right. \\ &+ 2(\varepsilon - 1) \frac{\alpha(q_{\parallel}) p_{\parallel} \alpha(p_{\parallel}) k_{\parallel}}{d_{p}(p_{\parallel})} g_{1}(p_{\parallel}|k_{\parallel}) - \left(\frac{\varepsilon - 1}{\varepsilon}\right) \frac{\alpha(q_{\parallel}) \alpha^{2}(p_{\parallel}) \alpha(k_{\parallel})}{d_{p}(p_{\parallel})} \left[g_{0}(p_{\parallel}|k_{\parallel}) - g_{2}(p_{\parallel}|k_{\parallel}) \right] \\ &+ (\varepsilon - 1) \left(\frac{\omega}{\varepsilon}\right)^{2} \frac{\alpha(q_{\parallel}) \alpha(k_{\parallel})}{d_{s}(p_{\parallel})} \left[g_{0}(p_{\parallel}|k_{\parallel}) - g_{2}(p_{\parallel}|k_{\parallel}) \right] \right\} \end{split}$$
(23)

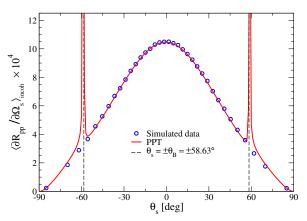


Figure 2. The contribution to the mean differential reflection coefficient from the in-plane, co-polarized p-polarized light scattered incoherently from a Gaussianly-correlated two-dimensional randomly rough dielectric surface as a function of the polar angle of scattering, obtained from computer simulations (circles) and from second-order phase perturbation theory (solid curve). The values of the surface roughness parameters assumed in these calculations are $\delta = 15.8$ nm, a = 158.20 nm, while the dielectric constant of the scattering medium is $\varepsilon = 2.64$, the wavelength of the p-polarized light incident on the surface is $\lambda = 632.8$ nm, and the polar angle of incidence is $\theta = 1.6^{\circ}$.

For in-plane $[\hat{\mathbf{q}}_{\parallel} \parallel \hat{\mathbf{k}}_{\parallel}]$ scattering and normal incidence, $\mathbf{k}_{\parallel} = \mathbf{0}$, Eq. (14) becomes

$$\left\langle \frac{\partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{0})}{\partial \Omega_{s}} \right\rangle_{\text{incoh}} = \frac{1}{2\pi} \left(\frac{\omega}{c} \right)^{2} \left(\sqrt{\varepsilon} - 1 \right)^{2} \frac{\left| f(q_{\parallel}) \right|}{\left| d_{p}(q_{\parallel}) \right|^{2}} \cos \theta_{s} \exp[-2M(\mathbf{q}_{\parallel} | \mathbf{0})] \\ \times \sum_{n=1}^{\infty} \frac{1}{n!} \left[4\delta^{2} \frac{\omega}{c} \frac{\alpha_{0}(q_{\parallel})\alpha^{2}(q_{\parallel})}{\left| f(q_{\parallel}) \right|} \right]^{n} \int_{0}^{\infty} du_{\parallel} u_{\parallel} J_{0}(q_{\parallel} u_{\parallel}) W^{n}(u_{\parallel}), \tag{24}$$

where

$$2M(\mathbf{q}_{\parallel}|\mathbf{0}) = -4\delta^2 \left(\varepsilon \frac{\omega}{c}\right)^{-\frac{1}{2}} \operatorname{Re} \left(\frac{\alpha_0(q_{\parallel})}{f(q_{\parallel})}\right)^{\frac{1}{2}} I(\mathbf{q}_{\parallel}|\mathbf{0})$$

with

$$I(\mathbf{q}_{\parallel}|\mathbf{0}) = -\frac{1}{2}\alpha(q_{\parallel}) \left[\alpha(q_{\parallel}) + \alpha(0)\right]\alpha(0) + \frac{1}{4\pi} \frac{\varepsilon - 1}{\varepsilon} \alpha(q_{\parallel}) \int_{0}^{\infty} dp_{\parallel} p_{\parallel} g_{0}(p_{\parallel}|0) \left[\alpha(p_{\parallel}) - \frac{\alpha^{2}(p_{\parallel})}{d_{p}(p_{\parallel})} + \varepsilon \frac{(\omega/c)^{2}}{d_{s}(p_{\parallel})}\right] \alpha(0).$$

$$(25)$$

There is a difficulty with the expression for $\langle \partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) / \partial \Omega_s \rangle_{\text{incoh}}$ given by Eq. (14). The function $f(q_{\parallel})$ Eq. (17), vanishes when $q_{\parallel} = (\omega/c) \sin \theta_s$ equals $(\omega/c) [\varepsilon/(\varepsilon+1)]^{\frac{1}{2}}$, i.e. when $\theta_s = \sin^{-1} [\varepsilon/(\varepsilon+1)]^{\frac{1}{2}} = \tan^{-1} \sqrt{\varepsilon}$. This angle is the Brewster angle θ_B at which the Fresnel reflection amplitude vanishes when a planar vacuumdielectric interface is illuminated from the vacuum by p-polarized light. Because of the presence of $f(q_{\parallel})$ in the denominator of the expression (18) for the function $2M(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel})$, the phase perturbation theory result for $\langle R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) / \partial \Omega_s \rangle_{\text{incoh}}$ has infinities rather than zeros at $\theta_s = \pm \theta_B$, independently of the angle of incidence θ_0 . This is illustrated by the result for $\langle \partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) \rangle_{\text{incoh}}$ calculated by second-order phase perturbation theory and plotted in Fig. 2. For comparison we have also plotted in this figure the result obtained by a rigorous numerical solution of the reduced Rayleigh equation for this scattering problem.⁴ It is seen that the result produced by phase perturbation theory agrees well with the one produced by the solution of the reduced Rayleigh equation, except in the immediate vicinity of the Brewster angles. In the remainder of this paper we will show that despite the presence of the singularities in $\langle \partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) / \partial \Omega_s \rangle_{\text{incoh}}$ to which it gives rise, second-order phase perturbation theory can still be used to invert experimental scattering data obtained in the angular interval $|\theta_s| < \theta_B$ to produce a good reconstruction of $W(|\mathbf{x}_{\parallel}|)$.

4. THE INVERSE PROBLEM

As was done in Ref. 1, and earlier in Ref. 6, to determine the function $W(x_{\parallel})$ from scattering data for $\langle \partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel}) / \partial \Omega_s \rangle_{\text{incoh, input}}$, we assume an analytic form for it that contains adjustable parameters. The values of these parameters, as well as the rms height δ , are determined by varying them to minimize a cost function. The cost function we use is

$$\chi^{2}(\mathcal{P}) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta_{s} \left[\left\langle \frac{\partial R_{pp}(\theta_{s})}{\partial \Omega_{s}} \right\rangle_{\text{incoh, input}} - \left\langle \frac{\partial R_{pp}(\theta_{s})}{\partial \Omega_{s}} \right\rangle_{\text{incoh, calc}} \right]^{2},$$
(26a)

where *in-plane* scattering data are defined as

$$\left\langle \frac{\partial R_{pp}(\theta_s)}{\partial \Omega_s} \right\rangle_{\text{incoh}} = \left\langle \frac{\partial R_{pp}(\mathbf{q}_{\parallel} | \mathbf{k}_{\parallel})}{\partial \Omega_s} \right\rangle_{\text{incoh}} \bigg|_{|\hat{\mathbf{q}}_{\parallel} \cdot \hat{\mathbf{k}}_{\parallel}| = 1}.$$
 (26b)

Here \mathcal{P} denotes the set of variational parameters used to characterize $\langle \partial R_{pp}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})/\partial \Omega_s \rangle_{\text{incoh,calc}}$. The minimization of this function with respect to the elements of \mathcal{P} was carried out by the use of the routine "Imdif1" contained in the Fortran package MINPACK which is part of the general purpose mathematical library SLATEC.⁷ The routine Imdif1 implements a modified version of the Levenberg-Marquardt algorithm,^{8,9} and it calculates the Jacobian by a forward-difference approximation.

In our reconstruction calculations for the input function $\langle \partial R_{pp}(\theta_s) / \partial \Omega_s \rangle_{\text{incoh,input}}$ we used results of rigorous nonperturbative, purely numerical solutions^{10, 11} of the reduced Rayleigh equation for the scattering amplitudes in the scattering of polarized light from a two-dimensional randomly rough dielectric surface.⁴ These calculations were carried out for an ensemble of N_p random surfaces generated¹¹ on the basis of expressions for $W(x_{\parallel})$ of either the exponential form

$$W(x_{\parallel}) = \exp\left(-\frac{x_{\parallel}}{a}\right),\tag{27}$$

or the Gaussian form

$$W(\mathbf{x}_{\parallel}) = \exp\left[-\left(\frac{x_{\parallel}}{a}\right)^2\right].$$
(28)

In both of these expressions the characteristic length a is the transverse correlation length of the surface roughness.

For the function $\langle \partial R_{pp}(\theta_s) / \partial \Omega_s \rangle_{\text{incoh,calc}}$ we used the expression for it, obtained by the use of second-order phase perturbation theory, given by Eq. (14), evaluated for the trial function assumed to represent $W(x_{\parallel})$. Three forms for this trial function were used in our calculations. They are the exponential,

$$W(x_{\parallel}) = \exp\left(-\frac{x_{\parallel}}{a^{\star}}\right),\tag{29a}$$

the Gaussian,

$$W(x_{\parallel}) = \exp\left[-\left(\frac{x_{\parallel}}{a^{\star}}\right)^2\right],\tag{29b}$$

and the stretched exponential,

$$W(x_{\parallel}) = \exp\left[-\left(\frac{x_{\parallel}}{a^{\star}}\right)^{\gamma^{\star}}\right].$$
(29c)

In the first two cases the variational parameters for the reconstruction are δ^* , a^* , and potentially ε^* . In the third case they are δ^* , a^* , γ^* , and potentially ε^* .

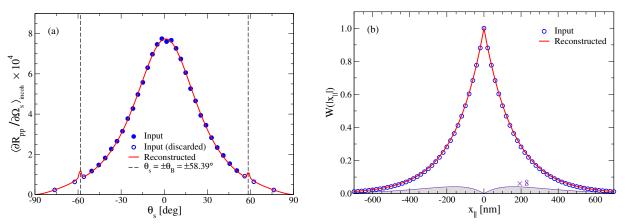


Figure 3. Reconstruction of the rms roughness δ^* and transverse correlation length a^* from scattering data obtained for an exponentially correlated dielectric surface. (a) The incoherent component of the in-plane, co-polarized (p-to-p) mean differential reflection coefficient $\langle \partial R_{pp} / \partial \Omega_s \rangle_{incoh}$ as a function of the polar angle of scattering θ_s obtained from computer simulations (circles) and from second-order phase perturbation theory, with the use of the reconstructed surface roughness parameters (solid curve), for a two-dimensional randomly rough dielectric surface defined by Eq. (27). The trial function for $W(|\mathbf{x}_{\parallel}|)$ in the reconstruction procedure has the exponential form given by Eq. (29a). The surface roughness parameters assumed in the computer simulations have the values $\delta = 9.50$ nm, and a = 158.20 nm. The reconstructed values of these parameters are $\delta^* = 9.45$ nm and $a^* = 160.465$ nm. The dielectric constant of the scattering medium is $\varepsilon = 2.64$, and the wavelength of the incident light is $\lambda = 632.8$ nm. The polar angle of incidence is $\theta_0 = 1.6^\circ$. (b) The input (open circles) and reconstructed (solid curve) surface height autocorrelation function $W(|\mathbf{x}_{\parallel}|)$ for the random surface. The shaded gray region represents the absolute difference between the input and reconstructed surface height autocorrelation functions.

5. RESULTS

We illustrate the inversion method presented here by applying it to the reconstruction of $W(|\mathbf{x}_{\parallel})$.

5.1 Exponentially Correlated Surface Roughness

For the first scattering system we consider it is assumed that the surface height autocorrelation function $W(|\mathbf{x}_{\parallel}|)$ is exponential, Eq. (27), and is characterized by a transverse correlation length a = 158.20 nm and an rms height $\delta = 9.50$ nm. The dielectric constant of the scattering medium is $\varepsilon = 2.64$, the corresponding Brewster's angle $\theta_B = 58.39^{\circ}$, the wavelength of the incident light is $\lambda = 632.8$ nm, and the polar angle of incidence is $\theta_0 = 1.6^{\circ}$. By the method of Ref. 11 the mean differential reflection coefficient was calculated as a function of the polar angle of scattering θ_s by averaging the results obtained from 5000 realizations of the surface profile function. The resulting mean differential reflection coefficient is presented by open circles in Fig. 3(a). These data constitute the input function $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh,input}}$ for the first set of reconstruction examples.

In our first example of a reconstruction based on this data set we assume that the trial function has the exponential form given by Eq. (29a). The set of variational parameters is therefor $\mathcal{P} = [\delta^*, a^*]$. By starting the minimization procedure with the values $\delta^* = 2.00$ nm, $a^* = 75$ nm, the values of these parameters that minimize the cost function $\chi^2(\mathcal{P})$, Eq. (26a), were found to be $\delta^* = 9.445$ nm and $a^* = 160.465$ nm. A comparison of these values with the values $\delta = 9.5$ nm and a = 158.20 nm used to generate the input data shows that the inversion is quite accurate. The function $\langle \partial R_{pp}/\partial \Omega_s \rangle_{\text{incoh,calc}}$ calculated with the reconstructed values of δ^* and a^* by means of second-order phase perturbation theory is plotted as the solid curve in Fig. 3(a), together with the input data, plotted as circles. The portion of the input data used in the inversion is indicated by the filled circles, while the open circles indicate the input data not used in the inversion. The agreement between the reconstructed and input data is excellent. The reconstructed $W(|\mathbf{x}_{\parallel}|)$ is nearly superimposed on the input $W(|\mathbf{x}_{\parallel}|)$ in Fig. 3(b). The shaded region in Fig. 3(b), and in the subsequent plots of $W(|\mathbf{x}_{\parallel}|)$, represents the magnitude of the difference between the input and reconstructed values of this function. It is seen to be very small.

In our second example we assume that the dielectric constant of the scattering medium is unknown. We take the input data from our first example, given by the filled circles in Fig. 3(a), so that the set of variational parame-

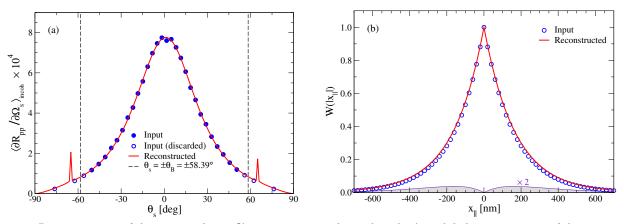


Figure 4. Reconstruction of the rms roughness δ^* , transverse correlation length a^* , and dielectric constant of the scattering medium ε^* from in-plane co-polarized scattering data. This figure is the same as Fig. 3 except now the dielectric constant of the scattering medium is also reconstructed. The reconstructed surface roughness parameters are $\delta^* = 5.930$ nm, $a^* = 166.508$ nm, and the reconstructed dielectric constant has the value $\varepsilon^* = 4.556$.

ters is now $\mathcal{P} = [\delta^*, a^*, \varepsilon^*]$. The results of the inversion carried out with the trial function given by Eq. (29a), are shown in Fig. 4, and it is seen that the resulting reconstruction is poor. By starting the minimization procedure with the values $\delta^* = 2.00$ nm, $a^* = 75$ nm, and $\varepsilon^* = 2.00$, the values of these parameters that minimize the cost function $\chi^2(\mathcal{P})$ were found to be $\delta^* = 5.930$ nm, $a^* = 166.508$ nm, and $\varepsilon^* = 4.556$. These are to be compared with the input values $\delta = 9.5$ nm, a = 158.20 nm, and $\varepsilon = 2.64$. The differences between the input and reconstructed values of these parameters are significant. Nevertheless, the function $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh,calc}}$ calculated with the reconstructed values of $\delta^*, a^*, \varepsilon^*$ by means of second-order phase perturbation theory, plotted as the solid curve in Fig. 4(a), and the reconstructed $W(|\mathbf{x}_{\parallel}|)$ plotted as the solid curve in Fig. 4(b), are in quite good agreement with the corresponding input curves.

We next consider a case where the trial function for $W(|\mathbf{x}_{\parallel}|)$ has a functional form that differs from the form assumed in generating the input data being reconstructed. As our third example we present results of calculations where the trial $W(|\mathbf{x}_{\parallel}|)$ is assumed to have the stretched exponential form given by Eq. (29c). The set of variational parameters is now $\mathcal{P} = [\delta^*, a^*, \gamma^*]$. We take the input data from our first example (Fig. 3(a)), and start the minimization procedure with the values $\delta^* = 2.00 \text{ nm}$, $a^* = 75.00 \text{ nm}$, and $\gamma^* = 2.00$. The values of these parameters that minimize the cost function were found to be $\delta^* = 10.545 \text{ nm}$, $a^* = 128.927 \text{ nm}$, and $\gamma^* = 0.891$. For comparison the input values were $\delta = 9.5 \text{ nm}$, a = 158.20 nm, and $\gamma = 1.00$. The values of δ^* and γ^* differ from the input values by approximately 10%, the value of a^* differs from that of a by approximately 20%. The importance of this example is that it shows that our minimization is able to distinguish a Gaussian form for the correlation function from an exponential form. The function $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh}}$, calculated by means of second order phase perturbation theory for the reconstructed values of δ^*, a^*, γ^* is plotted in Fig. 5(a) (solid curve) together with a plot of the input function (filled circles). The agreement between these two results is quite good. In Fig. 5(b) we present plots of the input (open circles) and reconstructed (solid curve) correlation functions $W(|\mathbf{x}_{\parallel}|)$. These two curves differ by less than 10%.

The reconstructed parameters obtained on the basis of in-plane p-to-p scattering of light from an exponentially correlated surface at a polar angle of incidence $\theta_0 = 1.6^{\circ}$ are summarized in Table 1.

5.2 Gaussianly-Correlated Surface Roughness

The second scattering system from which we will draw data for the purpose of inversion, is characterized by a *Gaussian* surface height autocorrelation function. In comparison with the preceding scattering system, in addition to the different form of $W(|\mathbf{x}_{\parallel}|)$ the only parameters that have changed are the rms height of the roughness and the dielectric constant of the scattering medium. They now have the values $\delta = 15.82$ nm and $\varepsilon = 2.6896$, respectively. The Brewster angle in this case is $\theta_B = 58.63^{\circ}$. Except for the angles of incidence, all other parameters characterizing the scattering system remain unchanged, i.e. a = 158.20 nm and $\lambda = 632.8$ nm.

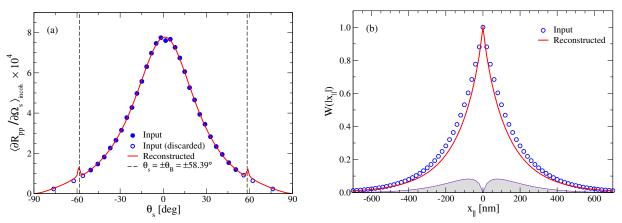


Figure 5. Reconstruction of the rms roughness δ^* , the transverse correlation length a^* , and the exponent γ^* from the in-plane co-polarized scattering data. This figure is the same as Fig. 3 except that now the trial function for $W(|\mathbf{x}_{\parallel}|)$ has the stretched exponential form given by Eq. (29c). The reconstructed surface roughness parameters have the values $\delta^* = 10.545$ nm, $a^* = 128.927$ nm, and $\gamma^* = 0.891$.

Table 1. Summary of the values reconstructed from in-plane scattering data obtained for the polar angle of incidence $\theta_0 = 1.6^{\circ}$ and corresponding to an exponentially correlated surface characterized by $\delta = 9.5$ nm and a = 158.20 nm. The dielectric constant of the substrate was $\varepsilon = 2.64$. When inverting for any of the parameters in the set $\{\delta^*, a^*, \varepsilon^*, \gamma^*\}$ the initial values used were $\{2 \text{ nm}, 75 \text{ nm}, 2, 2\}$, respectively.

δ^{\star} [nm]	$a^{\star} [nm]$	ε^{\star}	γ^{\star}	Comments
9.445	160.465			Fig. 3
5.930	166.508	4.556		Fig. 4
10.545	128.927		0.891	Fig. 5
10.517	129.057	2.645	0.892	

For these values of the parameters a computer simulation approach¹¹ was used to generate the input scattering data. Results for $\langle R_{pp}/\partial\Omega_s \rangle_{\rm incoh,input}$ obtained by averaging the results obtained from 5000 realizations of the surface profile function are presented as circles in Fig. 6(a) for a polar angle of incidence $\theta_0 = 14.8^{\circ}$. It is these data on which we base our inversions in this section, i.e. here this data set represents $\langle \partial R_{pp}/\partial\Omega_s \rangle_{\rm incoh,input}$

We present in Fig. 6 results for the reconstruction for $\mathcal{P}[\delta^*, a^*]$ when the trial function for $W(|\mathbf{x}_{\parallel}|)$ has the Gaussian form given by Eq. (29b). The reconstructed values of the surface roughness parameters were found to be $\delta^* = 15.357$ nm and $a^* = 163.178$ nm. These values are in good agreement with the values $\delta = 15.82$ nm and a = 158.20 nm assumed in generating the scattering data used in the inversion. The contribution to the mean differential reflection coefficient calculated for these reconstructed values of δ^* and a^* by means of the second-order phase perturbation theory are depicted by the solid curve in Fig. 6(a).

We next consider the inversion of the input data presented by the filled circles in Fig. 6(a) when the dielectric constant of the scattering medium is assumed to be unknown. In this case the set of variational parameters is $\mathcal{P} = [\delta^*, a^*, \varepsilon^*]$. The inversion of the scattering data generated by data by the use of the Gaussian trial function for $W(|\mathbf{x}_{\parallel}|)$ defined by Eq. (29b) yielded for the values of $\delta^*, a^*, \varepsilon^*$, that minimized the cost function $\chi^2(\mathcal{P})$, Eq. (26a), $\delta^* = 13.909$ nm, $a^* = 162.941$ nm, and $\varepsilon^* = 2.968$. These values differ from the input values $\delta = 15.82$ nm, a = 158.20 nm, $\varepsilon = 2.6896$, by less than 15%. The mean differential reflection coefficient $\langle \partial R_{pp}/\partial \Omega_s \rangle_{\text{incoh,calc}}$ calculated by second-order phase perturbation theory with the use of the reconstructed values of δ^*, a^* , a^* , and ε^* , is depicted by the solid curve in Fig. 7(a). It is in very good agreement with the input data. The input and reconstructed correlation functions, as well absolute difference between them, are depicted in Fig. 7(b). The agreement between the two function is quite good.

For our final example, assuming a Gaussian-correlated surface, we invert the input data depicted by filled

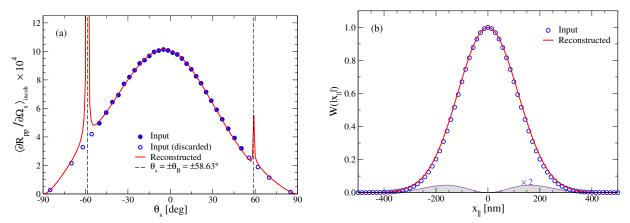


Figure 6. The same as Fig. 3, but now for a Gaussian-correlated surface, where the polar angle of incidence is $\theta_0 = 14.8^{\circ}$. The trial function for $W(|\mathbf{x}_{\parallel}|)$ assumed in the inversion method had the Gaussian form given by Eq. (29b). The values of the variational parameters obtained in this way were $\delta^* = 15.357$ nm, and $a^* = 163.178$ nm. The input data were characterized by $\delta = 15.82$ nm, a = 158.20 nm, $\varepsilon = 2.6896$, and $\lambda = 632.8$ nm.

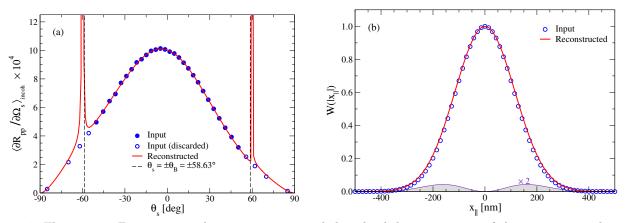


Figure 7. The same as Fig. 6, except that it is now assumed that the dielectric constant of the scattering medium is unknown. The set of variational parameters is now $\mathcal{P} = [\delta^*, a^*, \varepsilon^*]$, and the inversion of the input data represented by the filled circles in Fig. 6(a) is carried out with the use of the Gaussian trial function given by Eq. (29b). The values of the variational parameters obtained are $\delta^* = 13.909$ nm, $a^* = 162.941$ nm, and $\varepsilon^* = 2.968$. The input data were characterized by $\delta = 15.82$ nm, a = 158.20 nm, and $\varepsilon = 2.6896$.

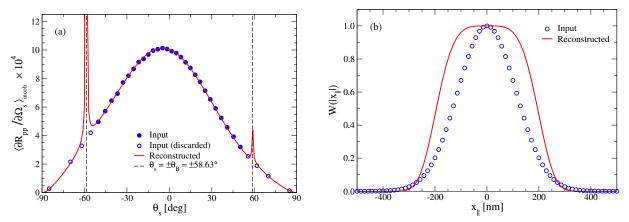


Figure 8. The same as Fig. 6, except that a stretched exponential trial function for $W(|\mathbf{x}_{\parallel}|)$ given by Eq. (29c) is used in carrying out the inversion of the input data represented by the filled circles in Fig. 6(a). The set of variational parameters is $\mathcal{P} = [\delta^*, a^*, \gamma^*]$. The reconstructed values of these parameters are $\delta^* = 12.211$ nm, $a^* = 212.293$ nm, and $\gamma^* = 4.307$.

Table 2. Summary of the values reconstructed from in-plane scattering data obtained for the polar angle of incidence $\theta_0 = 14.8^{\circ}$ and corresponding to a Gaussian correlated surface characterized by $\delta = 15.82$ nm and a = 158.20 nm. The dielectric constant of the substrate was $\varepsilon = 2.6896$. When inverting for any of the parameters in the set $\{\delta^*, a^*, \varepsilon^*, \gamma^*\}$ the initial values used were $\{2 \text{ nm}, 75 \text{ nm}, 2, 1\}$, respectively.

$\delta^{\star} [nm]$	a^{\star} [nm]	ε^{\star}	γ^{\star}	Comments
15.357	163.178			Fig. 6
13.909	162.941	2.968		Fig. 7
12.211	212.293		4.307	Fig. 8
12.028	199.754	2.902	3.202	—

circles in Fig. 6(a) with a trial function for $W(|\mathbf{x}_{\parallel}|)$ possessing the stretched exponential form given by Eq. (29c). The set of variational parameters in this case is $\mathcal{P} = [\delta^{\star}, a^{\star}, \gamma^{\star}]$. The values of these parameters that minimize the cost function, Eq. (26a), were found to be $\delta^{\star} = 12.211$ nm, $a^{\star} = 212.293$ nm, and $\gamma^{\star} = 4.307$. These values are in very poor agreement with the input values of these parameters. Despite this, the mean differential reflection coefficient $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh,calc}}$ calculated by means of second-order phase perturbation theory with the use of the reconstructed values of $\delta^{\star}, a^{\star}, \gamma^{\star}$, and represented by the solid curve in Fig. 8(a), is in very good agreement with the input data represented by the filled circles in this figure. The same is not true of the reconstructed correlation function $W(|\mathbf{x}_{\parallel}|)$ depicted by the solid curve in Fig. 8(b). It is seen to differ significantly from the input curve, depicted by the open circles in this figure.

The reconstructed parameters obtained on the basis of in-plane p-to-p scattering of light from a Gaussiancorrelated surface at a polar angle of incidence $\theta_0 = 14.8^\circ$ are summarized in Table 2.

5.3 Sensitivity to Noise

The reconstructions carried out in the preceding section have been based on the assumption that there is no noise in the input data. However, any experimental data set will contain some level of noise. It is therefore important to determine how sensitive the parameters reconstructed by the approach developed in this paper are to noise. We base our investigation of this sensitivity on the results obtained for a surface defined by a Gaussian height autocorrelation function, defined by the roughness parameters $\delta = 15.82$ nm and a = 158.20 nm, while the wavelength of the incident light is $\lambda = 632.8$ nm, the polar angle of incidence is $\theta_0 = 1.6^{\circ}$, and the dielectric constant of the scattering medium is $\varepsilon = 2.64$. The computer simulation result for $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh}}$ is depicted by the circles in Fig. 9(a), which coincide with the circles in Fig. 2. To this result we have added multiplicative Gaussian white noise of a standard deviation of 5%, (the gray erratic signal oscillating around zero in Fig. 9(a)). This produces the open squares in Fig. 9(a), that serve as the input data, $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh,input}}$, for the inversion procedure. The trial function for $W(x_{\parallel})$ used in minimizing the cost function, Eq. (26a), has the Gaussian form given by Eq. (29b). The set of variational parameters is therefore $\mathcal{P} = (\delta^*, a^*)$. The values of the parameters that minimize the cost function were found to be $\delta^* = 16.60$ nm and $a^* = 150.67$ nm, both within 10% of the input values. The initial values of these parameters in the minimization procedure were $\delta^* = 2.0$ nm and $a^* = 75$ nm. The use of these values in the phase perturbation theory expression for $\langle \partial R_{pp} / \partial \Omega_s \rangle_{\text{incoh,calc}}$, Eq. (14), produces the solid curve in Fig. 9(a). In Fig. 9(b) we present the input and reconstructed results for $W(x_{\parallel})$. The agreement between them is gratifyingly good.

6. DISCUSSION AND CONCLUSIONS

The contribution to the mean differential reflection coefficient from the in-plane co-polarized, diffuse scattering of p-polarized light from a two-dimensional randomly rough dielectric surface, calculated by second-order phase perturbation theory, displays singularities when the angle of scattering θ_s equals the Brewster angle θ_B . Nevertheless, we have shown in this paper that when the experimental values for the mean differential reflection coefficient as a function of θ_s are taken from only the region $|\theta_s| < \theta_B$, a good determination of the normalized surface height autocorrelation function, and other statistical properties of the surface roughness, can be achieved. The best reconstructions are of $W(\mathbf{x}_{\parallel})$ itself, in the sense of matching the input data. The reconstructed values

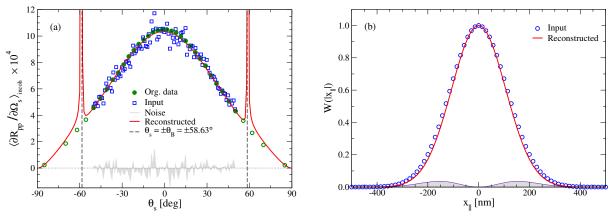


Figure 9. The sensitivity of the reconstruction to multiplicative Gaussian white noise of 5% standard deviation. (a) The contribution to the mean differential reflection coefficient for incoherent in-plane p-to-p scattering from a Gaussianly-correlated surface roughness. The circles indicate the original data set, which coincides with the data set represented by the circles in Fig. 2. The open squares represent the result of adding the multiplicative noise to the original data, and constitute the input data for the inversion. The irregular signal in gray oscillating around zero is the actual noise being added. The solid curve is the incoherent component of the mean differential reflection coefficient calculated with the reconstructed values of the variational parameters, $\delta^* = 16.60$ nm and $a^* = 150.67$ nm obtained by the use of a Gaussian trial function, Eq. (29b). (b) The input and reconstructed correlation function $W(x_{\parallel})$.

of δ^* , a^* , γ^* , and ε^* , agree with their input values less well, with errors as large as 15–20%. This is presumably due to the use of input values of $\langle \partial R_{pp}(\theta_s) / \partial \Omega_s \rangle_{\text{incoh,input}}$ taken from a limited range of scattering angles, namely $|\theta_s| < \theta_B$. The principal conclusion of the present work is therefore that although the inversion of scattering data, obtained by the use of p-polarized light, by means of second-order perturbation theory can yield good results for $W(x_{\parallel})$, the reconstructions of other statistical properties of a two-dimensional randomly rough dielectric surface are markedly poorer than those obtained by the use of s-polarized light, as demonstrated in Ref. 1.

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REFERENCES

- I. Simonsen, Ø. S. Hetland , J. B. Kryvi, and A. A. Maradudin, "Determination of the normalized surface height autocorrelation function of a two-dimensional randomly rough dielectric surface by the inversion of light scattering data," Phys. Rev. A. 99, 043829 (1–15) (2016).
- R. M. Fitzgerald and A. A. Maradudin, "A reciprocal phase perturbation theory for rough surface scattering," Waves in Random Media 4, 275–296 (1994).
- 3. A. R. McGurn and A. A. Maradudin, "Perturbation theory results for the diffuse scattering of light from two-dimensional randomly rough metal surfaces," Waves in Random Media **6**, 251–267 (1996). The relation between the scattering amplitudes and the elements of the scattering matrix $R_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel}) = [\alpha_0^{\frac{1}{2}}(k_{\parallel})/\alpha_0^{\frac{1}{2}}(q_{\parallel})]S_{\alpha\beta}(\mathbf{q}_{\parallel}|\mathbf{k}_{\parallel})$ is used in obtaining Eq. (10).
- 4. G. C. Brown, V. Celli, M. Haller, and A. Marvin, "Vector theory of light scattering from a rough surface: unitary and reciprocal expansions," Surf. Sci. **136**, 381–397 (1984).
- 5. I. Simonsen, J.B. Kryvi, and A. A. Maradudin, unpublished work, 2016.
- E. Marx and T. Vorburger, "Direct and inverse problems for light scattered by rough surfaces," App. Opt. 29, 3613–3626 (1990).
- SLATEC Common Mathematical Library, Version 4.1, www.netlib.org/slatec/ (also see http://people.sc.fsu.edu/jburkhardt/farc/slatec/slatec.html).

- K. Leverberg, "A method for the solution of certain non-linear problems in least squares," Quart. Appl. Math. 2, 164–168 (1944).
- D. W. Marquardt, "An algorithm for least squares estimation of nonlinear parameters," J. Soc. Indust. Appl. Math. 11, 431–441 (1963).
- T. A. Leskova, P. A. Letnes, A. A. Maradudin, T. Nordam, and I. Simonsen, "The scattering of light from two-dimensional randomly rough metal surfaces," Proc. SPIE 8172, 817209 (1–20) (2011).
- 11. T. Nordam, P. A. Letnes, and I. Simonsen, "Numerical simulations of scattering of light from twodimensional surfaces using the reduced Rayleigh equation," Front. Phys. 1, 8 (1–15) (2013).