The inversion of incoherent light scattering data to obtain statistical and optical properties of a two-dimensional randomly rough dielectric surface

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ABSTRACT

An approach to inverting experimental light scattering data for obtaining the normalized surface height autocorrelation function of a two-dimensional randomly rough dielectric surface, and its rms height is presented. It is based on the expression for the contribution to the mean differential reflection coefficient from the in-plane, co-polarized, light of s-polarization scattered diffusely from such a surface, obtained by phase perturbation theory. For weakly rough surfaces the reconstructions obtained by this approach are quite accurate.

Keywords: randomly rough surface, rough surface scattering, inverse scattering problem, surface height autocorrelation function, phase perturbation theory

1. INTRODUCTION

Statistical properties of randomly rough surfaces, such as the normalized surface height autocorrelation function, its Fourier transform, the power spectrum of the surface roughness, the probability density function of surface heights, and the root-mean-square (rms) height of the surface, are very useful characteristics of such surfaces. Efforts to determine these properties by inverting experimental measurements of light scattered into the far field from them, have been studied for many years because of the contactless nature of this approach, and because measurements in the far field are easier to make than measurements in the near field.

In this paper we present an approach to the determination of the normalized surface height autocorrelation function of a two-dimensional randomly rough dielectric surface from measurements of the angular dependence of the contribution to the mean differential reflection coefficient from the in-plane co-polarized light scattered incoherently (diffusely) from it. Our approach also enables us to obtain an estimate of the rms height of the surface from these data, as well as the dielectric constant of the scattering medium, if it is not known a priori.

This problem has been studied earlier by Chandley and by Marx and Vorburger. In the former work scalar diffraction theory and a thin random phase screen approximation were used to describe the interaction of light with the randomly rough surface. The use of this model allowed the inversion of the angular dependence of the mean intensity of the scattered light in the far field to be carried out by means of a Fourier transformation. However, the dielectric constant of the scattering medium does not appear in Chandley’s theory, so that it cannot be used to determine it from scattering data if it is not known in advance. In their work Marx and Vorburger applied the Kirchhoff approximation for the scattering of a plane wave from a two-dimensional randomly rough perfectly conducting surface to obtain the mean intensity of the scattered field. This expression was evaluated with the use of an expression for the surface height autocorrelation function of a particular analytical form, and the determination of the parameters defining it was carried out by a least squares fit of the theoretical mean intensity to the experimental result.

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In contrast, in this paper we use a vector theory of rough surface scattering, namely phase perturbation theory,\textsuperscript{7} to calculate the contribution to the mean differential reflection coefficient from the in-plane, co-polarized incoherently scattered light of s polarization incident normally on a two-dimensional randomly rough dielectric surface. The dielectric constant of the scattering medium is taken into account in this approach. This expression is evaluated with the use of an expression for the normalized surface height autocorrelation function that contains adjustable parameters. The values of these parameters are then determined through a least squares fit of the resulting expression to the corresponding experimental scattering data. The use of s-polarized light in this approach is prompted by the fact that it leads to a simpler expression for the mean differential reflection coefficient than does the use of p-polarized light, and because there is no Brewster effect in s polarization. Consequently a smoother function of the scattering angle is being inverted in s polarization than in p polarization.

2. THE SCATTERING SYSTEM

The system we study consists of vacuum in the region \( x_3 > \zeta(x_i) \) and a dielectric medium, characterized by a dielectric constant \( \varepsilon \), in the region \( x_3 < \zeta(x_i) \). It is assumed that \( \varepsilon \) is real, positive, and frequency independent. The vector \( x_i = (x_1, x_2, 0) \) is a position vector in the plane \( x_3 = 0 \). The surface profile function \( \zeta(x_i) \) is a single-valued function of \( x_i \) that is differentiable with respect to \( x_1 \) and \( x_2 \), and constitutes a stationary, zero-mean, isotropic, Gaussian random process defined by

\[
\langle \zeta(x_i)\zeta(x'_i) \rangle = \delta^2 W(|x_i - x'_i|) \quad (1a)
\]

\[
\langle \zeta^2(x_i) \rangle = \delta^2. \quad (1b)
\]

Here the angle brackets denote an average over the ensemble of realizations of \( \zeta(x_i) \), \( \delta \) is the rms height of the surface, and \( W(|x_i|) \) is the normalized surface height autocorrelation function. It has the property that \( W(0) = 1 \).

The surface profile function has a Fourier integral representation,

\[
\zeta(x_i) = \int \frac{d^2Q_i}{(2\pi)^2} \hat{\zeta}(Q_i) \exp(iQ_i \cdot x_i), \quad (2)
\]

where \( Q_i = (Q_1, Q_2, 0) \), so that

\[
\hat{\zeta}(Q_i) = \int d^2x_i \zeta(x_i) \exp(-iQ_i \cdot x_i). \quad (3)
\]

The Fourier coefficient \( \hat{\zeta}(Q_i) \) is a zero-mean Gaussian random process defined by

\[
\langle \hat{\zeta}(Q_i)\hat{\zeta}(Q'_i) \rangle = (2\pi)^2 \delta(Q_i + Q'_i)\delta^2 g(|Q_i|), \quad (4)
\]

where \( g(|Q_i|) \), the power spectrum of the surface roughness, is given by

\[
g(|Q_i|) = \int d^2x_i W(|x_i|) \exp(-iQ_i \cdot x_i). \quad (5)
\]

3. PHASE PERTURBATION THEORY

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

\[
E^{(i)}(x|\omega) = \left\{-\frac{c}{\omega} \left[ k_i\alpha_0(k_i) + \hat{x}_3 k_i \right] B_p(k_i) + \left( \hat{x}_3 \times k_i \right) B_s(k_i) \right\} \exp[i(k_i - \hat{x}_3\alpha_0(k_i)) \cdot x] \quad (6a)
\]

\[
E^{(s)}(x|\omega) = \int \frac{d^2q_i}{(2\pi)^2} \left\{ \frac{c}{\omega} \left[ \tilde{q}_i\alpha_0(q_i) - \hat{x}_3 q_i \right] A_p(q_i) + \left( \hat{x}_3 \times \tilde{q}_i \right) A_s(q_i) \right\} \exp[i(q_i + \hat{x}_3\alpha_0(q_i)) \cdot x]. \quad (6b)
\]
The subscripts p and s denote the p-polarized (TM) and s-polarized (TE) components of each of these fields with respect to the plane of incidence, defined by \( \mathbf{k}_0 \) and \( \mathbf{x}_3 \), and the local plane of scattering, defined by \( \mathbf{q}_\parallel \) and \( \mathbf{x}_3 \), respectively. The function \( \alpha_0(q_\parallel) \) in Eqs. (6) is \( \alpha_0(q_\parallel) = [(\omega/c)^2 - q_\parallel^2]^{1/2} \), with \( \text{Re}\alpha_0(q_\parallel) > 0, \text{Im}\alpha_0(q_\parallel) > 0 \).

Maxwell’s equations and the associated boundary conditions imply linear relations between \( A_\alpha(q_\parallel) \) and \( B_\beta(k_\parallel) (\alpha = p, s, \beta = p, s) \)

\[
A_\alpha(q_\parallel) = \sum_\beta R_{\alpha\beta}(q_\parallel|k_\parallel)B_\beta(k_\parallel). \tag{7}
\]

The scattering amplitudes \( \{R_{\alpha\beta}(q_\parallel|k_\parallel)\} \) play a central role in the present theory because the mean differential reflection coefficient is expressed in terms of them.

The differential reflection coefficient \( (\partial R_{\alpha\beta}(q_\parallel|k_\parallel)/\partial\Omega_s) \) is defined such that \( (\partial R_{\alpha\beta}(q_\parallel|k_\parallel)/\partial\Omega_s) d\Omega_s \) is the fraction of the total time-averaged flux in an incident field of \( \beta \) polarization, the projection of whose wave vector on the mean scattering plane is \( k_\parallel \), that is scattered into a field of \( \alpha \) polarization, the projection of whose wave vector on the mean scattering plane is \( q_\parallel \), within an element of solid angle \( d\Omega_s \) about the scattering direction defined by the polar and azimuthal angles \((\theta_s, \phi_s)\). It is given by\(^8\)

\[
\frac{\partial R_{\alpha\beta}(q_\parallel|k_\parallel)}{\partial\Omega_s} = \frac{1}{S} \left( \frac{\omega}{2\pi c} \right)^2 \frac{\cos^2\theta_s}{\cos\theta_0} \left| R_{\alpha\beta}(q_\parallel|k_\parallel) \right|^2,
\tag{8}
\]

with \( q_\parallel = (\omega/c)\sin\theta_s(\cos\phi_s, \sin\phi_s, 0) \) and \( k_\parallel = (\omega/c)\sin\theta_0(\cos\phi_0, \sin\phi_0, 0) \), where \((\theta_s, \phi_s)\) and \((\theta_0, \phi_0)\) are the polar and azimuthal angles of scattering and incidence, 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 we need the average of this function over the ensemble of realizations of the surface profile function. The contribution to this average from the light scattered incoherently is\(^8\)

\[
\left\langle \frac{\partial R_{\alpha\beta}(q_\parallel|k_\parallel)}{\partial\Omega_s} \right\rangle_{\text{incoh}} = \frac{1}{S} \left( \frac{\omega}{2\pi c} \right)^2 \frac{\cos^2\theta_s}{\cos\theta_0} \left[ \left| R_{\alpha\beta}(q_\parallel|k_\parallel) \right|^2 - \left\langle \left| R_{\alpha\beta}(q_\parallel|k_\parallel) \right|^2 \right\rangle \right].
\tag{9}
\]

When some typographical errors in the results presented in Ref. 7 are corrected, it is found that in the case of normal incidence \((k_\parallel = 0)\) and in-plane scattering \((q_\parallel = k_\parallel)\), the contribution to the mean differential reflection coefficient from the incoherent scattering of s-polarized light is given in phase perturbation theory by

\[
\left\langle \frac{\partial R_{ss}(q_\parallel|0)}{\partial\Omega_s} \right\rangle_{\text{incoh}} = \left\langle \frac{\partial R_{ss}(\theta_s)}{\partial\Omega_s} \right\rangle_{\text{incoh}}
\]

\[
= \frac{(\varepsilon - 1)^2}{(2\pi)^2} \left( \frac{\omega}{c} \right)^6 \frac{\cos\theta_s}{[d_s(q_\parallel)d_s(0)]^2} \exp[-2M(q_\parallel|0)]
\times \sum_{n=1}^{\infty} \frac{[4\delta^2\alpha_0(q_\parallel)\alpha_0(0)]^n}{n!} \int d^2u_\parallel W^n(u_\parallel) \exp(-iu_\parallel \cdot u_\parallel),
\tag{10}
\]

when the phase is calculated to second order in the surface profile function. The exponent \(2M(q_\parallel|0)\) is defined by

\[
2M(q_\parallel|0) = 2\delta^2[\alpha_0(q_\parallel)\alpha_0(0)]^{1/2} \left\{ (\alpha(q_\parallel) + \alpha(0)) - (\varepsilon - 1)\text{Re} \int_0^\infty dp_\parallel \alpha_0(p_\parallel)\alpha(p_\parallel) \left| d_s(p_\parallel) \right|^2 \int_0^\infty dx_\parallel x_\parallel J_0(p_\parallel x_\parallel)W(x_\parallel) \right\},
\tag{11}
\]

and \( J_0(x) \) is a Bessel function of the first kind and order zero. In writing these equations we have introduced the functions

\[
d_p(q_\parallel) = \varepsilon\alpha_0(q_\parallel) + \alpha(q_\parallel), \quad d_s(q_\parallel) = \alpha_0(q_\parallel) + \alpha(q_\parallel),
\tag{12}
\]

where the function \(\alpha(q_\parallel)\) is defined by \(\alpha(q_\parallel) = [\varepsilon(\omega/c)^2 - q_\parallel^2]^{1/2}\), with \(\text{Re}\alpha(q_\parallel) > 0, \text{Im}\alpha(q_\parallel) > 0\).
4. THE INVERSE PROBLEM

To use the preceding results to obtain $W(|x∥|)$ from scattering data for the trial function (14), we calculate the first derivative of the mean differential reflection coefficient with respect to the elements of $\mathcal{P}$ used in obtaining the simulation result is presented as open symbols in Fig. 1(a). This data set will serve as the input data, $\langle \partial R_{ss}(\theta_s)/\partial \Omega_s \rangle_{\text{incoh,input}}$, for the reconstruction. The corresponding correlation function assumed in obtaining the simulation result is presented as open symbols in Fig. 1(b). As a first example we assume that the variational parameters are $\delta^*, a^*$, and potentially also $\varepsilon^*$. This is not an overly restrictive form for the trial function, since the surface height autocorrelation function for non-fractal surfaces generally has the form $W(|x∥|) = 1 - (x∥/a^*)^2$ in the limit $x∥ \to 0$, which is captured by Eq. (14), or has a Gaussian form in this limit.

For the function $\langle \partial R_{ss}(\theta_s)/\partial \Omega_s \rangle_{\text{incoh,input}}$ we used the results of rigorous, non-perturbative, purely numerical solutions of the reduced Rayleigh equation for the scattering of polarized light from a two-dimensional randomly rough penetrable surface. These calculations were carried out for an ensemble of random surfaces generated on the basis of an expression for $W(|x∥|)$ of Gaussian form

$$W(|x∥|) = \exp \left[-(x∥/a)^2\right].$$

In this case the variational parameters are $\delta^*, a^*$ and potentially also $\varepsilon^*$. This is not an overly restrictive form for the trial function, since the surface height autocorrelation function for non-fractal surfaces generally has the form $W(|x∥|) = 1 - (x∥/a^*)^2$ in the limit $x∥ \to 0$, which is captured by Eq. (14), or has a Gaussian form in this limit.

The value of the rms height of the surface assumed in these calculations was $\delta = 9.50\ \text{nm}$, while the value of the transverse correlation length was chosen to be $a = 158.20\ \text{nm}$. The calculations were carried out for two values of the dielectric constant $\varepsilon$, namely $\varepsilon = 2.64$ (photoresist) and $\varepsilon = 12$ (silicon). The wavelength (in vacuum) of the s-polarized light incident normally onto the mean surface was $\lambda = 632.8\ \text{nm}$, and the co-polarized mean differential reflection coefficients were obtained after averaging over (at least) 5,000 surface realizations. The use of mean differential reflection coefficients generated by the use of a known $W(|x∥|)$ in our inversion approach enables us to assess the quality of the reconstructions we obtain.

5. RESULTS

To illustrate the inversion method developed here, we consider the reconstruction of $W(|x∥|)$ with the use of the trial function (14). First we assume $\delta = 9.50\ \text{nm}$, $a = 158.20\ \text{nm}$, and $\varepsilon = 2.64$ with the remaining experimental parameters as given in Sec. 4. For these parameters, we perform computer simulations of the mean differential reflection coefficients, and the in-plane variation of its s-to-s-polarized incoherent component is presented as open symbols in Fig. 1(a). This data set will serve as the input data, $\langle \partial R_{ss}(\theta_s)/\partial \Omega_s \rangle_{\text{incoh,input}}$, for the reconstruction. The corresponding correlation function assumed in obtaining the simulation result is presented as open symbols in Fig. 1(b). As a first example we assume that the variational parameters are $\mathcal{P} = \{\delta^*, a^*\}$. Under this assumption, a reconstruction of the surface parameters was performed by minimizing the cost function $\chi^2(\mathcal{P})$, Eq. (13), with respect to the elements of $\mathcal{P}$. The solid lines in Fig. 1 represent the (phase perturbation theory) reconstructed $\langle \partial R_{ss}/\partial \Omega_s \rangle_{\text{incoh}}$ [Fig. 1(a)] and $W(|x∥|)$ [Fig. 1(b)]. From Fig. 1 one observes a quite accurate inversion; for instance, the reconstructed $W(|x∥|)$ is nearly superimposed on the input $W(|x∥|)$. In particular, the gray region of Fig. 1(b) represents 10 times the absolute difference between the input and reconstructed $W(|x∥|)$. This minimization procedure estimated the surface parameters to be $\delta^* = 9.49\ \text{nm}$ and $a^* = 158.83\ \text{nm}$ which should be compared to the parameters $\delta = 9.50\ \text{nm}$ and $a = 158.20\ \text{nm}$ used to generate the input data.

*In the simulations, the polar angle of incidence was for technical reasons not zero, but instead $\theta_0 = 1.18^\circ$. 
These inversion results were found to be robust in the sense that the estimated values for the elements of $P$ did show little, or no, sensitivity towards the initial guess used to start the minimization procedure.

In the preceding example it was assumed that the dielectric constant $\varepsilon$ of the scattering medium was known. As a second example we take the input data from our first example, open symbols in Fig. 1, but in addition to the roughness parameters now also assume that the dielectric constant of the substrate is unknown. Therefore the variational parameter set now is $P = \{\delta^*, a^*, \varepsilon^*\}$. The results of the inversion are presented as solid lines in Fig. 2, and also in this case a rather good reconstruction is obtained. The parameters estimated in this way resulted in the values $\delta^* = 9.52$ nm ($9.50$ nm), $a^* = 159.2$ nm ($158.20$ nm), and $\varepsilon^* = 2.62$ (2.64), where the values in parentheses are the corresponding input values. A comparison of the absolute errors in the reconstruction of $W(|x_i|)$ from Figs. 1(b) and 2(b) shows that the error is larger in the latter case than in the former case. This is also to be expected since in the latter case, compared to the former, one inverts with respect to one additional parameter. However, what should be noticed, is that the addition of one extra variational parameter only slightly increase the error in the reconstruction of $W(|x_i|)$.

We now turn to the case of a high index substrate of dielectric constant $\varepsilon = 12$. All other parameters, including those of the surface roughness, are unchanged. In Fig. 3(a), as open symbols, we plot the numerical simulation result for the mean differential reflection coefficient, $\langle \partial R_{ss}(\theta_s)/\partial \Omega_s \rangle_{\text{incoh, input}}$, against the polar angle of scattering $\theta_s$. By comparing this result to its equivalents in Figs. 1 and 2 it is observed, as expected, that the incoherent scattering now is significantly increased (by a factor of about five). The solid lines in Fig. 3 correspond to the results for $\langle \partial R_{ss}(\theta_s)/\partial \Omega_s \rangle_{\text{incoh}}$ and $W(|x_i|)$ obtained by inversion of the scattering data with respect to the variational parameters $P = \{\delta^*, a^*\}$. In arriving at these results we obtained the reconstructed surface roughness parameters $\delta^* = 9.71$ nm and $a^* = 154.39$ nm. One observes that $\delta^*$ overestimates the surface roughness, while the correlation length is slightly underestimated. Even if these results are less accurate than those found for the $\varepsilon = 2.64$ case, the results are still rather satisfactory. Increasing the dielectric constant of the scattering medium significantly, making it strongly reflecting, has not seriously degraded the quality of the reconstruction of $W(|x_i|)$ and the corresponding surface roughness parameters. In passing we stress that also in this case, the values for $\delta^*$ and $a^*$ were robust to changes in the initial guess used to start the minimization.
Figure 2: Reconstruction of the rms-roughness $\delta^*$, the correlation length $a^*$, and the dielectric constant of the substrate $\varepsilon^*$ from scattering data: Same as Fig. 1 except now also the dielectric constant of the substrate is reconstructed. The reconstructed surface roughness parameters are $\delta^* = 9.52\,\text{nm}$, $a^* = 159.2\,\text{nm}$, and the reconstructed dielectric constant is $\varepsilon^* = 2.62$.

For the high index substrate case, an inversion of the scattering data with respect to the parameter set $\mathcal{P} = \{\delta^*, a^*, \varepsilon^*\}$ based on the cost function (13) has not been successful. This is contrary to what was observed for the $\varepsilon = 2.64$ case [see Fig. 2]. One may reproduce rather well the input data for some starting parameters of the minimization algorithm. However, for other choices, one seems to drift off into less physical relevant parameters while still getting a reasonable reproduction of the input data. At least when using the simple cost function Eq. (13), we have not been able to obtain robust inversion results with respect to $\varepsilon^*$ and the surface roughness parameters $\delta^*$ and $a^*$. An alternative form of the cost function $\chi^2(\mathcal{P})$ that, for instance, penalizes less physical parameters, could potentially cure this problem, but this will be left for further work.

Figure 3: Reconstruction of the rms-roughness $\delta^*$ and the correlation length $a^*$ from scattering data: Same as Fig. 1 except that the substrate is a high index material of dielectric constant $\varepsilon = 12$. The reconstructed surface roughness parameters are $\delta^* = 9.71\,\text{nm}$ and $a^* = 154.39\,\text{nm}$. Note that in Fig. 3(b) the error is multiplied by a factor of 2 (and not a factor 10 as in Figs. 1(b) and 2(b)).

6. DISCUSSIONS AND CONCLUSIONS

The preliminary results presented here indicate that second-order phase perturbation theory can yield a good approximation to the mean differential reflection coefficient from light scattered incoherently from a two-dimensional randomly rough dielectric surface. As a consequence it is expected that it should be effective in the inversion of experimental light scattering data to obtain the statistical properties of a random surface on which it depends. For weakly rough two-dimensional random dielectric surfaces this expectation has been borne out, as we have...
used it to determine the normalized surface height autocorrelation function $W(|x_\parallel|)$, the rms height of the surface $\delta$, the transverse correlation length $a$, and the dielectric constant $\varepsilon$ of the scattering medium. The function $W(|x_\parallel|)$ has been reconstructed quite accurately. The agreement between the reconstructed values of $\delta, a, \varepsilon$, and the values used in calculating the input scattering patterns is gratifyingly satisfactory.

The inversion approach outlined here needs to be explored to determine ranges of roughness, wavelength, and dielectric parameters for which it gives reliable results. Error estimates for the determined parameters should also be obtained. Moreover, the sensitivity to noise in the input data used in the inversion approach needs to be investigated. These issues will be explored in subsequent work.

ACKNOWLEDGMENTS

The authors are grateful to Dr. Tor Nordam for support in producing some of the simulation data used in this study. The research of S.C. was supported by the United States Army Research Office under Prime Contract No. W911NF-12-C0009 and Spectral Sciences, Inc. The research of I. S. was supported in part by The Research Council of Norway Contract No. 216699. The research of E. I. C. was supported in part by the Consejo Nacional de Ciencia y Tecnología under grant number 180654.

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