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The Scattering of Electromagnetic Waves from Two-Dimensional Randomly Rough Penetrable Surfaces

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An accurate and efficient numerical simulation approach to electromagnetic wave scattering from two-dimensional, randomly rough, penetrable surfaces is presented. The use of the Müller equations and an impedance boundary condition for a two-dimensional rough surface yields a pair of coupled two-dimensional integral equations for the sources on the surface in terms of which the scattered field is expressed through the Franz formulas. By this approach, we calculate the full angular intensity distribution of the scattered field that is due to a finite incident beam of p-polarized light. We specifically check the energy conservation (unitarity) of our simulations (for the non-absorbing case). Only after a detailed numerical treatment of *both* diagonal and close-to-diagonal matrix elements is the unitarity condition found to be well-satisfied for the non-absorbing case ($\mathcal{U} > 0.995$), a result that testifies to the accuracy of our approach.

PACS numbers:

The scattering of electromagnetic waves from two-dimensional randomly rough penetrable surfaces has been studied theoretically for more than five decades. The methods used in these studies in recent years, where attention has been directed toward multiple-scattering phenomena, have been either analytical in nature or computational. Chief among the former methods has been the small-amplitude perturbation theory [1–3], while several different computational methods have been used in solving the scattering problem. In the earliest calculation of this type [4] the system of coupled inhomogeneous integral equations for the tangential components of the total electric and magnetic fields on the rough surface obtained from scattering theory, was converted into a system of inhomogeneous matrix equations by the use of the method of moments [5], which was then solved by Neumann-Liouville iteration [6]. This is a formally exact approach but one that is computationally (and memory) intensive.

In subsequent work on this problem approximate solutions of the exact integral equations have been sought. In the sparse-matrix flat-surface iterative approach [7, 8] the matrix elements for two close points on the surface are treated exactly, while those connecting two widely separated points are treated approximately, in an iterative solution of the matrix equations.

Soriano and Saillard [9] have combined the sparse-matrix flat-surface iterative approach with an impedance approximation [10] to calculate co-polarized and cross-polarized bistatic scattering coefficients of aluminum randomly rough surfaces for comparison with results obtained from perfectly conducting surfaces.

An approach that combines the fast multipole method [11] and the sparse-matrix flat-surface iterative approach has been developed by Jandhyala *et. al* [12].

Despite these advances, the calculation of the scattering of electromagnetic waves from two-dimensional, penetrable, randomly rough surfaces, remains a computationally intensive problem, in need of further improvements in the methods used to solve it.

In this paper we use the Franz formulas of electromagnetic scattering theory [13, 14] to obtain expressions for the amplitude of the electromagnetic field scattered from a two-dimensional, rough, metallic or dielectric surface in terms of the tangential components of the total electric and magnetic fields on the surface. The independent elements of these tangential field components satisfy a system of four coupled inhomogeneous two-dimensional integral equations — the Müller equations [15, 16] — derived from Franz formulas. This system of four integral equations is reduced to a system of two integral equations by the use of an impedance boundary condition at a two-dimensional rough metallic surface [17], and its solution is used to calculate the mean differential reflection coefficient.

The approach to the scattering of an electromagnetic field from a rough metallic or dielectric surface outlined here is similar to the approach of Soriano and Saillard [5] in its use of an impedance boundary condition to reduce the number of coupled integral equations that have to be solved from four to two. However, there are still important differences between these two approaches. The first is that we do not use the sparse-matrix flat-surface iterative approach: the matrix elements connecting any two points on the surface are calculated accurately. Moreover, those connecting two nearby points are calculated more accurately than in the work of Soriano and Saillard. The second is that we calculate the full angular intensity distribution of the scattered field, which allows us to check the unitarity (energy conservation) of the scat-

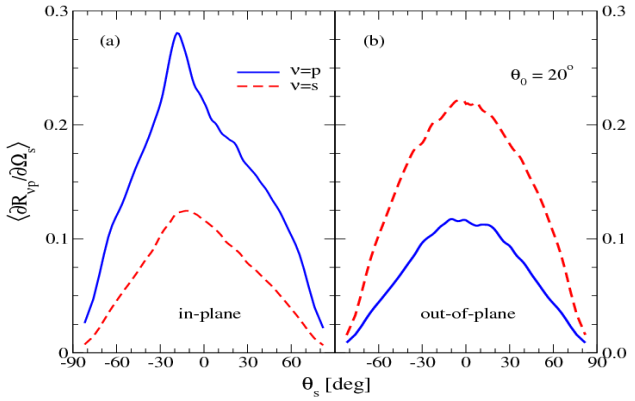

FIG. 1: (Color online) The mean differential reflection coefficients [20], $\langle \partial R_{\nu p}/\partial \Omega_s \rangle$ $(p \to \nu)$ for a p-polarized incident beam, whose polar angle of incidence is $\theta_0 = 20^\circ$, as functions of the polar scattering angle θ_s for the (a) in-plane and (b) out-of-plane scattering. See text for additional parameters.

tered field (for the non-absorbing case). This enabled the identification of critical aspects of the numerical implementation that, if not handled properly, could lead to erroneous results and/or a significant drop in accuracy. This important point seems to have been overlooked in previous publications. The third is that although the occurrence of hyper-singular kernels is avoided in both approaches by the use of the Müller equations [15, 16], some differences are found between our resulting matrix elements and those of Soriano and Saillard that appear to affect the unitarity of the scattered field[24]. Moreover, contrary to what was reported in Ref. [15], we find that matrix element terms containing the Green's function of the metal also have to be taken into account for some off-diagonal elements in order to produce accurate results. The fourth is that we do not use the beam decomposition method [19] for the incident beam in which a wide beam is represented by a weighted sum of shifted narrow beams. Instead we use a single wide incident beam.

The physical system that we consider consists of vacuum [$\varepsilon_0 = 1$] in the region $x_3 > \zeta(\mathbf{x}_\parallel)$ [where $\mathbf{x}_\parallel = (x_1, x_2, 0)$] and a non-magnetic metal in the region $x_3 < \zeta(\mathbf{x}_\parallel)$ that is characterized by a complex, frequency-dependent, dielectric function, $\varepsilon(\omega)$, for which $Re\,\varepsilon(\omega) < 0$ and $Im\,\varepsilon(\omega) > 0$. The surface profile function, $x_3 = \zeta(\mathbf{x}_\parallel)$, is assumed to constitute a zero-mean, Gaussian random process that is a single-valued function of $\mathbf{x}_\parallel$ and is differentiable with respect to x_1 and x_2 at least twice. It is defined by $\langle \zeta(\mathbf{x}_\parallel) \rangle = 0$ and $\left\langle \zeta(\mathbf{x}_\parallel)\zeta(\mathbf{x}'_\parallel) \right\rangle = \delta^2 W(|\mathbf{x}_\parallel - \mathbf{x}'_\parallel|)$, where δ is the root-mean-square roughness, $W(\cdot)$ denotes the (normalized) correlation function, and the angle brackets denote an average over the ensemble of realizations of $\zeta(\mathbf{x}_\parallel)$. In this work we will use an isotropic Gaussian correlation function $W(x) = \exp(-x^2/a^2)$ with a the correlation length.

The starting point of our approach is the Franz formulas of electromagnetic theory (or the dyadic form of Huygens principle) [13, 14]. By applying them to the vacuum region above the metal surface, and letting the observation point, $\mathbf{x}$, approach the surface $x_3 = \zeta(\mathbf{x}_\parallel)$, two coupled inhomogeneous integral equations for the tangential components of the electric and magnetic fields, $\mathbf{J}_E(\mathbf{x}_\parallel) = \hat{\mathbf{n}} \times \mathbf{E}(\mathbf{x})|_{x_3=\zeta(\mathbf{x}_\parallel)}$ and $\mathbf{J}_H(\mathbf{x}_\parallel) = \hat{\mathbf{n}} \times \mathbf{H}(\mathbf{x})|_{x_3=\zeta(\mathbf{x}_\parallel)}$, respectively, are obtained, where $\hat{\mathbf{n}}$ denotes the unit vector normal to the surface and directed into the vacuum. These equations contain double derivatives of the scalar Green's function $g_0(\mathbf{x}, \mathbf{x}') = \exp[ik_0 R]/4\pi R$ [$k_0 = \sqrt{\varepsilon_0(\omega)}\,\omega/c$, $R = |\mathbf{x} - \mathbf{x}'|$] resulting in non-integrable *hyper-singular* kernels that are sources of computational difficulties [9, 15, 16]. One way to obtain integrable kernels, is to combine in a suitable way the two sets of Franz formulas obtained separately for the vacuum and metal regions so that the resulting integral equations do not contain *any* hyper-singular terms. The resulting equations are known as the Müller integral equations [15], and the one satisfied by $\mathbf{J}_H(\mathbf{x}_\parallel|\omega)$ reads

$$\begin{aligned}\mathbf{J}_H(\mathbf{x}_\parallel|\omega) &= \mathbf{J}_H(\mathbf{x}_\parallel|\omega)_{inc} \\ &+ \mathcal{P}\int d^2x'_\parallel \left[\!\!\left[\hat{\mathbf{n}}(\mathbf{x}_\parallel) \times \{\boldsymbol{\nabla} \times [\mathcal{G}(\mathbf{x}|\mathbf{x}')\,\mathbf{J}_H(\mathbf{x}'_\parallel|\omega)]\}\right]\!\!\right] \qquad (1) \\ &- \frac{ic}{\omega}\int d^2x'_\parallel \left[\!\!\left[\hat{\mathbf{n}}(\mathbf{x}_\parallel) \times \{\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times [\mathcal{G}(\mathbf{x}|\mathbf{x}')\,\mathbf{J}_E(\mathbf{x}'_\parallel|\omega)]\}\right]\!\!\right],\end{aligned}$$

where the equation satisfied by $\mathbf{J}_E(\mathbf{x}'_\parallel|\omega)$ can be obtained from duality [14]. In writing Eq. (1) we have introduced $\mathcal{G}(\mathbf{x}_\parallel|\mathbf{x}'_\parallel) = g_0(\mathbf{x}_\parallel|\mathbf{x}'_\parallel) - g(\mathbf{x}_\parallel|\mathbf{x}'_\parallel)$ — the difference between the scalar Green's functions for the vacuum (subscript 0) and the metal; $[\![A(\mathbf{x}|\mathbf{x}')]\!] = A(\mathbf{x}|\mathbf{x}')|_{x_3=\zeta(\mathbf{x}_\parallel);x'_3=\zeta(\mathbf{x}'_\parallel)}$; $\mathcal{P}$ denotes the Cauchy principle value of an integral; and $\mathbf{J}_H(\mathbf{x}_\parallel|\omega)_{inc}$ is defined similarly to $\mathbf{J}_H(\mathbf{x}_\parallel|\omega)$ but for the incident field. Initially the kernel of Eq. (1) seems to be hyper-singular. However, because the leading term (when $R \to 0$) of the second derivative of the scalar Green's function is independent of medium parameters, the most divergent terms of the kernel cancel, rendering it integrable. By adopting the impedance boundary condition that relates the surface currents $\mathbf{J}_E(\mathbf{x}_\parallel|\omega)$ and $\mathbf{J}_H(\mathbf{x}_\parallel|\omega)$ via the (local) impedance tensor ($\mathbf{K}$) [17]: $\mathbf{J}_E(\mathbf{x}_\parallel|\omega)_i = K_{ij}(\mathbf{x}_\parallel|\omega)\mathbf{J}_H(\mathbf{x}_\parallel|\omega)_j$ $[i,j = 1,2]$, the dependence on $\mathbf{J}_E(\mathbf{x}_\parallel|\omega)$ can be removed from Eq. (1). Moreover, the resulting equation can be converted into a matrix equation for the two independent electric surface current components, say, $\mathbf{J}_H(\mathbf{x}_\parallel|\omega)_i$ $[i = 1,2]$, by the use of the method of moments [5]. The resulting linear system is then solved by the BiCGStab method [18] and the solution used to calculate the mean differential reflection coefficient that is averaged over an ensemble of realizations of the surface profile function (see Ref. [20] for details).

On the basis of the integral equation (1), and with the use of the impedance boundary condition, we have

performed numerical simulations for a p-polarized incident beam of wavelength $\lambda = 0.6328$ μm that is scattered from a Gaussian randomly rough silver surface. At this wavelength $\varepsilon(\omega) = -16.00 + i1.088$ [21]. The surface was characterized by a root-mean-square roughness of $\delta = \lambda/4$ and a correlation length $a = \lambda/2$. In the simulations it was assumed to cover an area of $16\lambda \times 16\lambda$, and the discretization interval was $\Delta = \lambda/7$ for both the x_1- and x_2-directions.

Figure 1 presents the mean differential reflection coefficients as functions of the polar scattering angle θ_s for the in-plane [Fig. 1(a)] and out-of-plane ($\phi_s = \pm 90°$) [Fig. 1(b)] scattered light due to a p-polarized Gaussian beam of width $w = 4\lambda$ incident on the surface at a polar angle $\theta_0 = 20°$. For the same parameters, Figs. 2 depict the full angular intensity distribution of the incident p-polarized light that is scattered into p- and s-polarized light (polarization not recorded) [Fig. 2(a)]; p-polarization [Fig. 2(b)]; and s-polarization [Fig. 2(c)]. The number of surface realizations used to obtain these results was $N_\zeta = 5000$. The simulations required for every surface realization 96 CPU seconds (on a 2.67GHz Intel i7 CPU) for each angle of incidence when calculating the scattered field on a 100×100 grid. The peaks observed in Figs. 1 and 2 at angular positions $\theta_s = -\theta_0$ (and $\phi_s = \phi_0 + \pi$) are due to the enhanced backscattering phenomenon, a multiple scattering effect [22]. The energy fraction of the incident light that is scattered by the surface was 94.7%, compared to 96.9% as predicted from the Fresnel coefficient of the corresponding flat interface scattering system. All the light scattered by the surface was essentially incoherent (diffuse) (about 99.98%).

In order to evaluate the accuracy of the simulations and to perform a self-consistency check of our approach, we have performed simulations using the parameters given above with the exception that the metal was assumed to be non-absorbing, *i.e.* we artificially put $\mathrm{Im}\,\varepsilon(\omega) \equiv 0$. Under this assumption, the total time-averaged power fluxes of the incident and scattered fields have to be equal, or in other word, one should require *energy conservation* (or equivalently unitarity of the scattered field, $\mathcal{U} \equiv 1$ where $\mathcal{U}$ denotes the fraction of the incident power flux that is scatted by the rough metal surface. It should be stressed that energy conservation is only a necessary, but not sufficient condition to guarantee the correctness of the simulation results for non-absorbing systems. It is still, however, a rather useful and non-trivial condition that can assist in detecting inaccuracies of the simulation approach as well as potential implementation errors. For the parameters used in the simulations reported in this work, we found $\mathcal{U} > 0.995$ for "non-absorbing" silver [$\varepsilon(\omega) = -16.00$], a result that testifies to the accuracy of our approach.

In order to achieve such good unitarity values, it turned out that great care had to be exercised when handling the matrix elements of the integral equation kernel

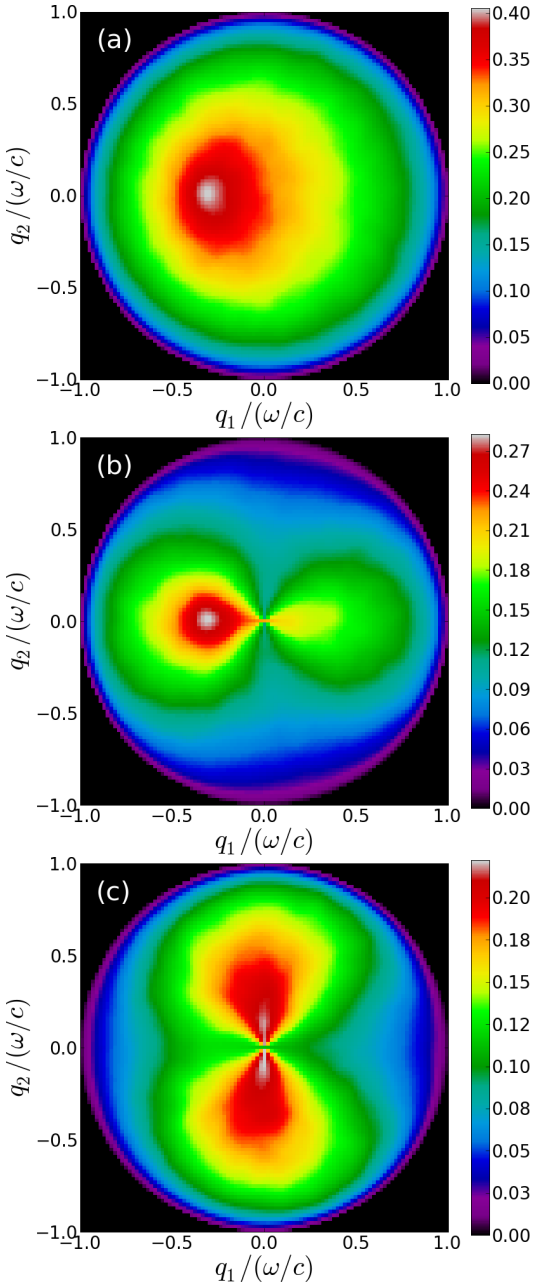

FIG. 2: (Color online) The same as Fig. 1, but now showing the full angular intensity distribution of the scattered field. (a) $p \to$ polarization not recorded; (b) $p \to p$; and (c) $p \to s$.

that were on, or close to, the diagonal. Soriano and Saillard [9] have previously pointed out one way of handling the diagonal matrix elements that contain the singularity (at $\mathbf{x}_\parallel = \mathbf{x}'_\parallel$) of the Green's function by separating it into two parts: one for which the integrand is singular but integrable and is handled analytically, and another that is regular and is handled numerically. These authors were not able within their approach to check the energy conservation of their calculations. We have

found, however, that in order to achieve good results for the energy conservation, also *close-to* diagonal matrix elements (in addition to those on the diagonal) have to be treated accurately even if the off-diagonal matrix elements are regular everywhere. These findings somewhat resemble results reported for volume integral equations where also close to diagonal volume-elements had to be handled with higher accuracy then more distant matrix elements[23]. For instance the use of the midpoint method for evaluating all off-diagonal matrix elements (as in Ref. [9]) and a more accurate method for the diagonal elements, would, for the surface parameters assumed here, result in about 16.4% ($\mathcal{U} = 0.834$) of the incident energy not being accounted for, a result that was found to be more-or-less independent of how accurately one treated the diagonal elements, or if the surface was rough or flat. Moreover, if in addition to the diagonal matrix elements, also the nearest-neighbor elements were treated accurately, the amount of energy that was not accounted for dropped to 4.9% ($\mathcal{U} = 0.951$). If, additionally, also next-nearest neighbor matrix elements were treated accurately, the unitarity condition started to become well satisfied ($\mathcal{U} > 0.995$), and treating accurately matrix elements that were even further apart contributed only insignificantly to the improvement of the unitarity condition [24]. It should be stressed that without performing the self-consistency check based on energy conservation, which requires the full angular distribution of the scattered light being available to us, it has probably not been realized that failing to treat close-to-diagonal matrix elements accurately could cause inaccuracies in the range of 10–20% even for flat interfaces. This is one of the main results of this Letter.

In conclusion, we have presented an accurate and high-performance simulation approach for the scattering of electromagnetic waves from two-dimensional penetrable metallic surfaces based on surface integral techniques. By this approach, the scattering of a p-polarized finite beam by a two-dimensional, randomly rough, silver surface was studied in the optical regime, and it gave rise to the well-known enhanced backscattering phenomenon. Due to the calculation of the full angular intensity distribution of the scattered light, it was possible for us to evaluate the accuracy of the simulation approach. It was found that high-quality simulation results required an accurate treatment of *both* the diagonal and close-to-diagonal matrix elements. This latter point seems to have been overlooked in previous studies. In this way, we were able to obtain results that respect energy conservation (unitarity) for the equivalent non-absorbing system, something that testifies to the accuracy of our approach.

The simulation approach presented in this Letter opens the door to a direct and detailed comparison of the full angle-resolved intensity distributions of the scattered light obtained experimentally and theoretically. Additionally, the approach provides the tools needed to predict the effect of surface roughness on the electromagnetic field in the near and far zone of the surface, and also to tailor surface structures towards specific applications (engineered surfaces). Such issues are of importance in numerous applications, like for instance, in the photovoltaic industry where surface roughness in solar cells is known to increase the efficiency of the cell, but the optimal surface structure, and the mechanism responsible for the increased efficiency, are still unknown [25].

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