Monte Carlo Calculation for Electromagnetic-Wave Scattering from Random Rough Surfaces

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A Monte Carlo calculation for light intensities scattered from a random Gaussian-correlated surface is presented for the first time. It is shown that small randomness on a grating surface can considerably change the intensities and, in particular, the surface polariton resonances. These results should be used to check perturbation-theory calculations.

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The study of surface properties by analyzing the scattered intensities of light from the surface is of current interest.[1] In particular, light scattering is used to study surface plasmons or polaritons on grating surfaces.[2,3] However, in modeling these surfaces it is essential to allow for a random roughness with a given correlation superimposed on the grating profile. It is also interesting to analyze the incoherent elastic scattering generated by the randomness of the surface to understand details of the light-surface interaction,[4] for example, the localization of surface plasmons. So far existing theories and calculations have relied on expansions of the scattering equations up to second order in the variance of the roughness[4,5] or on approximations whose validity is difficult to qualify because exact results are not known.

In this Letter, we present a Monte Carlo calculation that should be able to determine scattering intensities within the statistical error associated with this technique. The calculation is performed by taking statistical averages of a given set of scattering amplitudes obtained for surface profiles consistent with a Gaussian distribution of heights with a Gaussian lateral correlation function, generated according to precise numerical techniques. The scattering amplitudes of p-polarized light from each random sample are computed by using a generalization of the theory of Toigo *et al.*[6] with periodic boundary conditions.

The first step in constructing a sample surface is to generate an uncorrelated Gaussian distribution of random numbers $z_u(x)$, where x is the coordinate along the surface (assumed one-dimensional for simplicity) and z_u the corresponding random height. To a good approximation, this is achieved by considering[7]

$$z_u(x)=\sum_{j=1}^{M} a_{0j}(x)-\tfrac{1}{2}M, \tag{1}$$

where the $a_{0j}(x)$'s are equally distributed random numbers in the interval [0,1] with expectation value and correlation

$$\langle a_{0j}(x)\rangle=0.5,\quad \langle[a_{0i}(x)-0.5][a_{0j}(y)-0.5]\rangle=\tfrac{1}{12}\,\delta_{ij}\,\delta_{xy}, \tag{2}$$

so that

$$\langle z_u(x)\rangle=0,\quad \langle z_u(x)z_u(y)\rangle=\tfrac{1}{12}M\,\delta_{xy}. \tag{3}$$

In accordance with the central-limit theorem, $z_u(x)$ is Gaussian distributed for large M. In practice, M is restricted to only 12; this leads to very small absolute deviations in the tails of the distribution, and the prefactor $M/12$ in (3) becomes 1. The $a_{0j}(x)$'s are generated with the efficient shift-register random-number generator proposed by Kirkpatrick and Stoll.[8]

Next, to obtain the Gaussian-correlated profile $z_u(x)$ is convoluted by a Gaussian:

$$z_c(x)=L^{1/2}\pi^{-1/4}\int_{-\infty}^{+\infty}\exp[-(x-x')^2/2L^2]z_u(x')\,dx'. \tag{4}$$

With $M=12$, according to Eq. (3), we thus get

$$\begin{aligned}&\langle z_c(x)\rangle=0,\quad \langle z_c(x)z_c(y)\rangle=\exp[-(x-y)^2/4L^2],\\ &c_L^2=\int dx\,x^2\langle z_c(0)z_c(x)\rangle\Big/\int dx\,\langle z_c(0)z_c(x)\rangle=2L^2,\end{aligned} \tag{5}$$

so that the root-mean-square distance $c_L = \sqrt{2}L$. Because periodic boundary conditions are used in our actual calculations, we impose $z_c(x) = z_c(x + a)$ (this restriction will have no important physical consequences if the period of the grating $a >> c_L$). Therefore, Eq. (4) is transformed into a sum and evaluated by fast Fourier transformation of $z_u(x)$ using the fast-Fourier-transform (FFT) algorithm. The result is multiplied with the Fourier transform of the Gaussian (4), and finally an FFT backtransform performed to obtain $z_c(x)$. Note, however, that proper care has to be taken in choosing the appropriate prefactors at the FFT backtransform to ensure that relation (5) is satisfied.

The total corrugation function is assumed to be

$$D(x) = a[H\cos(2\pi x/a') + \sigma z_c(x)]. \quad (6)$$

H is the dimensionless strength of the grating profile with period a' on which $z_c(x)$ is superimposed, and σ is the standard deviation of the roughness. Calculations were performed with the same periods a' of the grating and a of the roughness profiles and also some with $a = 3a'$, a kind of supergrating, to check whether artifacts could occur at equal lengths of both periods. The elastic scattering conditions are defined by the incident wave vector $\vec{k}_0 = (\vec{K}, q_0)$, where K and q_0 are the components parallel and perpendicular to the surface. For the scattered waves, $\vec{k}_{\vec{Q}} = (\vec{K} + \vec{Q}, q_Q)$ is fixed by conservation of energy, $q_{\vec{Q}} = [k_0^2 - (\vec{K} + \vec{Q})^2]^{1/2}$, and by $\vec{Q} = 2\pi J/a$, the momentum transfer parallel to the surface, which is quantized because of the periodic boundary conditions imposed.

The scattering amplitudes are calculated by use of the extinction theorem,[6] previously applied by Garcia[9] to pure periodic profiles, in excellent agreement with experiments for Ag and Au gratings. In our case, however, the process of calculation is more complicated: For a given set of incident parameters (wavelength λ and angle of incidence θ), it is necessary to calculate $D(x)$ for many samples to obtain meaningful statistical averages. In our calculations, we kept fifty plane waves to represent the total scattered wave function and 1000 points to perform the necessary x integrals, and averaged the scattering amplitudes over 100 sample profiles for every set of parameters λ and θ. As will be seen, this procedure yields well convergent results. The material of the grating is described by a model dielectric constant $\epsilon(\omega)$.[10]

We first present numerical computations for particular values of the parameters. In Fig. 1(a), on the left-hand side, we present two typical random profiles generated for the parameters indicated in the figure. On the right-hand side, we show the corresponding moduli of the scattering amplitudes for a wavelength $\lambda = 5154$ Å for silver [described by $\epsilon(\omega) = -11 + 0.33i$].[10] In this example, $H = 0$, so that only specular ($\vec{Q} = 0$) reflection would occur without randomness; random roughness produces additional scattering accompanied by a reduction of the $\vec{Q} = 0$ amplitude. As in scattering by a pure periodic grating, these new amplitudes correspond to both propagating and evanescent waves. The former give rise to elastic incoherent scattering, while the latter represent excited surface modes. The specular reflectivity is large for small values of σ and c_L, as it should be on physical grounds.[4,5]

In Fig. 1(b), we plot the average specular intensity and scattered incoherent intensities $J = -1$ and $J = -2$ as a function of the incident angle θ. The randomness gives a continuous distribution of intensity in $\vec{Q}$ space, but in our model, because of the periodic boundary conditions, these intensities accumulate around the diffraction beams, and are defined by summing over samples, i.e.,

$$I(\vec{Q}) = \sum_{i=1}^{N} |A_{\vec{Q}}^{i}|^2/N, \quad (7)$$

where $N = 100$. Instead of error bars, the dimensions of the points indicate the statistical uncertainty of the calculation by increasing the number of waves in the expansion of the Green's function involved in the extinction condition[1] used to obtain the solution.

An interesting result is that at grazing incidence, $\theta = 90°$, the whole intensity is coherently reflected in the specular beam. This was previously obtained with a perturbation-theory approach up to fourth order; $q_0\sigma$ is then small and perturbation theory can be applied.[4]

We also considered the effect of the roughness on a well-defined surface polariton resonance. Quite recently, Garcia[9] studied the surface polariton resonance observed by Tsang and Kirtley[11] on a silver grating at $\theta \simeq 24°$ for $\lambda = 5145$ Å and $a = 8000$ Å. The maximum amplitude of the $J = 1$ polariton wave is obtained for $H = 0.02$ when $\sigma = 0$ in Eq. (6). It is interesting to find out what happens if σ is increased for a given value of $c_L << a$. The results are illustrated in Fig. 2(a), where samples of the random surface for $\sigma \neq 0$ are plotted on the left-hand side, and the corresponding scattering amplitudes on the right-hand side. It is clear that as σ increases from 0.000 31 to $0.02 = H$, the polariton amplitude is reduced from 13.2 to 2.5, and its intensity from 175 to 6, i.e., the surface polariton resonance essentially disappears. This is more evident

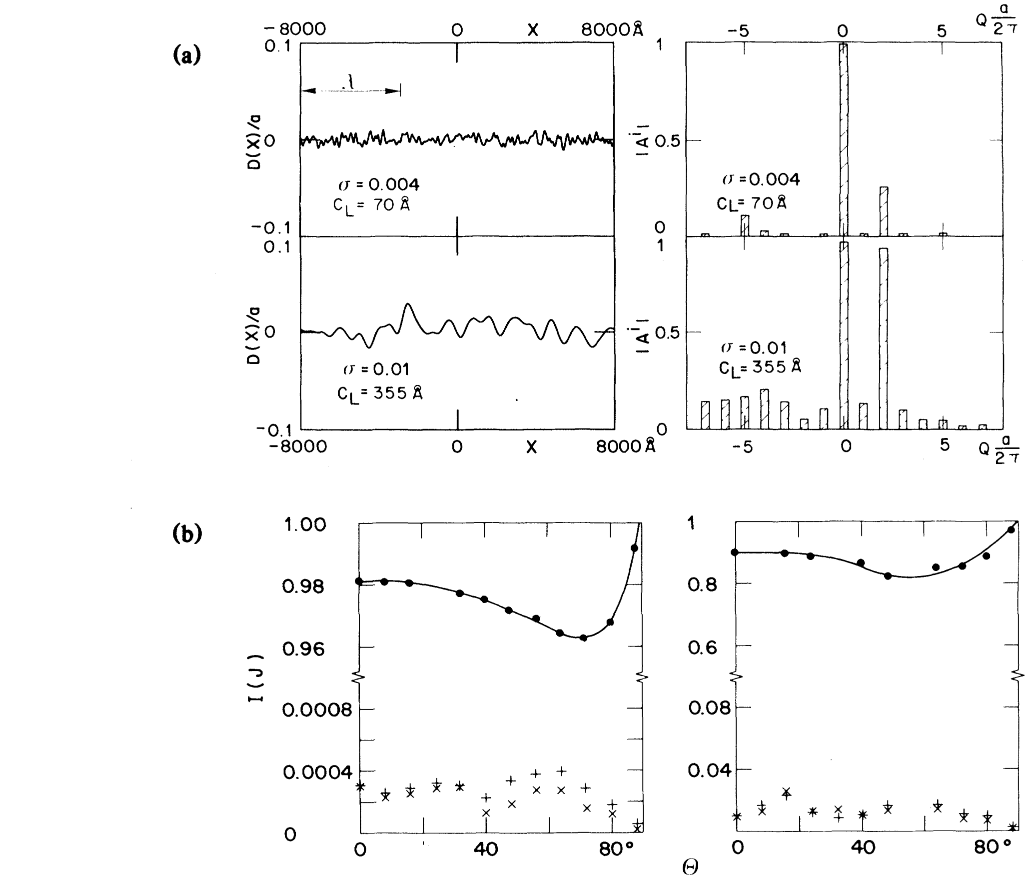

FIG. 1. (a) Left-hand side, two samples of random profiles with the parameters indicated on the figure. The period taken is $a = 16\,000$ Å while $H = 0$. Right-hand side, the corresponding moduli $|A'|$ of the scattering amplitudes of p-polarized light with $\lambda = 5154$ Å. Note the rising of a set of amplitudes when σ and c_L increase. (b) Averaged intensities [Eq. (7) for $N = 100$] for the left-hand side profiles. Circles, $J = Qa/2\pi = 0$; crosses, $= -1$; plusses, $= -2$.

from the averaged intensity versus θ plotted in Fig. 2(b).

In summary, from our calculations we conclude the following:

(i) For $\sigma = 0$, the scattered beam has a value near zero at $\theta_i \simeq 24°$, a result already obtained in Ref. 9.

(ii) The minimum of the specular beam shifts and its intensity grows as σ increases. The first- and second-order diffraction peaks increase; the latter even exhibits a maximum in its intensity versus θ.

(iii) The specular beam shows the same behavior for a pure sinusoidal grating when H increases from $H = 0.02$ to 0.06, but the effect on the first-order peak is different, i.e., a very small minimum remains in that case. The second-order peak follows the same trend as the specular.

(iv) It should be noted that the roughness σ has stronger effects than changes in H.[9] Because of nonlinear relations between the corrugation $D(x)$ and the scattering amplitudes A_J^i,[1] a small roughness superimposed on a sinusoidal grating must not be misinterpreted as being due to pure periodic gratings or to a grating with different Fourier components.

(v) Figures 1 and 2 show that upon increasing σ, higher-order evanescent amplitudes ($J \leq -3$, $J > 0$) build up and produce localized surface plasmons[12] near the corrugation minima. In our view, this happens as a result of the nonlinear relation between $D(x)$ and the A_J^i.[1] By increasing σ, we obtain many higher values $A_J^i (J \neq 0)$: This suggests that the surface plasmon is localized in contrast to what happens with $\sigma = 0$; only A_1^i is important in that case, giving a delocalized value. This conjecture remains to be confirmed by further investigations.

(vi) We performed calculations for $a = 16\,000$ and 24 000 Å, obtaining the same results as for $a = a' = 8000$ Å. This proves that equal lengths of

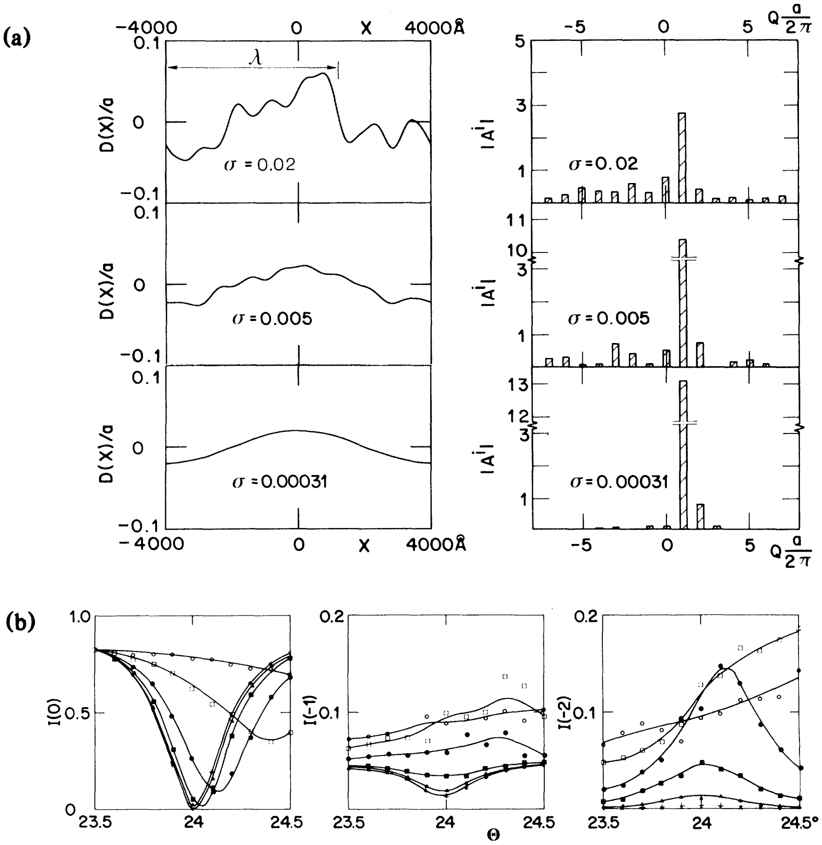

FIG. 2. (a) The same as Fig. 1(a) for $H = 0.02$, $c_L = 355$ Å, and $a = a' = 8000$ Å. Note the disappearance of the polariton amplitude ($J = Qa/2\pi = 1$) as σ increases, and the appearance of excitations at large $\vec{Q}$, i.e., localized plasmons. (b) The same as Fig. 1(b). Note the evolution of the surface resonance as σ increases. (Open circles, $\sigma = 0.02$; open squares, = 0.01; solid circles, 0.005; solid squares, 0.0025; triangles, 0.00125; plusses, 0.00062; crosses, 0.00031.) This has an effect similar to increased H (see Ref. 9).

the grating and roughness profiles do not affect the random scattering when $a \gg c_L$.

In conclusion, we have presented for the first time an exact Monte Carlo calculation for light scattered from a random rough surface with a Gaussian lateral correlation. The results presented here should be used to check perturbation calculations for the same problems, as well as to better characterize optical rough surfaces.

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