Periodicity and Disorder

Simeon D. Simeonov

Western Michigan University

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PERIODICITY AND DISORDER

by

Simeon D. Simeonov

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PERIODICITY AND DISORDER

Simeon D. Simeonov, Ph.D.

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We have studied four examples of periodicity and disorder in nature and the phenomena associated with them.

In the first chapter of the dissertation we present an introduction to this work.

In the second chapter, the photonic band structures of two types of zinc blend structures are computed using the plane wave expansion method. Both structures are formed from an array of dielectric spheres in a vacuum background. In a first type zinc blend structure the spheres have the same size but different dielectric constants. In a second type of structure we keep the dielectric contrast of the spheres the same but change their radii. The lowest frequency band gaps are studied as a function of the dielectric constant ratio in the first structure and as a function of the radii ratio in the second type of structure.

In the third chapter a numerical algorithm is used to generate two-dimensional randomly rough surfaces. The results are used to compute the probability density that the nearest maximum (minimum) to a given maximum (minimum) is at a certain distance. Results are presented for random surfaces defined by surface height correlation function specified by Gaussian, Lorentzian and a novel type of statistics. Results are also presented for a recently proposed one-dimensional random surface.
In the fourth chapter we study the effects of disorder on magnetic superlattices. We have presented two methods to calculate the dispersion relation for electromagnetic waves propagating through stochastically modulated superlattices. The first method is self-consistent method and the second one is based on the Green's functions approach.

In the fifth chapter a new Reverse Monte Carlo method for the determination of the surface profile statistics from differential reflection data for scattering of electromagnetic radiation from surface is presented. The method is used to extract the power spectrum of the surface profile from scattering data recently measured and from data generated by computer. Excellent agreement between the original and retrieved data was found.

In the sixth chapter we present the conclusions of this dissertation.
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Simeon D. Simeonov
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CHAPTER I

INTRODUCTION

There has been a lot of interest throughout recent years in the study of the propagation of electromagnetic waves in two different types of structures. The first is the propagation of electromagnetic waves through periodic structures [Yablonovich, E., 1987; Ho, K.M. et al., 1990] and the second is the scattering of light from surfaces [McGurn, A.R. et al., 1985]. A complete understanding of these processes is of great importance for the progress of the science and related fields of technology. There have been many examples in the history of science when the study of basic processes has generated new materials, new technologies [Ho, K.M. et al., 1990] and has inspired the development of novel devices [Zakhidov, A.A. et al., 1998] with applications which might have seemed unrealistic just a few years before their introduction. That is why the interest of the scientific community in the basic processes of scattering and propagation is still very strong. The phenomena of interactions between the electromagnetic waves and matter become even more challenging when the substance of interest has elements of disorder.

A growing number of scientists have invested considerable efforts in studying the propagation of light through periodic dielectric structures [Sozuer, H.S. et al., 1992; Yablonovich, E. et al., 1991; Maradudin, A.A. et al., 1993]. It has been less than a decade since theoretical physicists announced exciting results in this area [Ho,
These investigations evolved into the study of novel type of macroscopic crystals known as photonic crystals. Photonic crystals are formed of periodic dielectric media which is periodic on macroscopic (much larger than atomic dimension) scales. Due to the periodicity of photonic crystals the electromagnetic waves which propagate through the photonic crystals are characterized by a band structure. This band structure has ranges of frequencies (stop gaps) for which the photons cannot propagate in any direction through the photonic crystal and ranges of frequencies (pass bands) for which photons propagate through the photonic crystal. These ranges of frequencies are often referred as photonic band structures (PBS).

There are many one-, two- [Maradudin, A.A. et al.; 1993] and three-dimensional [Ho, K.M. et al., 1990; Haus, J.W. et al.; 1993] periodic dielectric systems which have been considered and found to exhibit a variety of interesting band structure for the propagation of electromagnetic waves. In addition to the theoretical efforts many experimental groups have fabricated [Yablonovich, E., 1987; Shawn-Yu. Lin et al., 1998] and confirmed the unusual properties of the photonic crystals. The stop gaps were reported first for periodic dielectric media formed of dielectric spheres which are placed at the lattice sites of diamond structure [Ho, K.M. et al., 1990]. Since then many other types of systems [Sozuer, H.S. et al., 1993; Haus, J.W. et al., 1992] have been shown to exhibit photonic band structure. The largest stop gaps (and hence most interesting) are in the diamond lattice. We will consider the study of a photonic crystal with the zinc-blend structure. This new type of structure is similar to the diamond-like structure but it is composed of two different types of atoms [Kittel, C..
We will show that this type of photonic crystal exhibits larger stop bands than does the diamond structure.

In practice we rarely deal with perfectly ordered systems. To study the stochastic component in a system, we would need a tool to describe the nature of the disorder in a random systems. One of the most basic systems to study are surfaces which have a small random component in their surface profile. These surfaces are known as Randomly Rough Surfaces. Methods for mathematical description and computer generation of one-dimensional randomly rough surfaces have been given [Maradudin, A.A., Michael, T., 1990] in the literature and adopted by the scientific community. In these publications, the authors presented mathematical description of the method for generation of one-dimensional randomly rough surfaces. The method is based on the correlation function of sets of randomly rough surfaces. The authors of the method have also used it to generate by computer sets of one-dimensional randomly rough surfaces and to calculate the transverse correlation length. They show that a very good measurement of the transverse correlation length is the average distance between nearest minima and maximum on these surfaces. We find challenging the task to develop ways to generate two-dimensional randomly rough surfaces characterized by a given set of statistical properties. These techniques could be used in extensive computer simulations to generate series of random surfaces with predefined statistical correlations. The results of these simulations could help the scientists to determine important additional statistical properties of randomly rough functions or to use these generated surfaces in computer simulations of scattering.
[Chaikina, E.I. et al., 1997] from, or transport along, rough surfaces. The prescriptions developed for surfaces could be applied to almost any kind of system with elements of disorder. This makes it a valuable tool for theoretical scientists.

It is of interest to study the effects of disorder on the perfectly periodic system and investigate its influence on the material's properties. In some cases we might even expect new phenomena to arise in these systems due to the disorder. One such an example is the propagation of electromagnetic waves through stochastically modulated superlattices. The problem has been recently proposed [Ignatchenko, V.A. et al., 1998] and studied within certain perturbation theory limitations. The results of these studies suggested the existence of interesting effects of the disorder on the band gaps in the dispersion relation of the propagation of electromagnetic waves through superlattices with elements of disorder. We will extend these considerations to studies of more general sets of parameters and develop techniques that will handle any type of stochastically modulated superlattices.

Once we learn how to describe the disorder in a system we might ask ourselves whether we can measure the disorder in a system. The solution of the problem could be connected to the efforts of the experimentalist working in the field. If we consider the task on the example of randomly rough surfaces, then in most experiments the classical way to measure the properties of a surface is to measure the scattering of light from the surface. We assume that this will be the initial data presented to us by experimentalists. Then we are presented with a task of determining the surface profile as a class of the inverse scattering problems. There have been
many efforts at solving the inverse scattering problem in the field of bulk scattering [McGreevy, R.L. et al., 1992]. It turned out the problem is not trivial, and there is no standard way to solve it. A method of interest to us, called Reverse Monte Carlo (RMC) has been applied before to bulk inverse problems considering liquids [Arai. T. et al., 1998], glasses [Montjoy, G. et al., 1998] superconductors and magnetic systems [Borchers, J.A. et al., 1994]. The implementation of the method starts with an initial guess for the configuration of interest, and a random change to the last one is made. Then a characteristic for the system function is computed and, based on a criteria the random change, is accepted, rejected or accepted with certain probability. The process is repeated until an error criteria is satisfied. We are going to apply the Reverse Monte Carlo method to two different types of surfaces. First we will extract information about the statistical properties of a set of randomly rough surface's profiles. The second application of the method which we are going to present is to retrieve the deterministic surface profile.

The problems described here are of special interest to us. A number of tools are available for us to solve these tasks. We will give a mathematical description of the problems, use different mathematical techniques from the numerical analysis to solve differential and integral equations, use matrix algebra and use interpolation and extrapolation of the data. In computing the PBS of the zinc-blend structure we will need methods for diagonalizing large matrixes. There are a large number of software packages which provide standard subroutines which give solution to the problem. We are going to use a subroutine from EISPACK for diagonalizing general matrices.
because we do not expect our eigenvalue problem to have any type of symmetry. To generate the randomly rough surface and apply the Reverse Monte Carlo method, we need a good random number generator. These are well described in the literature and readily provided in software libraries. Different methods for solving integral equations will be used in the calculation of the dispersion relation for the magnetic waves in stochastically modulated superlattices. These methods are developed and described in the mathematical literature. The results of the mathematical description are usually rather complicated equations or systems of equations which we solve using scientific computational techniques. We will use the latest and some of the best computers, including parallel supercomputer nCUBE2 and workstation DEC-Alpha 5300.

In the second chapter of this dissertation, we present the mathematical description of a method to calculate the photonic band gaps in three-dimensional zinc-blend type periodic dielectric media. First, a short description of the type of dielectric system which we are going to study is given. The zinc-blend structure is formed from an fcc lattice with a basis consisting of two non-identical dielectric spheres [Kittel, C., 1986]. Then the photonic band structure is described mathematically. The method is based on the numerical solution of the Maxwell's equations for the propagation of the electromagnetic waves in this type of periodic dielectric media. It is first shown how to obtain the corresponding wave equation. The wave equation is solved by expanding the reciprocal dielectric constant and the magnetic field vector in plane waves. The resulting problem is recognized as a standard eigenvalue problem. Then the final system of equations are used to solve the problem by
computer simulations. In our computer programs we make use of standard subroutines for diagonalization of large matrices. The corresponding systems of equations are solved for three different sizes of the matrices. This is done in order to check the convergence of the problem. We show that the solution converges for large enough sizes of the matrices. The results of these three different sizes of the problem are used to extrapolate the solution for an infinitely large matrix of equations. Two different types of zinc-blend structures are studied. In the first one, we study a system in which the spheres in the basis of the lattice have the same geometry but different dielectric constants. In the second type of dielectric system, we keep the dielectric constant the same for both spheres but change their radii. We use our simulations to study the dependence of the stop gaps on the dielectric constant ratio for the first type of structure and the ratio of the geometrical properties of the spheres for the second type of structure. We present results of the calculation of PBS in zinc-blend type of structure. These findings are compared to the similar results for the classical example of photonic crystals - the PBS for diamond-like structure. We find that dielectric systems that have the zinc-blend lattice type of symmetry can have stop gaps larger than those with diamond structure. These results are very important because they show the possibility to fabricate photonic crystals with band gaps that can be varied in greater limits.

In the third chapter we present a mathematical method to describe two-dimensional randomly rough surfaces and we use this method to generate series of surfaces and calculate important characteristics describing their statistics. One usually
describes the randomly rough surfaces by surface profile function. The mathematical
description is based on the correlation function among the series of surface profile
functions. The study and the generation of one-dimensional randomly rough surfaces
have been presented before our work. Our efforts were directed toward the
continuation of the studies in the field to include the generation of two-dimensional
randomly rough surfaces. We will present the theoretical consideration to describe
these surface and give a general prescription for how to generate by computer two-
dimensional randomly rough surfaces. The mathematical description allows us to
simulate surfaces which would have different correlation functions. The method is
used to generate by computer a series of surfaces characterized by the most common
types of statistical functions describing the correlation among the set of surface
profiles. The results of the generation could be used to calculate important parameters
of the series of the generated surface. One such parameter is the so called transverse
correlation length which is believed to represent how quickly the surface profile
changes and which could be a good measure of the roughness of the surface. We use
the generated series of profiles to measure the transverse correlation length for four
different types of correlation functions. In the process we use a random number
generator from the standard mathematical software package. The method requires the
generation of a large number of surface profiles in order to obtain good statistical
results and that is why the computations are very extensive. We use the parallel
supercomputer nCUBE2 for our simulations.

In the fourth chapter of this work, we present yet another example of disorder
studies. Our efforts in this chapter are directed toward computing the dispersion relations of the magnetic waves propagating through stochastically modulated superlattices. The superlattices are extremely important structures which have been well studied in the last twenty years. There are a number of interesting effects and numerous applications based on the propagation of electromagnetic waves through superlattices. We usually represent the superlattice as a series of layered materials with different properties stacked together to form a sandwich-like structure. It has been customary for most of the studies to assume that the substance in each layer is homogeneous and thus does not have a variation in its properties. Unfortunately, in practice that is rarely the case. This inspired a number of studies of superlattices that have elements of disorder. In some of these studies the authors presented solutions of the problem of propagation of electromagnetic waves through stochastically modulated superlattices based on perturbation theory. We find it challenging to develop general methods to solve the problem exactly. We will present our findings on the example of magnetic waves propagating through superlattice with elements of disorder in the magnetic anisotropy. A mathematical description of the problem is first presented in this chapter of the dissertation. Based on the mathematical description, we solved the problem in two different ways. The first approach is based on the self-consistent method, and the second one is exact method based on the Green’s functions theory. The two methods are used to calculate the dispersion relation of the electromagnetic waves, propagating through stochastically modulated lattices. Based on our computer simulations we were able to confirm the existence of band gaps in the dispersion
relation for a series of different parameters. The approach could be applied to almost any kind of electromagnetic system which is periodic on average and has a small random component.

In the fifth chapter of the dissertation we present a method to recover the surface profile of a deterministic surface and the surface profile statistics of randomly rough surfaces. We use the Reverse Monte Carlo method. The method is first applied to randomly rough surfaces with two types of correlation. The first set of one-dimensional randomly rough surfaces is computer generated, and we calculate the average differential reflection coefficient (which is proportional to the cross section) from these surfaces. The RMC is used to retrieve the surface structure factor (the Fourier transformation of the correlation function). Then the results of the computer simulations are compared with the surface structure factor used to generate the input set of randomly rough surfaces. In a second set of results, the input data is an actual experimental scattering cross section data. Again we apply the Reverse Monte Carlo method, and the results of the simulation are compared to experimental data. In both simulations, a very close match of the experimental and retrieved data is found. This method is also applied to deterministic surface profiles. A mathematical description is first given for the scattering of light from this type of surfaces. This description is used to generate scattering data. The generated data is then used to recover the surface profile. We show that the method could be used successfully to determine the shape of the surface.
CHAPTER II

PHOTONIC BAND STRUCTURES

Introduction

The idea of studying the possibility of band gaps (known as photonic band gaps) in the dispersion relations of electromagnetic waves propagating in periodic dielectric media was introduced by Yablonovich in 1987. The origin of this idea is in the analogy between the propagation of electromagnetic waves through a periodic dielectric medium and the rather well-known energy band behavior of the dispersion relation for electron waves propagating in crystals formed of periodic arrays of atoms. In systems exhibiting photonic band gaps it is clear that technological applications similar to those in the electron systems, which are based on band gaps in the electron dispersion relation, could be developed for photon systems. Specifically, the frequency gaps (photonic band gaps) in periodic dielectric media allow for the use of these structures as highly efficient frequency filters of electromagnetic waves. Consequently there has been much recent interest in the theoretical and experimental study of photonic band structures [Sozuer, H.S. et al., 1993; Yablonovich, E. et al., 1987] exhibiting band gaps in the electromagnetic dispersions relation. These structures, formed as a periodic array of dielectric media, are known as photonic crystals and are of interest due to the band structure exhibited by the dispersion relation of electromagnetic waves propagating in the periodic dielectric media.
To consider the propagation of electromagnetic waves in a periodic dielectric medium or photonic crystals, we start with the Maxwell's equations for the propagation of electromagnetic waves in a position dependent dielectric medium. These equations are [Jackson, J.D., 1975]:

\[ \nabla \times \mathbf{E} = \frac{i \omega}{c} \mathbf{H}, \quad (1.1a) \]

\[ \nabla \cdot \left( \varepsilon(\omega) \mathbf{E} \right) = 0, \quad (1.1b) \]

\[ \nabla \times \mathbf{H} = -\frac{i \omega}{c} \varepsilon(\omega) \mathbf{E}, \quad (1.1c) \]

and

\[ \nabla \cdot \mathbf{H} = 0, \quad (1.1d) \]

where for simplicity the magnetic susceptibility is taken to be one, \( \mu = 1 \).

Eliminating the electric field vector \( \mathbf{E} \) between equations (1.1c) and (1.1a), we find a single wave equation for the magnetic field \( \mathbf{H} \):

\[ \nabla \times \frac{1}{\varepsilon(\omega)} \nabla \times \mathbf{H} = \frac{\omega^2}{c^2} \mathbf{H}. \quad (1.2) \]

This is a wave equation describing the \( \mathbf{H} \) field of an electromagnetic wave propagating in the dielectric medium. We note that we could have derived a wave
equation involving the electric field vector $\vec{E}$ by eliminating $\vec{H}$ from equations (1.1c) and (1.1a). The resulting equation, however, turns out to be more difficult to handle from a computational point of view than equation (1.2). Consequently we will use equation (1.2) to calculate the photonic dispersion spectra in the results described below.

Band gaps have been obtained from equation (1.2) for a variety of periodic dielectric structures including the simple cubic [Sozuer, H.S. et al., 1993], bcc [Sozuer, H.S. et al., 1993], fcc [Ho, K.M. et al., 1990; Sozuer, H.S. et al., 1993] and diamond [Ho, K.M. et al., 1990] lattices. From these studies, the diamond lattice has been found to be most effective in generating large frequency gaps for small dielectric constants. Simple cubic, bcc and fcc structures mentioned above all exhibit small band gaps that require large dielectric contrasts for their generation. Structures with large band gaps are more useful for technological applications than are structures with small band gaps because they are used to block out a greater portion of the electromagnetic spectrum. Consequently, the simple cubic, bcc and fcc structures are less likely to be of technological interest than the diamond structure. In our work presented below we shall investigate new photonic crystals based on zinc-blend structures. We will show that these new photonic crystals can exhibit larger band gaps than those of diamond structure.

Photonic Band Structure of Zinc Blend Type Periodic Dielectric Media

In this part results for the photonic band structure of two types of zinc blend
structures are presented. The zinc blend structure [Kittel, C. 1986] is closely related to the diamond structure. The diamond structure is formed from an fcc lattice with a basis consisting of two identical spheres whereas the zinc blend is an fcc lattice with a basis consisting of two non-identical spheres [Kittel, C. 1986]. We shall see if improvements to the gap forming properties of the diamond lattice can be found in its modified zinc-blend form. Specifically, in one zinc blend structure we shall vary the dielectric contrast of the two spheres of equal radii forming the basis, taking the dielectric background to be a vacuum. In a second zinc blend structure we shall vary the relative radii of the two spheres of equal dielectric constants forming the basis, taking the dielectric background to be vacuum.

The photonic band structure is computed using the planewave method. In this method the electromagnetic wave equation for waves propagating in the periodic medium is expanded in planewaves. The dielectric constant ε is assumed to be periodic of the coordinates:

$$\varepsilon(\vec{r}) = \varepsilon(\vec{r} + \vec{m})$$  \hspace{1cm} (1.3)

where \(\vec{m} = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3\) and \(\vec{a}_1, \vec{a}_2, \vec{a}_3\) are the three noncoplanar primitive translational vectors and \(m_1, m_2\) and \(m_3\) are integers. The reciprocal of the dielectric constant is periodic function as well. This allows us to expand it in a Fourier series:

$$\frac{1}{\varepsilon(\vec{r})} = \sum_{\vec{G}} \hat{\varepsilon} (\vec{G}) e^{i\vec{G}\cdot\vec{r}}$$  \hspace{1cm} (1.4)
where:

\[ \mathbf{G} = h_1 \mathbf{a}_1^* + h_2 \mathbf{a}_2^* + h_3 \mathbf{a}_3^* \]  \hspace{1cm} (1.5)

is the reciprocal lattice vector of the photonic crystal lattice and \( \mathbf{K}(\mathbf{G}) \) is the atomic form factor of the basis. In equation (1.5) \( h_1, h_2 \) and \( h_3 \) are integers and

\[ \mathbf{a}_1^* = \frac{2\pi (\mathbf{a}_2 \times \mathbf{a}_3)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \]

\[ \mathbf{a}_2^* = \frac{2\pi (\mathbf{a}_3 \times \mathbf{a}_1)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \]

and

\[ \mathbf{a}_3^* = \frac{2\pi (\mathbf{a}_1 \times \mathbf{a}_2)}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \]

are the reciprocal lattice vectors.

In accordance with the Bloch-Floquet theorem the magnetic field vector \( \mathbf{H} \) can be expanded as a Fourier series:

\[ H_q(\mathbf{r}, \omega) = \sum_{\mathbf{G}'} A_q(\mathbf{k}, \mathbf{G'}) e^{i(\mathbf{k} \cdot \mathbf{G'} + \omega t)} \]  \hspace{1cm} (1.6)
where $\vec{k}$ is a wavevector in the first Brillouin zone of the reciprocal lattice. Substituting equations (1.5) and (1.6) in equation (1.2) we get an eigenvalue problem for the frequency $\omega$ in terms of $\vec{k}$. This eigenvalue problem for $\omega$ is solved for the band structure of the electromagnetic dispersion relation in the periodic medium.

We consider a periodic dielectric medium with a zinc blend structure consisting of a two non-identical sphere basis on an fcc Bravais lattice. The matrix equation obtained from a planewave expansion of the wave equation describing the magnetic field of the electromagnetic waves propagating through such a structure is [Maradudin, A.A. and McGurn, A.R., 1993]:

$$
\sum_\delta \sum_\beta M_{\alpha \beta} (\vec{k} + \vec{G}, \vec{k}' + \vec{G}') A_\beta (\vec{k}', \vec{G}') = \left( \frac{\omega}{c} \right)^2 A_\alpha (\vec{k}, \vec{G})
$$

(1.7)

where

$$M_{\alpha \beta} (\vec{k} + \vec{G}, \vec{k}' + \vec{G}') = - (k_\alpha + G_\alpha)(k'_\beta + G'_\beta) + \delta_{\alpha \beta} (k + G)(k' + G') \cdot K(G - G)
$$

(1.8)

and

$$K (\vec{G}) = \frac{1}{V_c} \int d^3r \frac{e^{i\vec{G} \cdot \vec{r}}}{\varepsilon(\vec{r})}.
$$

(1.9)

Here $\vec{G}$, $\vec{G}'$ are reciprocal lattice vectors of the fcc lattice; $\beta = 1, 2, 3$ sums over the $x_1$, $x_2$, $x_3$ orthogonal space axes, $V_c$ is the volume of the primitive lattice cell in the fcc lattice; and $\varepsilon(\vec{r})$ is the dielectric constant of the basis.
We have considered two different zinc blend structures. In the first type we have taken a basis of the form

\[ \varepsilon(r) = \varepsilon_A \theta \left( R - |r| \right) + \varepsilon_B \theta \left( R - \frac{a}{4} (\hat{x}_1 + \hat{x}_2 + \hat{x}_3) \right) \]  \hspace{1cm} (1.10a)

where \( R \) is the radii of the dielectric spheres of dielectric constants \( \varepsilon_a \) and \( \varepsilon_b \) and \( a \) is the lattice constant of the conventional (cubic) cell representation of the fcc lattice. In the second type we have taken a basis of the form

\[ \varepsilon(r) = \varepsilon \theta \left( R_1 - |r| \right) + \varepsilon \theta \left( R_2 - \frac{a}{4} (\hat{x}_1 + \hat{x}_2 + \hat{x}_3) \right) \]  \hspace{1cm} (1.10b)

where \( R_1 \) is the radius of one sphere, \( R_2 \) is the radius of the second and both spheres have dielectric constant \( \varepsilon \). These basis are placed on the fcc lattice with the sphere described by the first term on the right hand side of either equation (1.10a) or (1.10b) being centered on a point of the fcc lattice. In the preceding, this sphere (sphere centered at \( \bar{r}=0 \) in the basis) will be referred to as the Zn sphere. The remaining sphere (sphere centered at \( \bar{r}=\frac{a}{4} (\hat{x}_1 + \hat{x}_2 + \hat{x}_3) \) in the basis) of the basis will be referred to as the S sphere. The eigenvalue problem in equation (1.7) then yields the band structure of our periodic dielectric system.

Equation (1.7) is evaluated numerically by restricting the sum on \( \bar{G} \) to the \( N \) smallest \( \bar{G} \) in the system. This converts equation (1.7) into a \( 3N \times 3N \) matrix eigenvalue problem. A further reduction of this problem to a \( 2N \times 2N \) matrix eigenvalue problem can be made by the use of \( \vec{V} \cdot \vec{B} = 0 \) which requires
\[\sum_{\beta} (k_\beta + G_\beta) A_\beta (\vec{k}, \vec{G}) = 0 \quad (1.11)\]

Using equations (1.11) and (1.7) we find:

\[\sum_{\vec{\alpha}'} \left[ M_{\alpha_1} (\vec{k} + \vec{G}, \vec{k}' + \vec{G}') - \frac{(k_1 + G_1')}{(k_3 + G_3')} M_{\alpha_3} (\vec{k} + \vec{G}, \vec{k} + \vec{G}') \right] A_1 (\vec{k}', \vec{G}') + \]

\[+ \sum_{\vec{\alpha}'} \left[ M_{\alpha_2} (\vec{k} + \vec{G}, \vec{k}' + \vec{G}') - \frac{(k_2 + G_2')}{(k_3 + G_3')} M_{\alpha_3} (\vec{k} + \vec{G}, \vec{k} + \vec{G}') \right] A_2 (\vec{k}', \vec{G}') = \]

\[\left( \frac{\omega}{c} \right)^2 A_\alpha (\vec{k}, \vec{G}) \quad (1.12)\]

The eigenvalue solution of the resulting $2N \times 2N$ matrix eigenvalue problem is studied as a function of $N$ to extract via numerical means the $N \to \infty$ limit of the dispersion relation for the infinite photonic band structure.

The specific method we have used to determine the $N \to \infty$ limit of the dispersion relation of our system is as follows: Let $\omega_{N_1}, \omega_{N_2}, \omega_{N_3}$ be eigenvalues of the same photon mode computed using, respectively, $2N_1 \times 2N_1$, $2N_2 \times 2N_2$ and $2N_3 \times 2N_3$ matrices. Assume that for large $N$

\[\omega_N = \omega_- + \alpha \left( \frac{1}{N} \right)^\beta \quad (1.13)\]

where $\omega_-$ is the $N \to \infty$ limit of $\omega_N$ and $\alpha, \beta$ are constants. Using equation (1.12)
for $\omega_{N_1}$, $\omega_{N_2}$, $\omega_{N_3}$ we find from equation (1.13) that:

$$\left[\frac{(\omega_{N_1} - \omega)}{(\omega_{N_2} - \omega)}\right]^\delta = \frac{(\omega_{N_1} - \omega)}{(\omega_{N_3} - \omega)}$$  \hspace{1cm} (1.14)

where

$$\delta = \frac{\log (N_j/N_i)}{\log (N_j/N_i)}$$  \hspace{1cm} (1.15)

The solution of equation (1.14) for $\omega_\omega$ yields an approximate solution of $\omega_\omega$

Results

The zinc blend structures we initially study are based on the diamond structure formed of dielectric spheres in vacuum. The diamond structure was originally studied by [Ho, et al., 1990], and found to give the largest gap width to midgap ratio for the lowest frequency band gap for the simple cubic, bcc, fcc and diamond lattice studied to that date. The diamond structure with the largest gap width to midgap ratio corresponds to a system with $\epsilon = (3.6)^2$ and a single dielectric sphere filling fraction of 0.17. Beginning with the diamond structure we study zinc blend structures formed from this diamond structure by either of the first or second type of modifications of the diamond system as discussed above. The objects of the study of the zinc blend modifications to this diamond structure is to see if such modifications can improve the gap width to midgap ratio over this ratio as computed for the diamond structure.

In Figure 1 we present results for the lowest band gaps as a function of $\epsilon_j/\epsilon_{Zn}$ for fixed $\epsilon_{Zn}=(3.6)^2$ and a filling fraction of 0.17. (A copy of the program used in these computations is presented in the Appendix.) The regions of the frequency band
Figure 1. Lowest Photonic Band Gaps: Shaded Regions Between Solid Lines and Dashed Lines vs. Dielectric Constant Ratio. The Dashed Lines Indicate a Gap Between the Second and Third Bands and Solid Lines Indicate Gap Between the Fifth and Sixth Bands. The Filling Fractions are 17% for Both Types of Atoms.
gaps are indicated in this figure by shading. In obtaining the results in Figure 1 we used the extrapolation in equations (1.7) through (1.9) for $N_1=537$, $N_2=645$ and $N_3=749$. To facilitate the reader in understanding the results in Figure 1 we present results for the band structure along some symmetry directions in the Brillouin zone of the zinc blend structure in Figure 2 for $\epsilon_g/\epsilon_{Zn} = 0.111$, 0.605 and 2.334. These illustrate typical band structures found between $0 \leq \epsilon_g/\epsilon_{Zn} \leq 2.5$. The results in Figure 1 indicate that some advantages to the creation of large photonic band gaps are seen for large and small $\epsilon_g/\epsilon_{Zn}$ ratios in zinc blend structures.

It is interesting to note that for both large and small ratios of $\epsilon_g/\epsilon_{Zn}$ the lowest band gap occurs between the 5th and 6th bands. For intermediate values of $0.5 \leq \epsilon_g/\epsilon_{Zn} \leq 2.0$ a lowest gap exists between the 2nd and 3rd bands. Between $1.3 \leq \epsilon_g/\epsilon_{Zn} \leq 1.6$ we have indicated the positions of the two lowest band gaps. In addition we observe that for $\epsilon_g/\epsilon_{Zn} > 1.5$ the lowest band gap observed is greater than the lowest gap seen in the diamond lattice. Also at $\epsilon_g/\epsilon_{Zn} \equiv 0.1$ a large gap is observed in the zinc blend structure.

In Figure 3 we present similar results to those in Figure 1 but now for spheres with filling fractions of 0.1225. The lowest band gaps (shaded regions) are again presented as a function of the ratio $\epsilon_g/\epsilon_{Zn}$. In these results large band gaps are obtained in the zinc blend data for $\epsilon_g/\epsilon_{Zn} > 1.5$ while no band gaps are observed in the diamond structure. In this case we see that zinc blend structures based on dielectric contrasts favor the creation of band gaps over the diamond lattice counterparts.
Figure 2. Calculated Photonic Band Structures Along Important Symmetry Lines in the Brillouin Zone for Zinc Blend Structure Composed of Dielectric Spheres With Refractive Indexes 3.6 for Zn-placed Atoms and (a) 1, (b) 2.8 and (c) 5.5 for S-placed Atoms. The Band Gap Region Has Been Shaded in.
Figure 3. Photonic Band Gaps (Shaded Regions) vs. Dielectric Constant Ratio. The Filling Fractions Are 12.5 % for Both Types of Atoms.
In Figure 4 we present results obtained using the same extrapolation as in Figure 1 for the second type of zinc blend system described in equation (1.10b). For the results in Figure 4 we have taken $\epsilon=(3.6)^2$ and plotted the band gap (shaded region) as a function of $f_{Zn}f_S$ where $f_{Zn}$ is the filling fraction of the $Zn$ spheres and $f_S$ is the filling fraction of the $S$ spheres. In the region $f_{Zn}f_S<1$ we have fixed $f_S=0.17$ and varied $f_{Zn}$. In the region $f_{Zn}f_S>1$ we have fixed $f_{Zn}=0.17$ and varied $f_S$. The band gap is always found between the 2nd and 3rd bands and is greatest in the diamond structure. In this second type of zinc blend modification of the diamond lattice structure there is then no advantage in the gap forming properties over the original diamond lattice limit.
Figure 4. Photonic Band Upper Edge (Dashed Line) and Lower Edge (Solid Line) vs. Filling Fraction Ratio. The Refractive Indexes are 3.6 for Both Types of Atoms. For $f_{2a}/f_s > 1$ we have fixed $f_{2a} = 0.17$ and varied $f_s$. For $f_{2a}/f_s < 1$ we have fixed $f_s = 0.17$ and varied $f_{2a}$. The $f_{2a}/f_s > 1$ Results are Related by Symmetry to the $f_{2a}/f_s < 1$ Results and this Symmetry is Observed in the Numerical Data Displayed.
CHAPTER III

THE TRANSVERSE CORRELATION LENGTH FOR RANDOMLY ROUGH SURFACES: TWO-DIMENSIONAL ROUGHNESS

Introduction

There is much recent interest in studies involving the generation and investigation of the properties of so called randomly rough surfaces. The term randomly rough surface stands for a surface with a surface profile which can be characterized by a set of random profile functions with certain statistical properties. Precisely, this set of random profile functions is characterized by the mean root squared height of the surfaces about the average surface and by a set of surface profile correlation functions.

Our goal is to generate random surfaces characterized by a root mean squared height and a profile correlation function, and to investigate some of their other topographical properties. We will generate a set of random surface profiles using a set of random numbers in a generating program to create a set of random heights along the $x_1-x_2$ plane. The generating program will address the fact that the profiles we generate have to obey a set of specified statistical properties including a specification of the root mean squared mean height and the correlations of the surface profile functions. The profile correlation functions describe the relation between different heights of the surface at different points in the $x_1-x_2$ plane. On randomly rough
surfaces one can compute two types of correlation functions. One of them is the correlation between different points on the surface. A second type of correlation function is the one that describe the relation between different profile realizations. The former is the type of correlation we will be interested in our work.

Much progress has been made in the laboratory fabrication of one- and two-dimensional randomly rough surfaces [West, C.T. et al., 1995] for the study of optical scattering from such surfaces. In particular one- and two-dimensional surfaces with a given set of profile statistics can be made with photoresist technologies. The statistical properties of these surfaces have been thoroughly studied experimentally and correlated with the optical scattering from these surfaces. The results of the experimental measurements have been compared with theoretical results for the scattering from randomly rough surfaces, and very good agreement was found.

These experimental results were the motivation for us to extend the existing theoretical studies of the properties of one-dimensional rough surfaces to include the two-dimensional randomly rough surfaces. Two-dimensional surfaces are more commonly studied in measurements related to the scattering of light from rough surfaces than are manufactured one-dimensional rough surfaces. At the same time with the advance of modern technology we are presented by significant computational capabilities in the form of very fast and inexpensive computers to aid in the study of the scattering from two-dimensional rough surfaces. The goals of this work was to develop a precise theory for generation and reproduction of two-dimensional randomly rough surfaces and study the statistical properties of the generated surfaces for
probability distributions of different types of topographical features of the surface.

A very important characteristic of the randomly rough surfaces is the transverse correlation length. It is believed that it is a good estimate of the distance between the nearest peaks and valleys on the surfaces. One of the major goals of this work was to check the validity of this statement for the two-dimensional randomly rough surfaces.

A second goal of this work is to demonstrate a method for generating two-dimensional random surface profiles which can then be used in simulation of the scattering from rough surfaces.

Theory

Many theories developed for the properties of randomly rough surfaces assume that the surface profile function \( \xi(x_1, x_2) \) of the rough surface is a stationary, stochastic, Gaussian process and that averages over the surface roughness can be expressed as averages over a set \( \{ \xi(x_1, x_2) \} \) of stationary stochastic Gaussian functions which represent the statistical properties of the rough surface. The set of stationary, stochastic Gaussian functions \( \{ \xi(x_1, x_2) \} \) is defined such that the mean deviation from flatness is

\[
<\xi(\overline{x})> = 0
\]

and the correlation function is in the form

\[
<\xi(\overline{x}) \xi(\overline{x}')> = \sigma^2 g(|\overline{x} - \overline{x}'|)
\]
where $< >$ represents an average over $\{\xi(x_1, x_2)\}$, $\sigma^2 = <\xi(x)^2>$ and $g(|x|)$ is a correlation function. The correlation functions involving higher order products of $\xi$'s can be expressed in terms of the correlations in equations (2.1), using well known factorization techniques [Wick, G.C., 1950].

The assumption that a rough surface is described by a Gaussian process is particularly useful in Green's functions calculations of the scattering waves from or propagation of surfaces waves along rough surfaces as it allows for a Wick's [Wick, G.C., 1950] theorem factorization of averages over products of $\xi(x_1, x_2)$. This makes possible a Feynmann diagrammatic treatment of the perturbation theory for electromagnetic scattering from the surface in powers of the surface roughness profile $\xi$ [Gray, P.F., 1978; Brown, G. et. all, 1985]. Aside from these theoretical considerations, a number of experimental systems with Gaussian random statistics have recently been generated and studied experimentally [West, C.S. et. all, 1995]. For these reasons it is of interest to investigate the statistical properties exhibited by these surfaces which provide insight into the general topography of the surface roughness.

Recently, Micheal and Maradudin have presented [Maradudin, A.A., Micheal, T., 1990] such a study of the statistical properties of one-dimensional randomly rough surfaces, defined by $x_3 = \xi(x_1)$ where $\xi(x_1)$, which is independent of $x_2$, is a stationary, stochastic, Gaussian process. A central result of these studies was the determination, by means of computer simulation, of the probability density as a function of distance along the $x_1$-axis for finding nearest-neighbor maximum-
minimum pairs on the random surface. This probability density is very useful as an indication of the general character of the occurrence of minima and maxima along the one-dimensional rough surface. This distribution was computed for a number of different types of correlation functions $g(\tilde{x}_1-\tilde{x}_1')$. The physical features of $g(\tilde{x}_1-\tilde{x}_1')$ where related to the features of the computed probability density of nearest neighbor maxima-minima pairs. In the present work we extend the simulation efforts of Micheal and Maradudin to compute the probability density as a function of distance in the $x_1-x_2$ plane for finding nearest-neighbor maxima, minima and maximum-minimum pairs on a two-dimensional randomly rough surface defined by $x_3 = \xi(x_1,x_2)$ where $\xi(x_1,x_2)$ is a stationary, stochastic, Gaussian process.

A surface with a surface profile of the form $x_3 = \xi(x_1,x_2)$ where $\xi(x_1,x_2)$ is a stationary, stochastic, Gaussian process can be numerically simulated as follows: The axes $x_1$ and $x_2$ axes are discretized into segments of length $\Delta x$ such that a mesh is formed in the $x_1-x_2$ plane. The points of this mesh are then given by $(x_1(l), x_2(k)) = (l, k)\Delta x$. At each point of the mesh $(x_1(l), x_2(k))$ the height $x_3$ coordinate of the random surface is taken to be given by:

$$
\xi(x_1(l), x_2(k)) = \sigma \sum_{i=-N}^{N} \sum_{j=-N}^{N} W_{ij} X_{i-l, j-k}
$$

(2.2)

where $N \rightarrow \infty$. In Eq.(2.2) $X_{n,m}$ is a Gaussianly distributed random number with

$$
< X_{n, m} > = 0
$$

(2.3a)

$$
< X_{n, m} X_{i, k} > = \delta_{n, l} \delta_{m, k}
$$

(2.3b)
where $\delta_{ij}$ is the Kroneker delta function.

$$W_{i,j} = \Delta x \int \frac{d^2q}{(2\pi)^2} \hat{g}^{1/2}(q) e^{iq_1x_1(0)} e^{iq_2x_2(0)}$$ (2.4)

and

$$g(x) = \int \frac{d^2q}{(2\pi)^2} \hat{g}(q) e^{iq_1x_1} e^{iq_2x_2}$$ (2.5)

is the power spectra of the desired statistical distribution. Using equations (2.2) through (2.5) we compute the surface profile averages defined in equations (2.1) and find:

$$<\xi(x_1(l), x_2(k))> = 0$$ (2.6a)

$$<\xi(x_1(k), x_2(k'))\xi(x_1(k+l), x_2(k'+l'))> = \sigma \sum_{i,j=-N}^{N} W_{ij} W_{i-j,k-l'} g(|(x_1(k), x_2(l'))|)$$ (2.6b)

The higher order correlations can also be computed from equations (2.2) through (2.5) and are found correct to terms of order $\Delta x$, to be related to equations (2.6) by the well known factorization relations [Wick, G.C., 1950] for the surface profile correlation functions for stationary, stochastic, Gaussian random process. In particular, we find for the next higher correlation from Eq.(2.6b) that :

$$<\xi(x_1(k), x_2(k'))\xi(x_1(k+l), x_2(k'+l'))\xi(x_1(k+l), x_2(k'+l'))> = \Delta x \int \frac{d^2q}{(2\pi)^2} \int \frac{d^2p}{(2\pi)^2} \hat{g}^{1/2}(q) \hat{g}^{1/2}(p) \hat{g}^{1/2}(q+p)$$ (2.7)

which goes to zero as $\Delta x \rightarrow 0$. 

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A set of Gaussian random profiles can now be generated from equations (2.2), (2.4) and (2.5). Once $g(q)$ is determined from equation (2.5), $W_{ij}$ is obtained from equation (2.4). A surface profile with the desired statistical properties is then obtained from equation (2.2) where $X_{i+t_1+t_2}$ are a set of Gaussian distributed random numbers characterized by equation (2.3b).

Results

We have used the formulation in equations (2.2) to generate a set of stochastic Gaussian random surfaces and to compute the statistical distribution of the nearest neighbor maxima, minima and maxima-minima pairs on the set of random surfaces as a function of their separations in the $x_1-x_2$ plane. (A copy of the program for this generation can be found in the Appendix.) For this determination equation (2.2) was used to generate a single Gaussian random surface which satisfies equation (2.1), and the distribution of nearest neighbor maxima, minima and maxima-minima pairs and their separations was computed for the generated surface. The data from a large number of such generated surfaces was then used to obtain a numerical computation of the nearest neighbor maxima, minima and maxima-minima pairs distributions for the set of Gaussian random surface functions. In the results presented below we have used $N=6500$, $N=6000$ and $N=1000$ surfaces respectively to generate the distributions presented in Figures 5, 7 and 9. We have studied two-dimensional random surfaces which were computed using three different types of correlation functions. In a first study we took $g(|\vec{x}-\vec{x}'|) = \exp[-(\vec{x}-\vec{x}')^2/a^2]$; in a second study we took
\[ g(\|\vec{x} - \vec{x}'\|) = \frac{a^2}{(\vec{x} - \vec{x}')^2 + a^2} \] and in third study we examined a random surface with a spectral density [West, C.T. et al., 1995]

\[ \hat{g}(k_{11}) = \int d^2x \ e^{-ik_{11}^2} \langle \xi(0) \xi(\vec{x}) \rangle = \frac{4\pi \sigma^2}{k_2^2 - k_1^2} \Theta(|k_{11}| - |k_1|) \Theta(k_2 - |k_{11}|). \]

This last surface has recently been proposed as a surface which would be of interest in studying resonant scattering processes on two-dimensional rough surfaces [McGurn. A.R. et al., 1996] which are dominated by surface plasmon-polariton effects. In the results presented below for these surfaces, we have measured all lengths in units of \( a \) and have taken \( \Delta x = 0.05a \). The distribution of maxima, minima and maxima-minima pairs were obtained by considering a \( L \times L \) portion of the \( x_1 - x_2 \) plane with \( L = 7a \).

In Figure 5 we present results for the probability distribution \( P(x) \) for finding nearest neighbor maxima (Figure 5a), nearest neighbor minima (Figure 5b), nearest neighbor maxima-minima pairs (Figure 5c) separated by a distance \( x \) in the \( x_1 - x_2 \) plane for \( g(\vec{x}) = \exp[-\frac{x^2}{a^2}] \). The results in Figure 5a and Figure 5b should be the same as each generated surface \( \xi(x_1, x_2) \) and its reflection \( -\xi(x_1, x_2) \), is a member of \{ \( \xi(x_1, x_2) \) \}. In fact, Figures 5a and 5b are found to be in good agreement. The maximum value of \( P(x) \) in Figures 5a, 5b and 5c are at 1.675 \( a \), 1.675 \( a \) and 1.225 \( a \) respectively. We also determined the average distance between the minima-minima, maxima-maxima and minima-maxima on these surfaces to be 1.784 \( a \), 1.783 \( a \) and 1.400 \( a \) respectively. As a check of the accuracy of the set of computer generated surfaces as a representation of stochastic set of Gaussian random surfaces with \( g(\|\vec{x}\|) = \exp[-\frac{x^2}{a^2}] \), we have used the set of generated surfaces to compute \( g(\|\vec{x}\|) \).
Figure 5. The Probability Density Function (a) $P_1(x)$, (b) $P_2(x)$ and (c) $P_3(x)$ for the Two-dimensional Random Surface Defined by $g(|\bar{x}-\bar{x}'|) = \exp[-(\bar{x}-\bar{x}')^2/a^2]$. 
In Figure 6 we present \( g(|\vec{x}|) \) versus \( x \) computed from the numerically generated surfaces (solid line) and for the function \( g(|\vec{x}|) \) read into the simulation at the start of the computation (dashed line). The noise in the solid line decreases as \( 1/\sqrt{N} \) where \( N \) is the number of generated surfaces used to compute the numerical average for \( g(|\vec{x}|) \). The results obtained in Figure 5 were obtained for \( N=800 \).

In Figure 7 we present results for the probability distribution \( P(x) \) for finding nearest neighbor maxima (Figure 7a), nearest neighbor minima (Figure 7b), nearest neighbor maxima-minima pairs (Figure 7c) as a function of the spatial separation by \( a \) in the \( x_1-x_2 \) plane for \( g(|\vec{x}|) = \frac{a^2}{x^2+a^2} \). The maximum value of \( P(x) \) in Figures 7a, 7b and 7c are at 1.025\( a \), 1.025\( a \) and 0.925\( a \), respectively. We also determined the average distance between the minima-minima, maxima-maxima and minima-maxima on these surfaces to be 1.112\( a \), 1.108\( a \) and 0.964\( a \) respectively. For comparison we plot in Figure 8 \( g(|\vec{x}|) \) versus \( x \) computed from the numerically generated surfaces (solid line) and for the function \( g(|\vec{x}|) \) read into the simulation at the start (dashed line). For the numerical results in Figure 8, 1200 numerically generated surfaces were used. Aside from the noise in the results computed from the generated surfaces, the results from the generated surfaces approach zero for large increasing \( x \) faster than the read in Lorentzian correlator which is cutoff in range by the limiting size of the simulation region for the \( x_1-x_2 \) plane.

From Figures 5 and 7 we see that the \( P(x) \) as functions of \( x \) exhibit maxima for \( x \) of order \( a \). For the Lorentzian correlator, however the value of \( x \) for which \( P(x) \) are maximum are smaller than those for which the corresponding \( P(x) \) are
Figure 6. The Initial (Dashed curve) and Calculated (Solid Curve) Surface Height Autocorrelation Functions for the Two-dimensional Random Surface Defined by $g(|\vec{x}-\vec{x}'|) = \exp[-(\vec{x}-\vec{x}')^2/a^2]$. 

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Figure 7. The Probability Density Function (a) $P_1(x)$, (b) $P_2(x)$ and (c) $P_3(x)$ for the Two-dimensional Random Surface Defined by $g(|\bar{x}-\bar{x}'|) = \frac{a^2}{[(\bar{x}-\bar{x})^2+a^2]}$. 

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Figure 8. The Initial (Dashed Curve) and Calculated (Solid curve) Surface Height Autocorrelation Functions for the Two-dimensional Random Surface Defined by $g(|\vec{x} - \vec{x}'|) = a^2 / [(\vec{x} - \vec{x}')^2 + a^2]$. 

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maximum for the Gaussian correlator. In both systems the maxima in $P(x)$ for the
distribution in $x$ of maxima-minima nearest neighbor pairs occurs for a smaller $x$
separation than that for the maxima in $P(x)$ for the distribution in $x$ of the maxima-
maxima nearest neighbor pairs.

In Figure 9 we present results for the probability distribution $P(x)$ for finding
nearest neighbor minima (Figure 9a), nearest neighbor minima-maxima (Figure 9b),
nearest neighbor maxima pairs (Figure 9c) as a function of their spacial separation by
$a$ in the $x_1-x_2$ plane for a set of random surfaces described by the power spectrum
$g(k) = \frac{4\pi a^2}{k^2 - k_1^2} \Theta(k-k_1) \Theta(k-k_2).$ In evaluating $\hat{g}(k_1)$ we have taken

$$k_1 = \frac{2\pi}{\lambda} \left[ \sqrt{\frac{\epsilon}{\epsilon + 1} - \sin(\theta_m)} \right]$$

and

$$k_2 = \frac{2\pi}{\lambda} \left[ \sqrt{\frac{\epsilon}{\epsilon + 1} + \sin(\theta_m)} \right]$$

for $\lambda = 4579\lambda$, $\epsilon = -7.5$ and $\theta_m = 10^\circ$ which is a possible realization of this
surface on a silver surface. The maximum value of in $P(x)$ in Figures 9a, 9b and 9c
are at $0.375a$, $0.375a$ and $0.225a$, respectively. We also determined the average
distance between the minima-minima, maxima-maxima and minima-maxima on these
surfaces to be $0.368a$, $0.367a$ and $0.248a$ respectively. In Figure 10 we present
$\hat{g}(k_1)$ computed from the simulation surface using 600 surfaces and compare it with $\hat{g}(k_1)$
read into the simulation at the beginning. The "wings" on the simulation results

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Figure 9. The Probability Density Function (a) $P_1(x)$, (b) $P_2(x)$ and (c) $P_3(x)$ for the Two-dimensional Random Surface With Spectral Density Defined by $\hat{g}(k) = [4\pi a^2/(k_2^2-k_1^2)] \Theta(k-k_1) \Theta(k_2-k)$. 

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Figure 10. The Initial (Dashed Curve) and Calculated (Solid Curve) Surface Height Autocorrelation Functions for the Two-dimensional Random Surface With Spectral Density Defined by
\[ \tilde{g}(k) = \frac{4\pi a^2}{(k_2^2 - k_1^2)} \Theta(k-k_1) \Theta(k_2-k). \]
decrease with increasing $L$ and are a feature of the finite size of the region we consider in the $x_1$-$x_2$ plane for the generation of random surfaces.

In addition to the results presented above for the probability distribution of nearest neighbor maxima, minima and maxima-minima pairs on two-dimensional surfaces, we will now obtain results for the probability distribution of the nearest neighbor maxima-minima pairs for one-dimensional rough surface which has been of recent interest [West, C.T. et al., 1995] in the content of the experimental studies of the surface plasmon-polariton mechanism in the enhanced backscattering of light from rough surfaces. West and O'Donnell have fabricated an one-dimensional randomly rough gold surface which has a surface profile which is a stationary, stochastic, Gaussian process described by spectral density of the form

$$\hat{g}(k) = \int dx \; \langle \xi(0) \xi(x) \rangle \; e^{-ikx_1} = \frac{\pi}{k_2-k_1} \left[ \Theta(k-k_1)\Theta(k_2-k) + \Theta(-k-k_1)\Theta(k_2+k) \right].$$

where

$$k_1 = \frac{2\pi}{\lambda} \left[ \sqrt{\epsilon - \sin(\theta_m)} \right] \quad \text{and} \quad k_2 = \frac{2\pi}{\lambda} \left[ \sqrt{\epsilon + \sin(\theta_m)} \right].$$

In evaluating [West, C.T. et al., 1995] $\hat{g}(k)$; $\epsilon = -17.29$, $\lambda = 612\lambda$ and $\theta_m = 13.5^\circ$. The probability density $P(x)$ of the distribution of nearest neighbor maxima-minima for this surface can be computed using the technique developed by Micheal and Maradudin. In Figure 11 we present results from such a computation for $P(x)$ versus $x$. These are the parameters which characterize the surface studied experimentally in Ref.2. The distribution of the nearest neighbor maxima-minima pairs is seen to be sharply peaked about $\frac{\Delta k}{2} x = 0.6$ and to have a full width at half maximum of 0.1 in units of $\left( \frac{\Delta k}{2} \right)^{-1}$. As a check on this result, an estimate of the
Figure 11. The Probability Density Function \( P(x) \) for the One-dimensional Random Surface With Spectral Density Defined by

\[
\hat{g}(k) = \frac{\pi}{(k_2 - k_1)} [\Theta(k - k_1)\Theta(k_2 - k) + \Theta(-k - k_1)\Theta(k_2 + k)]
\]
value of $x$ at the peak in the $P(x)$ distribution can be obtained if we consider that the spectral density of the rough surface is an almost periodic function with an approximate periodicity described by the wavenumber $k_{av} = \frac{1}{2}(k_1+k_2)$. The separation in $x$ between nearest neighbor maxima-minima pairs, $\Delta x$, for a periodic sinusoidal function of wavenumber $k_{av} = \frac{1}{2}(k_1+k_2)$ is given by $k_{av} \Delta x = \frac{\pi}{2} \frac{\Delta k}{k_{av}} = 0.69$ which is in reasonable agreement with the value of 0.6 obtained from Figure 11. In addition a good estimate for the nearest neighbor minima maxima separation on one-dimensional West-O'Donnell surfaces is also provided by the reciprocal of the density of zeroes $<d>$ of the random surface profile function $\xi(x)$. For our surface is 0.665, which is in very good agreement with the results in Figure 11. As an additional check of our numerical work, we present in Figure 12 a plot of $\hat{g}(k_{1/})$ versus $k$ for the $\hat{g}(k_{1/})$ computed from the surfaces generated by the computer simulation. Good agreement is found between these two $\hat{g}(k_{1/})$. 

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Figure 12. The Initial (Dashed Curve) and Calculated (Solid Curve) Power Spectra for the One-dimensional Random Surface With Spectral Density Defined by

\[ \hat{g}(k) = \left[ \frac{\pi}{(k_2 - k_1)} \right] [\Theta(k-k_1)\Theta(k_2-k) + \Theta(-k-k_1)\Theta(k_2+k)]. \]
CHAPTER IV

DISPERSION RELATION OF RANDOMLY MODULATED MAGNETIC SUPERLATTICES

Introduction

There has been a lot of recent interest [Ignatchenko, V.A. et. al., 1998; Borchers, J.A. et. all, 1994] in the study of phenomena associated with optical and magnetic superlattice structures. These efforts have dealt both with perfect periodic superlattice structures and superlattice structures which are perturbed by stochastically modulated disorder. During the last decade, the general properties of perfect periodic superlattice structures have been very well investigated [Kittel, C., 1986] and a thorough theoretical explanation has been given. The general features of perfect periodic superlattice are selective transmission of electromagnetic waves within a series of band widths, spontaneous emission of coherent light, quantum-mechanical phenomena related to the quantum well nature of these structures.

Unfortunately, in practice, it is very difficult to fabricate perfectly ordered superlattices. The real structures can exhibit fluctuations in layer thickness [Clements, B.A. et. al., 1987] from layer to layer. This is one type of disorder. Another type of disorder arises from inhomogeneities and can be associated with the quality of the material used to fabricate the superlattice. It is very difficult to produce a perfectly ordered crystal lattice without any distortion, vacancies or impurity atoms incorporated.
into it. We can expect inhomogeneities would influence the electrical, optical or magnetic properties of the material of interest. These facts lead several authors to attempt to describe theoretically the effects of disorder [Mader, K. et. al., 1995] contributing to a randomly modulated superlattice structure. Experimental measurements [Borchers, J.A. et. al., 1994] have also been made to determine the effects of disorder on superlattice. Results of these investigations have shown some very interesting effects for the electron, photon [Ignatchenko. V.A. et. al., 1998] and spin-wave [Pang, G. et. al., 1988] propagation through superlattices.

The authors of Reference [Ignatchenko. V.A. et. al., 1998] have presented a perturbation theory treatment of the dispersion relation of electromagnetic waves propagating through stochastically modulated superlattices. This method is based on the description of the superlattice by a periodic function the period of which is modulated by a random field with certain statistical properties. Several solutions of the problem are presented in the perturbation theory limit, based on different statistical assumptions. Although easily applicable and computational inexpensive the perturbation theory possesses certain limitations. It usually gives precise results only in one limiting case of the parameters, and one has to be very careful not to violate these perturbation theory limits. If we have to obtain a general solution, we need to look for other methods to approach the problem. One method that could be applied is the self-consistent perturbation theory. This method is effective in solving the problem by representing the solutions of interest in an iteratively generated series. The most precise way to calculate the dispersion relation for the electromagnetic waves
propagating through randomly modulated superlattice, however, is to solve the resulting integral equation numerically. The last two methods are computationally more costly but produce precise results over a greater range of parameters. The objective of our work is to use the last two methods to calculate the dispersion relation of electromagnetic waves propagating through stochastically modulated superlattices. The self-consistent approach should extend the range of the perturbation theory and the computer simulation approach will give a solution over all range of the parameters.

Self-consistent Approach

In this part of our presentation we will describe the model to be studied. We will then discuss the perturbative self-consistent method for calculating the dispersion relation in the system. The computer simulation study of this model will be presented at the end of this section.

We consider a random one-dimensional system which is periodic on average. The system can be a magnetic system with magnetic excitations or a dielectric system with electromagnetic excitations. The mathematics of either of the systems are essentially the same. Both are superlattice structures with an additional element of random disorder. We shall begin by developing the theory of magnetic systems. Afterwards we will indicate the small changes needed to describe the dielectric system.

The Hamiltonian of the magnetic system is given by [Landau, L.V., 1953]:

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Here $H_m$ represent the magnetic energy density. $\vec{M}$ is the magnetization, $\vec{H}$ is the magnetic field, $\alpha$ is the exchange parameter, $\beta$ is the magnetic anisotropy and $\vec{b}$ - the direction of the anisotropy axis. In homogeneous materials all of the parameters are constants which characterize the nature of the material. A periodic superlattice is formed by choosing the $\alpha$ and $\beta$ to be periodic functions in space, and, with the addition of impurities to the superlattice, the parameters become random functions of coordinates which are periodic on average.

One can consider a series of different parameters $\alpha$ and $\beta$ in equation (3.1), each of which exhibits a different type of stochastic behavior. Each case of random disorder will correspond to a different type of inhomogeneities. Let us consider an inhomogeneous magnetic anisotropy of the form:

$$\beta(x) = \beta(1 + \gamma \rho(x))$$

(3.2)

where $\beta$ is the average values of the magnetic anisotropy and $\gamma$ is the relative rms fluctuation. The function of the form of equation (3.2) represents an anisotropy which has a certain average value and a random component superimposed on it. In equation (3.2) $\rho(x)$ is a random function which is periodic on average and can be expressed in terms of a Fourier transform as:

$$\rho(x) = \int \rho(k) e^{ikx} dk$$

(3.3)
For stochastic functions \( \rho(x) \) which are periodic on average the spectral density \( S(k) \) is then written as:

\[
\langle \rho(k)\rho(k') \rangle = S(k)\delta(k-k')
\]  

(3.4)

where the function \( S(k) \) is peaked in k-space about the Fourier components for which \( \rho(x) \) is periodic on average. The spectral density \( S(k) \) determines the form of the correlation of the random function and it will be used in our work to describe the stochastic component of the inhomogeneities in the system.

The ferromagnet dynamics obtained from equation (3.1) is given by the Landau-Lifshitz equation:

\[
\frac{\partial \mathbf{M}}{\partial t} = -g \left[ -\frac{\partial H_m}{\partial \mathbf{M}} + \frac{\partial}{\partial x} \left( \frac{\partial H_m}{\partial (\partial \mathbf{M}/\partial x)} \right) \right]
\]  

(3.5)

where \( g \) is the gyromagnetic ratio.

Choosing \( \mathbf{H} \) and \( \mathbf{b} \) to be in z-direction and \( \mathbf{m} = M_x + iM_y \) one can obtain from equation (3.5) the following differential wave equation which describes the propagation of magnetization waves through the periodic stochastically modulated superlattice:

\[
\nabla^2 \mathbf{m} + (\nu - \epsilon \rho(x))\mathbf{m} = 0.
\]  

(3.6)

In equation (3.6), \( \nu = (\omega - \omega_j/\alpha g M) \) is related to the frequency \( \omega \) of the magnetic excitation and \( \epsilon = \gamma \frac{\beta}{\alpha} \) describes the ratio of the magnetic anisotropy to the magnetic exchange parameter.
Fourier transforming of the equation (3.6) one finds:

\[
(v - k^2)m(k) = \int dq \rho(q-k)m(q) \tag{3.7}
\]

where

\[
\rho(k) = \frac{1}{2\pi} \int dx \rho(x) e^{-ikx}. \tag{3.8}
\]

In order to determine the spectrum of the frequency we have to solve the above integral equation in equation (3.7). If we average equation (3.7) we find:

\[
<m(k)> = G_0 U(k)<m(k)> \tag{3.9}
\]

where

\[
G_0(k) = \frac{1}{v-k^2}. \tag{3.10}
\]

Here \(U(k)\) is a self-consistent solution of the equation:

\[
U(k,v) = \eta^2 \int dq \frac{S(k-q)}{v-q^2-U(q,v)} \tag{3.11}
\]

and \(\eta = \gamma v\). The dispersion relation is then given by the relation of:

\[
v - k^2 = U(k,v) \tag{3.12}
\]

We are solving the equation above for a stochastic function with a power spectra:
This \( S(k) \) represents a system which has an average periodicity described by the wavevector \( k \). For a purely periodic system with \( \rho(x) \propto \cos(kx) \), we would replace the two Gaussian functions in equation (3.13) by delta function centered about \( k \) and \(-k\).

The spectrum of electromagnetic waves in stochastically modulated periodic medium will have to satisfy the same equations with different parameters. The dielectric constant of the system is assumed to be a random on average harmonic function of \( x \) in the form \( \epsilon(x) = [1 - \gamma \rho(x)] \). Here \( \rho(x) \) is some stochastic function which is periodic on average and \( \nu = \epsilon(\omega^2/c^2) \).

The dispersion relation of the magnetic waves propagating through stochastically modulated superlattice is determined by solving equation (3.11) for \( U(k,\nu) \) self-consistently and then substituting the values of \( U(k,\nu) \) in equation (3.12). To facilitate the readers understanding about the approach, we first solved equation (3.11) by using the Bourret approximation first. This approximation is essentially representing the self-consistent potential \( U(k,\nu) \) in the form:

\[
U(k,\nu) = \frac{\eta^2}{2\sqrt{\pi}} \int dq \frac{S(k-q)}{\nu - q^2}.
\]  

Equation (3.14) is then solved for a given value of the wavevector \( k \).

In order to determine the dispersion relation for the magnetic systems, one needs to find the poles of the Green's function of the form:
To determine the poles of the last equation we plot $G(k,v)$ as a function of the wavevector $v$ for a given $k$. In Figure 13a and Figure 13b we present the real and imaginary part of the Green's function for $k=0.48$. One can notice the presence of two distinct poles in Figure 13a and Figure 13b. The position of these poles corresponds to points in the dispersion curve. Furthermore we can extract information about the imaginary part of the frequency of propagation which represents the absorption of the propagating waves. Assuming the presence of two poles of the Green's function, we can represent the real and imaginary part of equation (3.15) as:

$$G(k,v) = \frac{1}{v - k^2 - M(k,v)}.$$  \hspace{1cm} (3.15)

$$\text{Re}(G(k,v)) = \frac{A(v-v_0)}{(v-v_0)^2 + \Gamma_0^2} + \frac{B(v-v_1)}{(v-v_1)^2 + \Gamma_1^2}$$  \hspace{1cm} (3.16)

$$\text{Im}(G(k,v)) = \frac{A\Gamma_0}{(v-v_0)^2 + \Gamma_0^2} + \frac{B\Gamma_1}{(v-v_1)^2 + \Gamma_1^2}$$  \hspace{1cm} (3.17)

where the $A, B$ are some real constants, $\omega_0$ and $\omega_1$ are the real parts of the frequencies, and $\Gamma_0$ and $\Gamma_1$ are the imaginary parts of the frequencies of propagation. Using the above written expressions one can try to fit the expressions in equations (3.16) and (3.17) to the curves representing the real and imaginary part of the Green’s function. Our attempts to do so did not prove to be very successful because of numerical round-off errors issue.

Another approach to the problem will be to try to consider the absolute value
Figure 13. Plot of the (a) Real Part and (b) Imaginary Part of the Green's Function Given by equation (3.17). The Presented Plot is for wavevector $k=0.48$. 

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of the Green’s function. A function in the form:

$$F(A, B, v_0, v_1, \Gamma_0, \Gamma_1) = \sum_{i=1}^{N} \left[ Im(G(k, v_i)) - \frac{A \Gamma_0}{(v_i - v_0)^2 + \Gamma_0^2} - \frac{B \Gamma_1}{(v_i - v_1)^2 + \Gamma_1^2} \right]^2 + \left[ Re(G(k, v_i)) - \frac{A(v_i - v_0)}{(v_i - v_0)^2 + \Gamma_0^2} - \frac{B(v_i - v_1)}{(v_i - v_1)^2 + \Gamma_1^2} \right]^2$$

(3.18)

is then constructed. Then $F(A, B, v_0, v_1, \Gamma_0, \Gamma_1)$ is treated as a function of six independent variables, and it is minimized with respect to these variables. The successful inaction of the minimization will result in determination of both the real $v_0$, $v_1$ and imaginary parts $\Gamma_0$, $\Gamma_1$ of the Green’s function’s poles and effectively calculating the dispersion relation and the absorption function for the system of interest which is one of the goals of this paper. The proposed minimization can be done using standard subroutines from computer packages for mathematical and statistical calculations. In Figures 14a and 14b we present the results of the magnetic superlattice band calculation using the Bourret approximation. A band gap was clearly observed in the real part of the dispersion relation, plotted in Figure 14a, which corresponds to region of energies where the magnetic waves cannot propagate along any given direction. The observation of the gap in the first order perturbation calculations is very important because it gave us a good idea of the region of frequencies where one can expect to find interesting phenomena. Bad gap was not observed in the imaginary part of the dispersion relation, plotted in Figure 14b.

More precise results were obtained using the self-consistent method. This
Figure 14. Plot of the Dispersion Relation of Electromagnetic Waves, Computed Using Bourret Approximation. The Presented Plot is for $\eta=0.016$. 

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method is similar to the Bourret approximation which was described above. In solving the integral equation in equation (3.7) one represents the $U(k,v)$ using equation (3.11) and solving it self-consistently by iterative methods. A special attention should be paid on the convergence of the series when doing that because different regions of the spectra could require different number of iterations. Once the self-consistent potential is determined, we proceed in the same manner as described for the Bourret approximation. The results of the simulation are given if Figures 15a and 15b, Figures 16a and 16b which correspond to the real and imaginary part of the dispersion relation. Again we observed a well defined band gap for the magnetic waves and no gap in the absorption. The results are consistent with the ones obtained by the Bourret approximation but much more precise. To help the reader understand better the process the presented plots in Figure 15 and Figure 16 are for different values of the parameter $\eta$ which are 0.016 and 0.16. One can notice that the increment of the disorder corresponds to increase in the band gap. The reader should also notice that although very encouraging the last results are limited by the very nature of the self-consistent method and this effectively limits the range of the disorder which could be studied using this method.

Exact Solution

Although very helpful in studying and understanding the nature of the band gaps for the magnetic waves propagating in stochastically modulated superlattices, the methods described in the previous part of this chapter are perturbative in their nature
Figure 15. Plot of the (a) Real Part and (b) Imaginary Part Dispersion Relation for Magnetic Waves Calculated by the Self-Consistent Approach for \( \eta = 0.016 \).
Figure 16. Plot of the (a) Real Part and (b) Imaginary Part Dispersion Relation for Magnetic Waves Calculated by the Self-Consistent Approach for $\eta = 0.16$. 

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and exhibit all the intrinsic limitations of that class of methods. The ultimate goal when studying a problem is to find an approach which will enable us to find a general solution of the problem applicable for any combination of input parameters and existing conditions. This portion of our work is devoted to describing such a method which we have developed to study the dispersion relation for the magnetic waves.

We are going to solve the differential equation of equation (3.6) using the Green's functions method which states that it should be written as:

$$\nabla^2 G(x,x') + (\nu - \epsilon \rho(x))G(x,x') = \delta(x - x')$$  \hspace{1cm} (3.19)

where $\delta(x - x')$ is the delta function.

Following the procedure described in the previous chapter from equation (3.19), we obtain the integral equation in the form:

$$(\nu - k^2)G(k) = 1 + \epsilon \int dq \rho(q-k)G(q).$$ \hspace{1cm} (3.20)

Let's represent the integral in equation (3.20) as a sum::

$$\int dq \rho(q-k)G(q) = \sum_r \Delta_r \rho_{k,r} g_{r,\alpha}$$ \hspace{1cm} (3.21)

Then the integral equation in equation (3.20) could be rewritten by representing as:

$$\sum_r \left[(\nu - k^2)\delta_{k,r} - \epsilon \Delta_r \rho_{k-r} g_{r,k}\right] g_{r,\alpha} = \delta_{k,\alpha}$$ \hspace{1cm} (3.22)

or by denoting the expression in the brackets by:
\[ P_{kr} = (v - k^2)\delta_{kr} - \epsilon \Delta_r \rho_{k-r} \]  

(3.23)

One can express equation (3.22) in matrix notation:

\[ P g = I \]  

(3.24)

From equation (3.24) we can find the discrete Green's function as:

\[ g = P^{-1} \]  

(3.25)

The last equation is the one that will allow us to compute the dispersion relation for the propagating magnetic waves. This could be seen from equation (3.23) from which we can get:

\[ g(k,r) = \frac{1}{v - k^2 - \epsilon \Delta_r \rho_{k-r}}. \]  

(3.26)

Essentially the poles of equation (3.26) will allow us to compute exactly the dispersion relation of the electromagnetic waves propagating through stochastically modulated superlattices. We proceed in the following way. First we use equation (3.23) to compute the elements of the matrix \( P \). In the process we take advantage of the method for generation of one-dimensional randomly rough surfaces described in chapter two of this thesis to generate a set of randomly rough functions which would represent our system. Then we compute the power spectra of the averaged set which is denoted in equation (3.23) by \( \rho_{k-r} \). In the next step of our computations, we construct the matrix \( P \). The reverse matrix \( P^{-1} \) is computed using standard
subroutines from the software package LAPACK. The diagonal elements of the matrix $g$ given by equation (3.25) are then plotted as a function of the wavevector $k$. The poles of the Green’s function $g(k,r)$ are determined from the plot. As a result of the described above process we would be able to determine the dispersion relation for the electromagnetic waves propagating through stochastically modulated superlattice.

In Figure 17 we present a typical plot of the diagonal elements of the matrix $g$ versus the wavevector $k$. One can clearly determine the poles of the Green’s function for that particular set of parameters. We used the method described above to compare our results of the self-consistent method with the results of the exact solution of the dispersion relation.

In Figure 18 we present a plot of the dispersion relation calculated by the self-consistent method (plotted by lines) and the results from the exact solution of the problem (plotted by single points). The presented results are calculated for the same parameters as the dispersion relation given in Figure 16a. We observed very good agreement for that particular set of parameters. The method we have presented in this chapter of the dissertation is a very useful tool for calculation of the dispersion relation of electromagnetic waves propagating through stochastically modulated superlattices with any set of parameters describing the process.
Figure 17. Typical Plot of the Diagonal Elements of the Matrix $g$. The Presented Data is for $\eta=0.16$, $a=0.05$, $b=1.0$ and Wavevector $r=0.29$
Figure 18. Plot of the Poles (shown as crosses) of the Green's Function Given by equation (3.29) for $\eta=0.16$, $a=0.05$ and $b=1.0$. The Poles are Marked With Crosses and Are Shown on the Same Graph as the One Presented in Figure 16a.
CHAPTER V

DETERMINATION OF THE SURFACE PROFILE STATISTICS FROM THE SCATTERING DATA

Introduction

A new method known as Reverse Monte Carlo (RMC) has recently been introduced and applied to the determination of the structures of amorphous and polymer materials from X-ray scattering data [McGreevy, R.L. et. al., 1992]. This method uses Monte Carlo techniques to generate possible atomic structures which reproduce the scattering data obtained experimentally from disordered systems. These generated structures then act as models for the atomic arrangement in these types of materials. In this chapter we present a new application of RMC, namely the determination of the power spectrum of a randomly rough surface from the differential reflection coefficient of electromagnetic waves scattered from such a surface, i.e. from far-field experimental data. In addition, these techniques are used to determine the surface profile of a scratch or bump on an otherwise flat surface using the data from the scattering from surfaces containing these features.

In contrast with the standard Monte Carlo approach, where for a given statistical distribution of random configurations one calculates some physical value, in the Reverse Monte Carlo simulations for a given physical value (in our case this is the differential reflection coefficient) we calculate the quantities describing the
surfaces. This approach originates from the work by McGreevy and Howe. They applied it to the determination of the structures of amorphous and polymer materials from X-ray scattering data [McGreevy, R.L. et. al., 1992]. We apply the RMC method to the determination of a surface profile from its scattering data.

The RMC method for extracting surface profile statistics from scattering data works as follows: First Monte Carlo techniques are used to generate surfaces with various surface statistics (power spectrum, surface profile function). The Differential Reflection Coefficient that describes the angular distribution of the scattered field for the generated surfaces with these simulated properties, is then calculated. (Perturbation theory or direct numerical simulation is used to compute the differential reflection coefficient for the given power spectrum.) Next the RMC employs a maximum entropy approach that allows for the determination from the generated surfaces of those surfaces that best fit the experimental data. This allow us to sort out previously generated surfaces and construct new surfaces which closely fit the experimental data. Using this generation procedure we obtain a surface statistics or profile that matches the experimental data to within experimental error.

In a first case we study a one-dimensional random surface with the surface profile $x_3 = \xi(x_1)$ and treat the profile function $\xi(x_1)$ as a Gaussian random process with the following statistical properties:

$$<\xi(x_1)> = 0$$  \hfill (4.1a)
where the angular brackets <> represent averaging over the rough surface or a set of realizations of the rough surfaces, and \( W(x_i) \) is the autocorrelation function of the surface profile functions. We shall be particularly interested in the power spectrum of the Gaussian surface profiles \( \tilde{g}(k) \), which is defined as the Fourier transform of \( W(x_i) \).

\[
W(x_i) = \int \frac{dq_1}{(2\pi)^2} \tilde{g}(q) e^{iqx_i}
\]  

Our goal will be to extract \( \tilde{g}(k) \) for random rough surfaces from the optical scattering data from such surfaces.

To compare the measured and computed differential reflection coefficient, we introduce the functional \( \chi \) defined below:

\[
\chi = \sum_i \sum_{\alpha,\beta} \int d\Omega_s [\sigma(\Omega_i,\Omega_s)]^{-2} \left( \frac{dR_{\alpha,\beta}(\Omega_i,\Omega_s)}{d\Omega_s} \right)_{\text{exp}} - \left( \frac{dR_{\alpha,\beta}(\Omega_i,\Omega_s)}{d\Omega_s} \right)_{0} \right)^2
\]  

Here \( (dR_{\alpha,\beta}(\Omega_i,\Omega_s)/d\Omega_s)_0 \) is the DRC computed by theory, \( (dR_{\alpha,\beta}(\Omega_i,\Omega_s)/d\Omega_s)_{\text{exp}} \) is the experimentally measured DRC, and \( [\sigma(\Omega_i,\Omega_s)]^{-2} \) is the variance of the experimental data about their mean, the indices \( \alpha,\beta = 1,2 \) label \( s \) and \( p \) polarization, \( \Omega_i \) are angles of incidence and \( \Omega_s \) are scattered angles. The sum on \( i \) allows for the use of scattering data from more than one angle of incidence. The problem of fitting the surfaces profiles will then be the problem of minimizing \( \chi \). The exact power
spectrum $\hat{g}^0(k)$ gives $\chi = 0$ when substituted into the RMC as a guess.

The problem of determining $\hat{g}(k)$ to match the measured DRC is transformed to the problem of the minimization of $\chi[\hat{g}(k)]$. We introduce an ensemble $\{ \hat{g}_i(k) \}$ of computer generated realizations of $\hat{g}(k)$. These are generated by a random Monte Carlo process, described below, and each realization $\hat{g}_i(k)$ gives a possible $\hat{g}(k)$. The power spectra for which $\chi = 0$, will reproduce exactly the experimental spectra. Each realization $\hat{g}_i(k)$ gives some value $\chi_i$ and a maximum entropy approach is used to generate from $\hat{g}_i(k)$ the next realization $\hat{g}_{i+1}(k)$ which gives $\chi_{i+1} \leq \chi_i$. At the end of this sequence we will have generated the most probable solution for $\hat{g}(k)$ consistent with experimental data including the error limits of the experimental data. For this state the entropy of the probability distribution of the $\{ \hat{g}_i(k) \}$ takes its maximal value.

We now discuss the details of the maximum entropy sampling approach.

The RMC approach is much different than the standard iterative approach for finding a minimum of $\chi$. The standard procedure typically includes the following steps:

1. We generate an initial guess $\hat{g}_0(k)$ which allows to compute the DRC

   $(dR_{a,b}(\Omega_p,\Omega_p)/d\Omega_p)_0$ and $\chi_0$. The initial configuration could be chosen randomly.

2. A random change is then made to $\hat{g}_0(k)$ which creates $\hat{g}_1(k)$ and the new power spectrum yields a new DRC $(dR_{a,b}(\Omega_p,\Omega_p)/d\Omega_p)_1$ and a new value for our error function $\chi_1$.

3. If $\chi_1 < \chi_0$ then $\hat{g}_1(k)$ is retained over $\hat{g}_0(k)$ as a good guess for the Fourier transformation of the correlation function. Otherwise the changes made in $\hat{g}_0(k)$ are
rejected and the generation process continue starting with the original power spectrum \( \hat{g}_0(k) \). The iterations continue in the manner described above using the \( \hat{g}(k) \) generated in the previous iteration, until certain criteria (e.g. minimal error, maximum count) are met. The final best guess for \( \hat{g}(k) \) is then kept as the true function \( \hat{g}(k) \).

Although very useful, this approach presents some problems associated with it. The main disadvantage of the standard iterative approach is that the computations could become trapped near a local minima of the function \( \chi \). This would produce false result. This fact makes our computations dependent on the initial guess \( \hat{g}_0(k) \). These are major problems with the standard iterative method if we are to apply it to any type of problem involving the minimization of \( \chi \). That is why it is advisable to make certain changes in the method which will allow us to search for global, rather than local maxima of the function \( \chi \). The maximum entropy method is a development which is used to help us reach a global minimum.

In the maximum entropy approach, not only are the Monte Carlo generated \( \hat{g}_i(k) \) retained which decrease \( \chi_i \) but some generated \( \hat{g}_i(k) \) are retained which increase \( \chi_i \). This allows the \{ \hat{g}_i(k) \} to hop out of local minima. A well known prescribed Monte Carlo sampling procedure exists for choosing which generated configurations \( \hat{g}_i(k) \) that increase \( \chi_i \) are to be retained in the sampling. This procedure is based on the assumption that the experimental data has a Gaussian sampling error.

In a second study we applied the Reverse Monte Carlo method to deterministic surfaces such as scratch or bump on a flat surface. More specifically we looked at profiles described by the following functions
\[ \xi(x_1) = \sigma_1 x_1 e^{\frac{x_1^2}{a^2}}. \]  

The method was applied in a similar way to the one described above but, instead of calculating the differential reflection coefficient for scattering from ensemble of surfaces, we looked at a single deterministic profile. Then the scattering from such a profile was calculated and compared to the "experimental" data and the quantity \( \chi \) was determined. Then a random change was made to the surface profile function depending on the error function \( \chi \). The decision to keep the change was made in the same fashion as the one described for the randomly rough surfaces. Several improvements of the method were implemented in order to increase its efficiency. Random changes are being made only to those regions of the scratch Fourier spectra which contribute to the differential reflection coefficient. The region of wavevectors which we use in our computations is divided onto subregions depending on the probability of each subregion to contribute to the scattering cross section. The absolute value of the random change is made depending on the contribution of that subregion to the total error \( \chi \).

Application of The RMC Method to the Randomly Rough Surfaces

We consider a one-dimensional randomly rough surface defined by the equation \( x_3 = \zeta(x_1) \). The surface profile function \( \xi(x_1) \) is assumed to be a single-valued function of \( x_1 \) that is differentiable as many times as is necessary, and that constitutes a stationary, zero-mean, isotropic, Gaussian random process defined by equation (4.1).
The roughness is assumed to be weak \((\sigma < \lambda)\) compared to the wavelength of the light.

The contribution to the mean differential reflection coefficient (mdrc) from the diffuse component of the light scattered from such surfaces depends explicitly on the spectral density \(\tilde{g}(k)\) of the \(\{\zeta(x_i)\}\). In those cases where the roughness is weak, the Differential Reflection Coefficient can be calculated and depends implicitly on \(\tilde{g}(k)\).

When the roughness is strong, a computer simulation approach to the evaluation of the Differential Reflection Coefficient is required [Nieto-Vesperinas, M. et. al, 1990].

We are looking to extract the surface statistics \(\tilde{g}(k)\) that is the most probable, i.e. that maximizes the entropy of the distribution of \(\chi\) from a set of scattering data. Entropy is a concept in probability theory, and the maximum entropy method is applicable when we are determining a function that can be treated as a Gaussian probability distribution centered about some mean function. The probability of each particular configuration is then given by the Boltzmann's factor:

\[
P \propto \exp(-\chi) \tag{4.6}
\]

where \(\chi\) is the comparison function in equation (4.3). Equation (4.6) follows from the maximal entropy theory, and it is similar to the Boltzman factor in statistical mechanics. The probability from equation (4.6) satisfies the following basic relation:

\[
P(\chi_1 + \chi_2) = P(\chi_1)P(\chi_2) \tag{4.7}
\]

which reflects that fact that entropy \(< -P \log P>\) is an extensive value.

The RMC is applied in the following way:
1. Let \((dR_{\alpha,\beta}(\Omega_p,\Omega_s)/d\Omega_s)_{\text{exp}}\) be the experimental data for contribution to the mdrc from diffuse component of the scattered EM waves of polarization \(\alpha\) and angles of incidence \(\Omega_i\) are scattered into waves of polarization \(\beta\) and scattered angles \(\Omega_s\).

2. If \(\hat{g}_0(k)\) is an initial guess at the power spectrum and if \((dR_{\alpha,\beta}(\Omega_p,\Omega_s)/d\Omega_s)_{0}\) is the contribution to the mdrc computed by theory or computer simulation from \(\hat{g}_0(k)\) then we can compute \(\chi_0\) using the expression given by equation (4.3).

3. A random change then is made in \(\hat{g}_0(k)\) to create a new guess power spectra \(\hat{g}_1(k)\), and \(\chi_1\) is computed from equation (4.3) is computed.

4. If \(\chi_1 < \chi_0\) then \(\hat{g}_1(k)\) is retained over \(\hat{g}_0(k)\) as a good guess for the power spectrum.

5. If \(\chi_1 \geq \chi_0\) then \(\hat{g}_1(k)\) is retained over \(\hat{g}_0(k)\) with a probability \(p = \exp(\chi_0 - \chi_1)\).

6. At the end of the cycle, when \(\chi_1 < \) (some criterion), the final \(\hat{g}_1(k)\) is taken as the \(\hat{g}(k)\).

The final guess for \(\hat{g}(k)\) is taken to represent the true power spectrum. The iterations \(\hat{g}_i(k)\) converge to \(\hat{g}(k)\) when \(i \to \infty\) or when the final results satisfies a given minimum error criteria. In view of the Monte Carlo sampling on which the RMC method is based, we expect that it converges to the true power spectrum with an error that decreases inversely with the square root of the number of Monte Carlo comparisons used.

We apply the method just described to the determination of the power
spectrum of weakly rough, one-dimensional, random metal surfaces (i.e. surfaces for which \( \xi(x) \) is independent of \( x_2 \), for which an analytic expression for the mean differential reflection coefficient in terms of the power spectrum exists [McGurn, A.R. et. al., 1985]. It has been obtained by an infinite—order perturbative calculation in the small roughness approximation. The plane of incidence is assumed to be the \( x_1-x_3 \)-plane, and the incident light is \( p \)-polarized. In this scattering geometry there is no cross-polarized scattering. The contribution to the mean differential reflection coefficient from the diffuse component of the scattered light is related to the power spectrum \( g(k) \) by [McGurn, A.R. et. al., 1985]:

\[
<\partial R_p(\theta_s,\theta_i)/\partial \theta_s>_{\text{diff}} = \frac{\omega}{4\pi^2 c} \cos(\theta_s)(I^{(L)}(q|k)+I^{(c)}(q|k))
\]  

(4.8)

where \( q=\frac{\omega}{c}\sin(\theta_s) \), \( k=\frac{\omega}{c}\sin(\theta_i) \). The values \( I^{(L)}(q|k) \) and \( I^{(c)}(q|k) \) are given in [McGurn, A.R. et. al., 1985] and are related to the ladder and crossed term respectively. They are expressed as:

\[
I^{(c)}(q|k)_{\text{diff}} = 8\pi \alpha_0(q) \alpha_0(k) \frac{G(q)}{G(k)} |G(q)|^2 |G(k)|^2 \times \\
\times \frac{C^2}{(q+k)^2+4(\Delta_{\text{tot}})^2} \left[ \frac{1}{1-(\Delta_{\text{tot}})^2} K(k,K_{sp} K(k,K_{sp})+\frac{1}{2} K^2(k,K_{sp} + K^2(k,K_{sp}))) \right]
\]

where

\[
K(q|k) = \delta^2 g(q-k)|\epsilon(\omega)-1/\epsilon^2(\omega)|^2 |\epsilon(\omega)qk-\alpha(q,\omega)\alpha_{lpla}(k,\omega)|^2,
\]

with \( \epsilon(\omega) \) the dielectric function of the metal;

\[
\alpha(q,\omega) = |\epsilon(\omega)(\omega/c)^2-q^2|^{1/2}, \text{ Re } \alpha(q,\omega) > 0, \text{ Im } \alpha(q,\omega) > 0
\]
and $\Delta_{sp}$ is defined by

$$\Delta_{sp} = 2\pi \delta^{2}C_{1}^{2}(\omega)[(\epsilon_{i}(\omega) - 1)/\epsilon_{i}(\omega)]^{2}K_{sp}^{4}(\omega)g(2K_{sp}(\omega)).$$

where

$$C_{1}(\omega) = (-\epsilon_{i}(\omega))^{3/2}[\epsilon_{i}^{2}(\omega) - 1], \quad K_{sp}(\omega) = (\omega/c)[\epsilon_{i}(\omega)[\epsilon_{i}(\omega) + 1]]^{1/2},$$

and $\epsilon_{i}(\omega) = Re \ e(\omega)$.

Results of the Application of the RMC Method to the Randomly Rough Surfaces

We have used the theoretical results of [McGurn, A.R. et. al., 1985] to generate "experimental" mdrc data for the scattering of p-polarized light of wavelength $\lambda = 457.9$ nm from a silver surface ($\epsilon(\omega) = -7.5 +0.24$) characterized by the power spectrum $\hat{g}(k)$ with roughness parameters $\delta = 5$ nm and $a = 100$ nm. The angles of incidence were arbitrarily chosen to be $\theta_{i} = 10^\circ$ and $18^\circ$. The RMC method was then used to extract $\hat{g}(k)$ from these data. In order to use the least amount of information about the power spectrum, the initial guess for $\hat{g}(k)$ in the RMC reconstruction from the scattering data was $\hat{g}(k) = 0$, and in making subsequent guesses we used the general properties $\hat{g}(k) \geq 0$ and $\hat{g}(k) = -\hat{g}(-k)$. For $k$ in the interval $(0, 2.95 \omega/c)$, $\hat{g}(k)$ was broken up into a histogram with 200 channels, and was allowed a random change in one channel for each Monte Carlo comparison described above. For $k > 2.95 \omega/c$ the value of $\hat{g}(k)$ does not affect the computed mdrc, so we took $\hat{g}(k) = 0$ in this region. A total of 20,000 Monte Carlo comparisons was used in obtaining the reconstructed power spectrum depicted in Figure 19, where it is compared with the exact power spectrum $g(k)$ used in generating the "experimental"
Figure 19. Plot of $g(k)$ Versus $ka$. The Curves Shown are for the Experimental Power Spectrum (Dashed Curve) $g(k)=\sqrt{\pi} \exp[-(ka)^2/4]$ and for the RMC Extraction of it (Solid Curve).
data. These calculations required 33 minutes of CPU time on a VAX 6000-620. Good agreement between the exact and reconstructed power spectra is observed, although better agreement could be obtained with longer runs.

As a stringent test of the effectiveness of the RMC method for recovering the $g(k)$ from scattering data, we have applied it to scattering data recently measured by West and O'Donnell [West, C.S. et. al., 1995]. These authors fabricated a weakly rough, one-dimensional, random gold surface and measured the contribution to the mdrf from the incoherent component of the scattered light for p-polarized light of wavelength $\lambda = 612 \mu m$ incident at $\theta = 0^\circ$, $10^\circ$, and $18^\circ$ from the normal to the mean surface. The surface was fabricated in a manner that assured that the surface profile would obey Gaussian statistics.

As the surface studied in [West, C.S. et. al., 1995] is a weakly rough surface, we used in our RMC method the perturbation theory of McGurn [McGurn, A.R. et. al., 1985] to express the differential reflection coefficient in terms of the guessed $g(k)$. In Figure 20 we present the results in dimensionless units for $\hat{g}(k)$ versus $ck/\omega$ obtained in Reference [West, C.S. et. al., 1995] by contact profilometry and by our application of the RMC method discussed above. The RMC result for $\hat{g}(k)$ was obtained by using the scattering data in Figure 19 of [West, C.S. et. al., 1995] for angles of incidence $\theta = 10^\circ$ and $18^\circ$. Again, the initial guess for $\hat{g}(k)$ was taken to be $\hat{g}(k)=0$, and 20,000 Monte Carlo comparisons were used. In presenting both sets of data, we have taken $\delta = 109 \AA$, which is the value obtained in Reference [West, C.S. et. al., 1995] for this parameter. The value of $\delta$ is used to normalize the power.
Figure 20. Plot of the \( g(k) \) as a Function of \( ck/\omega \). These Curves Represent the Profilometry Results in (C.S. West, et. all, 1995) (Dashed Curve) and Our RMC Results (Solid Curve).
spectrum and does not affect the RMC computation of \( g(k) \). Good agreement is observed between our RMC results and the profilometry results.

For the results in Figures 19 and 20 no values of \( \sigma(\theta_p, \theta_s) \) were available. In such cases, by trial and error we chose \( \sigma \) small enough to reproduce the published data closely, but large enough to allow the maximum entropy component of our computer routine to operate efficiently. Scattering data for \( \theta = 10^\circ \) and \( 18^\circ \) were necessary to obtain accurate RMC results for \( g(k) \).

Application of the Rmc Method to Deterministic Profiles

In this section we are presenting yet another application of the Reverse Monte Carlo method — recovery of the surface profile for deterministic surfaces. The method is based on calculating the differential reflection coefficient using a first- and second-order perturbation theory in which the surface profile function is treated as a small perturbation.

We are interested in calculating the scattering of a Gaussian beam of p-polarized light incident on a one-dimensional scratch or bump on a metal surface. The surface profile is given by:

\[
x_3 = \xi(x_1)
\]

where \( \xi(x_1) \) is a deterministic function.

The magnetic field vector of a p-polarized electromagnetic wave with frequency \( \omega \) and wavevector \( k \) is given by:

\[
H_2^{\text{out}}(x_1, x_3) = e^{i(kx_1 - \omega_0(k)x_3)} + \int \frac{dq}{(2\pi)} R(q, k) e^{i(qx_1 - \omega(q)x_3)} \tag{4.9}
\]
where \( \alpha_0(k) = [(\frac{\omega}{c})^2 - k^2]^\frac{1}{2} \).

The Gaussian beam in our discussions below is then formed as a Fourier composition of the planewaves in equation (4.9).

The magnetic field vector of the incident light for a \( p \)-polarized electromagnetic wave, is given by:

\[
H_{2m}^{im}(x_1,x_3) = \int \frac{dp}{(2\pi)} A(p,k) e^{i(px_1 - a(p)x_3)}
\]  

(4.10)

where \( A(p,k) \) is proportional to the amplitudes of the field inside the metal and

\[
\alpha(k) = [\epsilon(\frac{\omega}{c})^2 - k^2]^\frac{1}{2}.
\]

In both of these expressions, \( R(q,k) \) can be determined by studying the planewave solution in equations (4.1) and (4.2) solving the boundary value problem for each \( \omega, k \) planewave solution. In doing this we take the dielectric constant of the surface of the metal to be represented as having real part and imaginary part which represents the penetration of the electromagnetic waves in the media:

\[
\epsilon = \epsilon_1 + i\epsilon_2
\]

To first order perturbation theory Reflection Coefficient in the system has the form:

\[
R(q,k) = 2\pi \delta(q-k)R_0(k) + R_1(q,k)
\]  

(4.11)

where \( R_0(k) \) is the flat surface result and \( R_1(q,k) \) is the lowest order correction in \( \zeta(x_1) \).

For the field in the metal the first order perturbation theory is gives:
\[ A(q,k) = 2\pi \delta(q-k)A_0(k) + A_1(q,k) \]  

where \( A_0(k) \) is the flat surface result and \( A_1(q,k) \) is the lowest order correction in \( \zeta(x_1) \).

The standard approach in solving the problems of this type is to apply the boundary conditions between equations (4.8) and (4.9). The boundary conditions for the normal component of the magnetic field vector and the tangential component of the electric field vector on the surface are given by [Jackson, J.D., 1975]:

\[ H_{2n}^{\text{out}}|_{x_3 = \xi(x_3)} = H_{2n}^{\text{in}}|_{x_3 = \xi(x_3)} \]  

\[ E_{2t}^{\text{out}}|_{x_3 = \xi(x_3)} = E_{2t}^{\text{in}}|_{x_3 = \xi(x_3)} \]

First let's look at the first boundary condition equation (4.13) and substitute equation (4.14) in equation (4.9).

\[ H_2^{\text{out}}(x_1,x_3) = e^{i(kx_1 - a_0(k)x_3)} + \int \frac{dq}{(2\pi)} R(q,k)e^{i(qx_1 - a_0(q)x_3)} = \]
\[ = e^{ikx_1}
  \left(1 - i\alpha_0(k)\xi(x_1)\right) + \int \frac{dq}{(2\pi)} \left[ (2\pi \delta(q-k))R_0(k) + R_1(q,k)e^{-i\alpha_0(1 + i\alpha_0(q)\xi(x_1))} \right] \]  

Now let's look at the field inside the metal.

\[ H_2^{\text{in}}(x_1,x_3) = \int \frac{dp}{(2\pi)} A(p,k) e^{ipx_1 - a(p)x_3} = \]
\[ = \int \frac{dp}{(2\pi)} \left( 2\pi \delta(p-k)A_0 + A_1(p,k) \right) e^{ipx_1} \left(1 + i\alpha(p)\xi(x_1)\right) \]  

After substitution of equations (4.15) and (4.16) in equation (4.13) and separating the
coefficients of different orders of the surface profile Fourier transformations we get from the coefficients of $\hat{g}^{(0)}$.

$$1 + R_0(k) = A_0(k)$$  \hspace{1cm} (4.17)

From the coefficients involving $\hat{g}^{(1)}$:

$$A_1(q,k) - R_1(q,k) = i \frac{2\alpha(k)\alpha_0(k)(\varepsilon - 1)}{\varepsilon\alpha_0(k) + \alpha(k)} \hat{g}^{(1)}(q-k)$$  \hspace{1cm} (4.18)

where:

$$\hat{g}^{(n)}(k) = \int \frac{dk}{2\pi} \hat{e}^{(n)}(x)e^{ikx}.$$

Now we are going to use equation (4.14) to determine two additional equations which will allow us to determine closed form expressions for the coefficients $A_i(q,k), R_i(q,k)$ where $i = 0,1$. From the time-dependent Maxwell's equations, we can obtain an expression for the electric field vector, using the magnetic field vector as:

$$\frac{\partial H_2}{\partial x_1} = -\frac{i\omega}{c}\varepsilon E_3$$  \hspace{1cm} (4.19)

$$\frac{\partial H_2}{\partial x_3} = i\frac{\omega}{c}\varepsilon E_1.$$  \hspace{1cm} (4.20)

The unit vector, tangential to the surface will have the form:
\[ \mathbf{t} = \frac{1}{\sqrt{1 + \xi^2(x_1)}} [\hat{x}_1 + \hat{x}_3] \]  

(4.21)

where \( \hat{x}_1 \) and \( \hat{x}_3 \) are the unit vectors along our coordinate axes. Applying the boundary condition in equation (4.14) and using equations (4.19), (4.20) and (4.21) we can arrive at the expression at the boundary:

\[ \left( \frac{\partial}{\partial x_3} - \xi' \frac{\partial}{\partial x_2} \right) H_{2}^{\text{out}} = \frac{1}{\varepsilon} \left( \frac{\partial}{\partial x_3} - \xi' \frac{\partial}{\partial x_2} \right) H_{2}^{\text{in}}. \]  

(4.22)

Substituting (4.9) and (4.10) in (4.22) we get the following equations:

\[ i\alpha_0(k)\varepsilon(R_0(k) - 1) = -i\alpha(k)(R_0(k) + 1) \]  

(4.23)

and

\[ \varepsilon\alpha_0(q)R_1(q,k) + \alpha(q)A_1 = i(\varepsilon - 1)\xi^{(1)}(q-k)A_0 \]  

(4.24)

Then we use equations (4.18), (4.24) and get the following expressions for the zero-order Reflection and Absorption Coefficients:

\[ R_0(k) = \frac{\alpha_0(k)\varepsilon - \alpha(k)}{\alpha_0(k)\varepsilon + \alpha(k)}. \]  

(4.25)

\[ A_0(k) = \frac{2\alpha_0(k)\varepsilon}{\alpha_0(k)\varepsilon + \alpha(k)}. \]  

(4.26)

The first order perturbation theory results have the form:
In a similar fashion we can proceed to calculate the second order perturbation theory coefficients. We express (4.11) to the second order reflection coefficient:

\[ R(q,k) = 2\pi \delta(q-k)R_0(k) + R_1(q,k) + R_2(q,k). \]  

(4.29)

One can perform similar calculations and get, for the second order reflection coefficient, the following expression:

\[ R_2(q,k) = \frac{\alpha_0(k)}{(\varepsilon \alpha_0(q) + \alpha(q))(\varepsilon \alpha_0(k) + \alpha(k))} \left[ (\varepsilon - 1)(\alpha(q) + \alpha(k))(qk - \alpha(q)\alpha(k))\xi^{(2)}(q-k) + 2\varepsilon - 1 \varepsilon - 1 \int \frac{dp}{2\pi} \xi^{(1)}(q-p)\xi^{(1)}(p-k). \right. 

\left. + \frac{\varepsilon \alpha_0(p)\alpha(q)\alpha(p)\alpha(k) + \varepsilon p^2 \alpha(p)\alpha(k) - \varepsilon^2 p^2 qk}{\varepsilon \alpha_0(p) + \alpha(p)} \right] \]  

(4.30)

The presented forms of the reflection coefficients can be used to calculate the differential cross section and study the scattering of monochromatic light from deterministic surfaces. The problem is rather straightforward, and we used it as intermediate state for our final goal — the determination of the profile of scratch or bump using the scattering data for a beam of light with Gaussian distribution of the
different wavevectors. A Gaussian beam of light is considered then with the following equation describing the distribution of the modes:

\[ g(k) = \sigma e^{-\frac{(k-k_0)^2}{a^2}}. \]  

Then the total cross section will be:

\[ R = \frac{\int \frac{dk}{(2\pi)} e^{-a^2(k-k_0)^2} \int \frac{dq}{(2\pi)} \alpha_0(q) R(q,k) e^{i\alpha_1} \int \frac{dk'}{(2\pi)} R^*(q,k') e^{-a^2(k'-k_0)^2}}}{\int \frac{dk}{(2\pi)} \alpha_0(k) e^{-2a^2(k-k_0)^2}}. \]  

The integration in equation (4.32) in the \(k\)-wavevector space represents the contribution of all the frequency components of the incident Gaussian beam of light. We are interested in the differential cross section, and thus we have to determine the differential reflection coefficient, calculated as the derivative of the total cross section with respect to the scattering angle. Performing the necessary differentiation we get the expression:

\[ \frac{\partial R(q)}{\partial \theta} = \frac{\omega}{2\pi c} \alpha_0(q) \cos(\theta) \frac{\int \frac{dk}{(2\pi)} e^{-a^2(k-k_0)^2} R(q,k) \int \frac{dk'}{(2\pi)} R^*(q,k') e^{-a^2(k'-k_0)^2}}{\int \frac{dk}{(2\pi)} \alpha_0(k) e^{-2a^2(k-k_0)^2}}. \]  

Equation (4.33) can be used to calculate the differential reflection coefficient. This will allow us to simulate scattering of Gaussian beam of light from deterministic profile. The results obtained using equation (4.33) represents the scattering cross section and will be used to generate the initial data for our Reverse Monte Carlo.
simulations. In performing the actual retrieval of the surface profile we are going to use equation (4.25) again together with the expressions for the reflection coefficient in first- or second- order perturbation theory. The first order perturbation theory reflection coefficient is given by equation (4.10) and the second order perturbation theory result is presented in equation (4.29).

The RMC is applied in the following way:

1. Let \((\partial R(q)/\partial \theta)_{\text{exp}}\) be the experimental data for contribution to the DRC from the scattered at angle \(\theta\) EM waves.

2. If \(\hat{g}_0(k)\) is an initial guess at the power spectrum and if \((\partial R(q)/\partial \theta)_0\) is the contribution to the DRC computed by theory or computer simulation from \(\hat{g}_0(k)\), then we can compute \(\chi_0\) using the expression given by:

\[
\chi_i = \left( (\frac{\partial R(q)}{\partial \theta})_{\text{exp}} - (\frac{\partial R(q)}{\partial \theta})_0 \right)^2
\]

for \(i = 0\).

3. A random change then is made in \(\hat{g}_0(k)\) to create a new guess power spectra \(\hat{g}_1(k)\) and \(\chi_1\) is computed from equation (4.34) is computed.

4. If \(\chi_1 < \chi_0\) then \(\hat{g}_1(k)\) is retained over \(\hat{g}_0(k)\) as a good guess for the power spectrum.

5. If \(\chi_1 \geq \chi_0\) then \(\hat{g}_1(k)\) is retained over \(\hat{g}_0(k)\) with a probability

\[
p = \exp(\chi_0 - \chi_1).
\]

6. At the end of the cycle, when \(\chi_1\) is sufficiently small, the final \(\hat{g}_1(k)\) is taken as the \(\hat{g}(k)\).

In addition to the described above procedure we made a few modifications to
our program in order to speed up the procedure. At the very beginning of the computations we eliminated these regions in the wavevector $k$ space which do not contribute significantly to the DRC. We also made changes only to the positive portion of $k$-wavevectors and then used the condition which provides a real surface profile:

$$g(k) = g^*(-k).$$

The equations described in this chapter will be used in the Reverse Monte Carlo computer simulations.

Results of the Application of the RMC Method to Deterministic Surfaces

We have used the formulas described in the previous chapter to retrieve the profile of a scratch or a profile from the scattering data of light. The problem of retrieving the surface profile using a monochromatic light was first investigated. The Reverse Monte Carlo method easily converges to the expected solution in this case.

We found it more challenging to investigate the retrieval of the surface profile consisting of a scratch and a bump from the scattering data of a Gaussian beam of light. A profile consisting of a scratch and a bump on a surface is described by the equation:

$$\xi(x) = -x \sigma e^{-\frac{x^2}{a^2}}$$

One can notice that the surface described by equation (4.34) represents a scratch in
the region where $x_1<0$ and a bump in the region where we $x_1>0$. We used profile with parameters $a = 1000 \text{ Å}$ and $\sigma_1 = 50 \text{ Å}$ in our studies. A Gaussian beam (given by 4.31) of light centered at wavelength $\lambda = 4579 \text{ Å}$, beam width $\sigma = 4 \lambda$ is considered to be incident at angle $\theta = 23^\circ$ on silver surface. For this wavelength the dielectric constant was taken to be $\varepsilon = -7.5 + i 0.24$. The DRC for the system described above was first calculated using second order perturbation theory. The results of the computations were then taken to be the original (i.e. experimental in real life) data. The Reverse Monte Carlo Method was applied then in a manner described in part IV of this chapter. We used first order perturbation theory with 6600 steps, followed by 600 steps of second order perturbation theory which took about 2 hours and 10 minutes of computation on VAX -6000.

In Figure 21 we present the results of the RMC calculations. The dotted line in Figure 21 represents the original (read-in) cross section, and the solid line represents the cross section retrieved by RMC. Although there is difference in the presented data, we were able to get good agreement between the calculated and original curves. We attribute the small difference between the curves in Figure 21 to the small number of second order perturbation theory calculation steps taken in our simulations. As we would see on the next figure, our results were good enough to reproduce the shape original power spectra $\hat{g}(k)$.

In Figure 22 we plot the original (dashed curve) and the retrieved (solid line) power spectra $\hat{g}(k)$ of a scratch and a bump on a flat surface. We found very good agreement between the absolute values of the read-in data and the results of the RMC.
Figure 21. Plot of the Original (Dashed Curve) and Retrieved by RMC (Solid Curve) Scattering Cross Section From the Scattering of a Gaussian Beam of Light From a Surface With a Profile Given by Equation (4.35).
Figure 22. Plot of the Original (Dashed Curve) and Retrieved by RMC (Solid Curve) Power Spectra of a Deterministic Surface Given by Equation (4.35).
This is a very good example for how Reverse Monte Carlo could be successfully applied to determine the shape of deterministic surfaces. For this particular example we chose parameters such that the perturbation condition $\sigma < \lambda$ is not violated. In this case the contribution of the second order perturbation theory result given by equation (4.33) is insignificant. This contribution is the one that contains information about the phase of the surface (being able to distinguish bumps and scratches on the surface). We would expect to get even better results for surfaces for which the perturbation condition is not that strongly fulfilled. The method could be improved also by including the third order perturbation theory results for the reflection coefficient in our calculations.
CHAPTER VI

CONCLUSIONS

In the present dissertation we have presented several different problems. In describing every task we have examined dielectric systems or series of surfaces which are of significant interest to the scientific community and have helped the reader understand important properties of the system of interest. The outcome of our studies is the introduction of novel applications of existing methodology for describing phenomena in nature.

In the second chapter we have studied two zinc blend modifications to diamond lattice photonic band structures. Changes in the relative radii of the two-spheres basis are seen to decrease the lowest frequency photonic band size of the gaps from that of the diamond structure. Changes in the relative dielectric constants of the two-sphere basis can enhance the size of the band gaps over those found in the diamond lattice. In addition, in zinc blend structures composed of spheres with different dielectric constants, the lowest band gap is found to occur between different indexed bands dependent on the relative dielectric contrast of the spheres in the two spheres basis.

Recently, dielectric structures such as those discussed in the first chapter of this dissertation have been fabricated and shown in laboratory experiments to exhibit photonic band structures. These structures have been created [Yablonovich, E., 1993;
Zakhidov, A.A. et al., 1999] by setting an array of dielectric spheres, drilling cylindrical holes in dielectric media or by stacking layers of periodic dielectric media. We expect that, with the advancing interest in photonic crystals which yield large photonic band gaps, means will become available to fabricate photonic crystals based on our discussions above. In the context of illustrating the wide variety of possible photonic crystal geometries, we would like to point out some recent very nice work on layered systems [Ho, K.M. et. al., 1994] and spherical sphere systems in A7 geometries [Chan, C.T. et. al., 1994]. These too are possible structures for future fabrication of Photonic Crystals. A copy of the published paper on this project is included in the Appendix B.

In the third chapter of this dissertation, a method has been presented for numerically generating a set of stationary, stochastic, Gaussian random surfaces which reproduce given representations of the functions $g(x)$ or $g(k)$. This method has been used to study the distribution of nearest neighbor maxima, minima and maxima-minima pairs. The maxima in $x$ of the probability distribution $P(x)$, for these pair distributions found for the Gaussian and Lorentzian forms of $g(x)$ to be of order of the correlation lengths of these surfaces. A study of the West O'Donnell one-dimensional randomly rough surface has been made. The maxima in $P(x)$ for the distribution of maxima-minima pairs has been explained by regarding the West O'Donnell surface as being almost periodic.

The results of this study could be used in the perturbational studies of the scattering of randomly rough surfaces. This is a very important aspect of the science
because it has practical application in many areas of the science: physics, microelectronics, meteorology, oceanography and others. The method for generation of two-dimensional randomly rough surfaces is also a very useful research tool for the study of different hypotheses in the theoretical investigations of the basic properties of scattering from such surfaces and the surfaces themselves as well. A copy of our paper appearing in the Proceedings of SPIE (International Society of Optical Engineers) is given in the Appendix D.

In the fourth chapter of this dissertation, we have studied the propagation of the electromagnetic waves through stochastically modulated superlattices. The study was performed on the example of magnetic waves propagating through superlattices with elements of disorder in the magnetic anisotropy. In addition to the perturbation theory approach published by other group of authors, we have presented two additional methods to calculate the dispersion relation for the magnetic waves. The first method, the self-consistent approach, extends the limits of parameters for which we can calculate the dispersion relation with comparison to the approach based on the perturbation theory assumptions. We have shown using the self-consistent method that there exists a gap in the dispersion relation of the real part of the propagating waves frequencies. A gap in the absorption of the magnetic waves was not observed. The other approach which we tested was the complete solution of the problem based on the Green's functions method. A good agreement was found between the results of the self-consistent approach simulations and the complete solution of the problem. As a result of our investigations we were able to confirm the existence of band gaps in
the frequency spectra of the magnetic waves which can propagate through stochastically modulated superlattices. This gap in the dispersion relation is a direct result of the presence of random components in the otherwise periodic system. The result of our simulations is another example of the importance of the stochastic processes in periodic system. The method could easily be modified to calculate the dispersion relation for the electric field vector through periodic system with elements of disorder in the dielectric constant.

In the fifth chapter of this dissertation we have presented an application of the Reverse Monte Carlo method to determine surface statistics from scattering data. Although clearly much can be done to improve the efficiency of the method, we have demonstrated how RMC techniques can be used to extract the power spectrum of a randomly rough surface from measured results for the mdrc of light scattered diffusely from randomly rough surfaces. Existing methods for obtaining the power spectrum from diffuse scattering data (see, e.g. [Stover, J.C., 1990]) are based on a single-scattering approximation to the mdrc, which could not be used in reconstructing the West-O'Donnell power spectrum, because it produces surfaces from which single scattering processes are largely suppressed [West, C.S. et al., 1995]. The RMC method in the present work is based on a multiple-scattering theory. As a result, the power spectrum $g(k)$ can be obtained for a larger range of $k$ than is possible with a single-scattering theory.

In addition, the RMC method contains two important improvements over routines which compute $g(k)$ by a straightforward minimization of $\chi$ [Daniel, G.D.,
1991:

1. the Monte Carlo component of the RMC offers an efficient way to minimize $\chi$ approximately.

2. The maximum entropy component of the RMC sorts out from all of the local minima of $\chi$ the most probable solution for $g(k)$. In this regard, the more scattering data (more experimental points and more angles of incidence) used, the more probable is the agreement of the $g(k)$ computed by the RMC with the actual $g(k)$. It is important along with a study of the convergence of the RMC routine itself to study the change in the computed $g(k)$ as data from additional angles of incidence are added.

The method we have presented is readily generalized to treat surfaces that are defined by surface profile functions that are not Gaussian random processes. One generalization of the RMC method is the extraction of deterministic surface profiles from scattering data. In this work the differential reflection coefficient is expressed in terms of the surface profile function and the random guesses in the RMC method are made of $g(k)$ rather than of the power spectrum as in the random surface RMC.

In the case that an analytic result for is not available, the RMC method can still be used to determine the power spectrum $g(k)$ at the expense of additional computational effort. For each choice of $g(k)$ an ensemble of several hundred profiles would have to be generated by a standard method [McGurn, A.R. et. al.. 1985], the results for partial $R(\theta_p,\theta_s)$ for each member of the ensemble would have to be averaged, and the result used in the RMC algorithm.
In a second application of the Reverses Monte Carlo method we used the method to recover a deterministic surface profile. The method was successfully applied to a scratch, a bump and a combination of a bump and a scratch. We were able to determine the shape of the surface profile using the Reverse Monte Carlo method in a way very similar to the one described for the determination the statistical properties of sets of randomly rough surfaces. This application of the method has very important practical realization because it provides a way for nondestructive profile measurement. This is very significant if we compare it with the classical method for measuring the surface profiles — contact profilometry. The method requires minimal computational resources and this makes it applicable in almost any environment in science and technology. A copy of our published paper on the RMC is to be found in the Appendix E.

In this dissertation we have studied the propagation of electromagnetic waves through periodic dielectric systems, the generation of randomly rough surfaces, extraction of important information about surfaces and the propagation of electromagnetic waves through stochastically modulated superlattices. These problems play significant role in the better understanding of the physical processes in the nature and help us in our future investigations. We have also pointed out some of possible practical applications of the described processes. The importance of these phenomena requires further investigations of the tasks presented in this work. Although we believe we have presented a complete study of the problems described in this dissertation, we can anticipate the observation of new phenomena when one studies similar but more
complex systems than the ones presented in this work. This will be our inspiration to continue our investigations in the field.
Appendix A

Copy of the Program Used in Computing the Photonic Band Structure of Zinc Blend Type of Periodic Dielectric Media
integer reso, order, np
parameter
(reso=10, lowest=12, range=3., np=537, order=np*2)
integer ierr, nx, ax
complex
min(lowest), ww, el(2, 2), e(order, order), eval(order)
real ea, eb, pi, pi2, gg(3), gp(3), ak(3), gl(3, np), rty
double precision ar(order, order), ai(order, order)
double precision wi(order), wr(order)
double precision fvl(order), fv2(order), fv3(order)
data ak/0., 0., 0./
do 8 i=1, order
do 8 j=1, order
e(i, j)=0
8 continue
c ea=dielectric const of shpere1, eb=dielectric const of vacuum
c ea2=dielectric const of the shpere2
c background
eb=1.
ea=3.6*3.6
ea2=ea
f2=0.17
f1=0.17
write(20, 20) f1, f2
20 format(1x, 2e15.8)
pi=4.*atan(1.)
c pi=3.1415926
r1=(3.*f1/(16.*pi))^**(1./3.)
r2=(3.*f2/(16.*pi))^**(1./3.)
c r= the radii of the spheres in the fcc lattice
nx=0
pi2=2.*pi
c do 1 creates a set of reciprocal lattice vectors
(note: the
c lattice constant is a=1). Specifically the vectors
are contained
c within a sphere centered about the origin. By
changing the
c value of rty the radius of the sphere is changed. The
total
number of reciprocal lattice vectors generated is nx.
do 1 h=-10, 10, 1
do 1 k=-10, 10, 1
do 1 l=-10, 10, 1
h2=h-k+1
k2=h+k-1
l2=-h+k+1
rty=h2*h2+k2*k2+l2*l2
rty=sqrt(rty)
if(rty.gt.8.0) go to 1
nx=nx+1
 gl(1,nx)=pi2*h2
 gl(2,nx)=pi2*k2
 gl(3,nx)=pi2*12

 c gl(1,n) is the x component of the nth recip lattice
 vector
 c gl(2,n) is the y component of the nth recip lattice
 vector
 c gl(3,n) is the z component of the nth recip lattice
 vector
120 format(1x,3e15.8)
1 continue
 write(20,30) nx
30 format(1x,i9)
c c the gl are a duplicate set of reciprocal lattice
 vectors
do 234 ax=1,2
do 29 ind=0,reso
 c The vector (ak(1),ak(2),ak(3)) is a k vector in the
 first
 c Brillouin Zone. We plot the frequency spectra as a
 function
 c of (ak(1),ak(2),ak(3)) in the first Brillouin zone.
c write(40,71)ind
 if(ax.eq.1) goto 15
 if(ax.eq.2) goto 25
 if(ax.eq.3) goto 35
 if(ax.eq.4) goto 45
 if(ax.eq.5) goto 55
 if(ax.eq.6) goto 65
goto 979
15 ak(1)=pi2*ind/reso
 ak(2)=0.
 ak(3)=0.
x=ak(1)
goto 979

c c the up ak is along the X direction
25 ak(1)=pi2
 ak(2)=ind*0.5*pi2/reso
 ak(3)=0.
x=pi2+ak(2)
goto 979

c c the up ak is along the XW direction
35 ak(1)=pi2*(1.-ind*0.25/reso)
 ak(2)=pi2*(0.5+ind*0.25/reso)
 ak(3)=0.
x=pi2+ak(2)*2-pi
goto 979

c c the up ak is along the WK direction
\begin{verbatim}

45 \text{ak}(1) = \pi \text{ind/reso}
\text{ak}(2) = \text{ak}(1)
\text{ak}(3) = \text{ak}(1)
x = -2 \times \text{ak}(1)
goto 979

c the up \text{ak} is along the \text{L} direction
55 \text{ak}(1) = \pi/2 \times (0.5 + 0.5 \times \text{ind/reso})
\text{ak}(2) = \pi/2 \times (0.5 - 0.25 \times \text{ind/reso})
\text{ak}(3) = \text{ak}(2)
x = -\pi - \text{ak}(1)
goto 979

c the up axis is along the LA direction
65 \text{ak}(1) = \pi/2
\text{ak}(2) = \pi/2 \times (0.25 - 0.25 \times \text{ind/reso})
\text{ak}(3) = \text{ak}(2)
x = -2 \times \pi/2 + \text{ak}(2) \times 2

c the up axis is along the AX axis
979 continue

\text{write (40,70)ind}
\text{write(40,80) ak}\text{(1), ak}\text{(2), ak}(3)
do 3 i=1,nx
do 3 j=1,nx
\text{gg}(1) = \text{gl}(1,i)
\text{gg}(2) = \text{gl}(2,i)
\text{gg}(3) = \text{gl}(3,i)
\text{gp}(1) = \text{gl}(1,j)
\text{gp}(2) = \text{gl}(2,j)
\text{gp}(3) = \text{gl}(3,j)
call \text{am}\text{(ea2, ea, eb, f1, r1, f2, r2, ak, gg, gp, el, ax)}
c The subroutine \text{am} generates the matrix elements of the
\text{matrix}
c to be diagonalized in order to get the electromagnetic
\text{frequency}
c spectrum

do 4 ki=1,2
do 4 kj=1,2
li=2*(i-1)+ki
lj=2*(j-1)+kj
e\text{(li, lj)} = \text{el}\text{(ki, kj)}
c e is the matrix to be diagonalized in order to get the
\text{c frequency spectra of the e&m waves.}
4 continue
3 continue
n=order
\text{do 7 i=1,order}
\text{do7 j=1,order}
\text{ar(i, j)} = \text{dble(e(i, j))}
7 \text{ai(i, j)} = \text{dble(aimag(e(i, j))})
\end{verbatim}
matz=0
call
cg(order,order,ar,ai,wr,wi,matz,fv1,fv2,fv3,ierr)
c  write(6,70) ind
  if (ierr.ne.0) then
  77    format(1x,'CG Error:',i9)
  write(6,77) ierr
  stop
endif
do 88 i=1,order
  eval(i)=cmplx(wr(i),wi(i))
c up is an EISPACK routine which generates the
eigenvalues
c in eval
  itext=0
  do 5 i=1,lowest
     do 89 j=1,order-i
     ww=csqrt(eval(j))/pi2
     if(cabs(ww).lt.0.01) go to 89
     ww=csqrt(eval(j+1))/pi2
  if(real(eval(j)).gt.real(eval(j+1)).and.cabs(ww).gt.0.01) goto 81
  ww=eval(j+1)
  eval(j+1)=eval(j)
  eval(j)=ww
  81  ww=csqrt(eval(j+1))/pi2
  c ww are the lowest 12 eigenvalues in units of
  w*a/(2*pi*c)
  89  continue
     min(i)=ww
  5  continue
  write(20,40) (min(i),i=1,lowest)
  40  format(3(2f9.6,lx,':',lx))
  50  format(lx,f7.3,' ',f7.4,' ',f7.4,' ',f7.4,' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ','f7.4',' ',write(40,*)x,real(min(i))
  6  continue
  write(55,50)x,(real(min(i)),i=1,lowest)
  29 continue
  234 stop
  end
  subroutine
  am(ea2,ea,eb,f1,r1,f2,r2,ak,gg,gp,ee,ax)
  real ea2,ea,eb,ak(3),gg(3),gp(3)
  real a1,a2,a3,b1,b2,b3

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complex e(3,3), bk, q, bkp, ee(2,2)
integer ax
call
form(ea2, ea, eb, gg, gp, f1, r1, f2, r2, bk, q, bkp, pi)
al = ak(1) + gg(1)
a2 = ak(2) + gg(2)
a3 = ak(3) + gg(3)
b1 = ak(1) + gp(1)
b2 = ak(2) + gp(2)
b3 = ak(3) + gp(3)
e(1,1) = (a2*b2 + a3*b3)*bk
e(1,2) = -a2*b1*bk
e(1,3) = -a3*b1*bk
e(2,1) = -a1*b2*bk
e(2,2) = (a1*b1 + a3*b3)*bk
e(2,3) = -a3*b2*bk
e(3,1) = -a1*b3*bk
e(3,2) = -a2*b3*bk
e(3,3) = (a1*b1 + a2*b2)*bk
if (ax.eq.2.or.ax.eq.6) goto 26
if (ax.eq.3) goto 3
if (ax.eq.5) goto 5
  if (bl.eq.0.) then
  ee(1,1) = 0.
ee(1,2) = 0.
ee(2,1) = 0.
ee(2,2) = 0.
  else
  ee(1,1) = e(2,2) - b2*e(2,1)/bl
  ee(1,2) = e(2,3) - b3*e(2,1)/bl
  ee(2,1) = e(3,2) - b2*e(3,1)/bl
  ee(2,2) = e(3,3) - b3*e(3,1)/bl
  endif
goto 45
26 if (b2.eq.0.) then
  ee(1,1) = e(2,2) - b2*e(2,1)/bl
  ee(1,2) = e(2,3) - b3*e(2,1)/bl
  ee(2,1) = e(3,2) - b2*e(3,1)/bl
  ee(2,2) = e(3,3) - b3*e(3,1)/bl
else
  ee(1,1) = e(1,1) - b1*e(1,2)/b2
  ee(1,2) = e(1,3) - b3*e(1,2)/b2
  ee(2,1) = e(3,1) - b1*e(3,2)/b2
  ee(2,2) = e(3,3) - b3*e(3,2)/b2
endif
goto 45
3 ee(1,1) = e(1,1) - b1*e(1,2)/b2
ee(1,2) = e(1,3) - b3*e(1,2)/b2
ee(2,1) = e(3,1) - b1*e(3,2)/b2
ee(2,2) = e(3,3) - b3*e(3,2)/b2
5

    ee(1,1)=e(1,1)-b1*e(1,3)/b3
    ee(1,2)=e(1,2)-b2*e(1,3)/b3
    ee(2,1)=e(2,1)-b1*e(2,3)/b3
    ee(2,2)=e(2,2)-b2*e(2,3)/b3

12

    format(lx,i9)

45

    return

end

subroutine

form(ea2,ea,eb,gl,gp,f1,r1,f2,r2,bk,q,bkp,pi)

    c The subroutine form generates the structure factor
    c for a spherical ball in the fcc lattice.
    real ea,eb,a1,a2,a3,g,a,gl(3),gp(3),fp,pi,f
    complex bk,q,bkp
    q=cmplx(0.,1.)
    a1=gl(1)-gp(1)
    a2=gl(2)-gp(2)
    a3=gl(3)-gp(3)
    g=sqrt(a1*a1+a2*a2+a3*a3)
    if(g.lt.0.00001) go to 1
    pi=4.*atan(1.)
    ap=g*r2
    bkp=3.*((sin(ap)-ap*cos(ap))/(ap*ap*ap))
    a=g*r1
    if(a.lt.0.00001) go to 1
    bk=3.*((sin(a)-a*cos(a))/(a*a*a))
    write(10,*)bk
    bk=f1*(1./ea-1./eb)*bk
    bk=bk+f2*(1./ea2-1./eb)*b kp*cexp(q*(a1+a2+a3)/4.)
    return

1

    f=f1+f2
    bk=1./eb+f1*(1./ea-1./eb)+f2*(1./ea2-1./eb)
    return

end

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Appendix B

Copy of the Paper Published in *Physica B*
Photonic band structure of zinc blende type periodic dielectric media

Simeon Simeonov, Ulrich Bass, Arthur R. McGurn*

Department of Physics, Western Michigan University, Kalamazoo, MI 49008, USA

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Abstract

The photonic band structures for two types of zinc blende structures are computed using the plane wave expansion method. Both structures are formed from an array of dielectric balls in a vacuum background. In the first type of structure the basis on the FCC lattice is composed of two balls of equal radii but of different dielectric composition. In the second type of structure the basis is composed of two balls of different radii which are composed of identical dielectric materials. The lowest frequency band gaps are studied in the first system as a function of the dielectric contrast ratio of the balls and in the second system as a function of the filling fraction ratio of the balls. In the first system it is found that by increasing the difference of the dielectric constants, the frequency gap can be increased from that observed in the limit of the diamond structure. In the second system the largest gap is observed in the limits of the diamond structure.

Keywords: Photonic; Photonic band structure; Electromagnetic filters; Band structure; Optical dispersion

There has been much recent interest in the theoretical and experimental study of photonic band structures [1–7]. These structures are formed as a periodic array of dielectric media and are of interest due to the band structure exhibited by the dispersion relation of electromagnetic waves propagating in the periodic dielectric media. Specifically, frequency gaps (photonic band gaps) can be opened up in the frequency spectrum, allowing for the use of these structures as highly efficient frequency filters of electromagnetic waves. Such band gaps have been exhibited by a variety of periodic dielectric structures including the simple cubic [4], BCC [4], FCC [2, 3, 5], and diamond [2] lattices. The diamond lattice, however, is found to be most effective in generating, for small dielectric constants, large frequency gaps in its photonic band structures. Simple cubic, BCC and FCC structures mentioned above all exhibit small band gaps that require large dielectric contrasts for their generation and are, hence, less likely to be of technological interest than the diamond structure.

In this paper we present results for the photonic band structure of two types of zinc blende structures. The zinc blende structure [8] is closely related to the diamond structure. The diamond structure is formed from an FCC lattice with a basis consisting of two identical balls whereas the zinc blende is an FCC lattice with a basis consisting of two non-identical balls [8]. We shall also see if improvements to the gap-forming properties of the diamond lattice can be found in its modified zinc blende form. Specifically, in one zinc blende structure we shall vary the dielectric contrast of the two balls of equal radi forming the basis, taking the dielectric background to be vacuum. In a second

*Corresponding author.

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zinc blende structure we shall vary the relative radii of the two balls of equal dielectric constants forming the basis, taking the dielectric background to be vacuum.

The photonic band structure is computed using the plane-wave method. In this method the electromagnetic wave equation for waves propagating in the periodic medium is expanded in plane waves. The resulting eigenvalue problem is solved for the band structure of the electromagnetic dispersion relation in the periodic medium. Specifically, we consider a periodic dielectric medium with a zinc blende structure consisting of a two non-identical ball basis on an FCC Bravais lattice. The matrix equation obtained from a plane-wave expansion of the wave equation describing the magnetic field of the electromagnetic waves propagating through such a structure is [9]

\[
\sum \sum M_{ij}(k - G_i, k - G_j)A_{iG} = \left( \frac{1}{\epsilon} \right)^{\frac{3}{2}} A_{iG} \cdot G_i
\]

where

\[
M_{ij}(k - G_i, k - G_j) = [-i k_i G_{ij} k_j G_{ij} - G_{ij}]
\]

\[
K(G) = \frac{1}{\epsilon} \int \frac{e^{-iG \cdot r}}{\epsilon r} d^3r
\]

Fig. 1: Lowest photonic band gaps: shaded regions between solid lines and dashed lines versus dielectric constant ratio. The dashed lines indicate a gap between the second and third bands and solid lines indicate a gap between the fifth and sixth bands. The tilting fractions are \(100\)\% for both types of atoms.
G, G' are reciprocal lattice vectors of the FCC lattice: \( \beta = 1, 2, 3 \) sums over the \( x, y, z \) orthogonal space axes. \( \varepsilon_i \) is the volume of the primitive lattice cell in the FCC lattice, and \( \alpha \) is the dielectric constant of the basis. The eigenvalue problem in Eq. (1) then yields the band structure of our periodic dielectric system.

Numerically, Eq. (1) is evaluated by restricting the sum on \( G \) to the \( N \) smallest \( G \) in the system. This converts Eq. (1) into a \( 3N \times 3N \) matrix eigenvalue problem. A further reduction of this problem to a \( 2N \times 2N \) matrix eigenvalue problem can be made by the use of \( V \cdot \beta = 0 \) which requires

\[
\sum_{j} \langle k \mid G_j \rangle \eta_j \langle k \mid G \rangle = 0. \tag{4}
\]

The eigenvalue solution of the resulting \( 2N \times 2N \) matrix eigenvalue problem is studied as a function of \( N \) to extract via numerical means the \( N \rightarrow \infty \) limit of the dispersion relation for the finite photonic band structure.

The specific method we have used to determine the \( N \rightarrow \infty \) limit of the dispersion relation of our system is as follows: Let \( \omega_y, \omega_z, \omega_x \), be eigenvalues of the same photon mode computed using, respectively, \( 2N_1 \times 2N_1, 2N_2 \times 2N_2 \), and \( 2N_3 \times 2N_3 \) matrices. Assume that for large \( N \), \( \omega_y = \omega_z = 2 \left( \frac{1}{N} \right) \), \( \omega_x \) is the \( N \rightarrow \infty \) limit and \( \alpha, \beta \) are constants. Using Eq. (5) for \( \omega_y, \omega_z, \omega_x \), we find that

\[
[\omega_y - \omega_x](\omega_y - \omega_z) = (\omega_y - \omega_z)(\omega_y - \omega_x), \tag{6}
\]

where

\[
\delta = \text{int}(N_1, N_3) / \text{int}(N_2, N_1). \tag{7}
\]

yields an approximate solution of \( \omega_x \).

We have considered two different zinc blende structures. In the first type we take a basis of the form

\[
\alpha \beta = \sqrt{\omega_y(\beta^2 - |\beta|)} - \sqrt{\omega_z(\beta^2 - |\beta|)} (\bar{c}_1 - \bar{c}_2), \tag{8a}
\]

where \( R \) is the radius of the dielectric balls of dielectric constants \( \varepsilon_i \) and \( \varepsilon_m \), and \( \alpha \) in the lattice constant of the conventional cubic-cell representation of the FCC lattice. In the second type we take a basis of the form

\[
\alpha \beta = \beta (R_1 - R) - \beta (R_2 - R - d/4 (\bar{c}_1 - \bar{c}_2 - \bar{c}_3)), \tag{8b}
\]

Fig. 2. Calculated photonic band structures along important symmetry lines in the Brillouin zone for zinc blende structure composed of dielectric spheres with refractive indexes 3.6 for Zn-placed atoms and 1.5 for Sn-placed atoms. The band gap region has been shaded in.

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where \( R_1 \) is the radius of one ball, \( R_2 \) is the radius of the second and both balls have dielectric constant \( \varepsilon \). These basis are placed on the FCC lattice with the ball described by the first term on the right-hand side of either Eq. (8a) or (8b) being centered on a point of the FCC lattice. In the preceding, this ball (ball centered at \( r = 0 \) in the basis) will be referred to as the Zn ball. The remaining ball (ball centered at \( r = \frac{1}{3} a (\hat{x}_1 + \hat{x}_2 + \hat{x}_3) \) in the basis) of the basis will be referred to as the S ball.

The zinc blende structures we initially study are based on the diamond structure formed of dielectric balls in vacuum which Ho et al. [2] found to give the largest gap width to midgap ratio for the lowest frequency band gap. This diamond structure corresponds to a system with \( \varepsilon = 3.6 \) and a single dielectric ball filling fraction of 0.17. We study zinc blende structures formed from this diamond structure by either of the first or second type of modifications of the diamond system as discussed above. The objects of the study of the zinc blende modifications to this diamond structure is to see if such modifications can improve the gap width to midgap ratio over this ratio as computed for the diamond structure.

In Fig. 1 we present results for the lowest band gaps as a function of \( \varepsilon / \varepsilon_{Zn} \) for fixed \( \varepsilon_{Zn} = 3.6 \) and a filling fraction of 0.17. The regions of the frequency band gaps are indicated in this figure by shading. In obtaining the results in Fig. 1 we used the extrapolation in Eqs. (5) and (7) for \( \varepsilon_2 = 537, \varepsilon_4 = 645 \) and \( \varepsilon_3 = 749 \). To facilitate the reader in understanding the results in Fig. 1 we present results for the band structure along some symmetry
directions in the Brillouin zone of the zinc blende structure in Fig. 2 for \( \varepsilon_s/\varepsilon_{Zn} = 0.111, 0.605 \) and 2.334. These illustrate typical band structures found between \( 0 \leq \varepsilon_s/\varepsilon_{Zn} \leq 2.5 \). The results in Fig. 1 indicate that some advantages to the creation of large photonic band gaps are seen for large and small \( \varepsilon_s/\varepsilon_{Zn} \) ratios in zinc blende structures.

It is interesting to note that for both large and small ratios of \( \varepsilon_s/\varepsilon_{Zn} \), the lowest band gap occurs between the 5th and 6th bands. For intermediate values of \( 0.5 \leq \varepsilon_s/\varepsilon_{Zn} \leq 1.6 \), a lowest gap exists between the 2nd and 3rd bands. Between \( 1.3 \leq \varepsilon_s/\varepsilon_{Zn} \leq 1.6 \) we have indicated the positions of the two lowest band gaps. In addition, we observe that for \( \varepsilon_s/\varepsilon_{Zn} > 1.5 \) the lowest band gap observed is greater than the lowest gap seen in the diamond lattice. Also at \( \varepsilon_s/\varepsilon_{Zn} = 0.1 \) a large gap is observed in the zinc blende structure.

In Fig. 3 we present similar results to those in Fig. 1 but now for balls with filling fractions of 0.125. The lowest band gaps (shaded regions) are again presented as a function of the ratio \( \varepsilon_s/\varepsilon_{Zn} \). In these results large band gaps are obtained in the zinc blende data for \( \varepsilon_s/\varepsilon_{Zn} > 1.5 \) while no band gaps are observed in the diamond structure. In this case we see that zinc blends structures based on dielectric contrasts favor the creation of band gaps over the diamond lattice counterparts.

In Fig. 4 we present results obtained using the same extrapolation as in Fig. 1 for the second type of...
of zinc blende system described in Eq. (8b). For the results in Fig. 4 we have taken $c = (3.6)^2$ and plotted the band gap (shaded region) as a function of $f_{Zn}/f_S$ where $f_{Zn}$ is the filling fraction of the Zn balls and $f_S$ is the filling fraction of the S balls. In the region $f_{Zn}/f_S < 1$ we have fixed $f_S = 0.17$ and varied $f_{Zn}$. In the region $f_{Zn}/f_S > 1$ we have fixed $f_{Zn} = 0.17$ and varied $f_S$. The band gap is always found between the 2nd and 3rd bands and is greatest in the diamond structure. In this second type of zinc blende modification of the diamond lattice structure there is then no advantage in the gap-forming properties over the original diamond lattice limit.

In this paper we have studied two zinc blende modifications to diamond lattice photonic band structures. Changes in the relative radii of the two balls basis are seen to decrease the lowest frequency photonic band size of the gaps from that of the diamond structure. Changes in the relative dielectric constants of the two ball basis can enhance the size of the band gaps over those found in the diamond lattice. In addition, in zinc blende structures composed of balls with different dielectric constants, the lowest band gap is found to occur between different indexed bands dependent on the relative dielectric contrast of the balls in the two balls basis.

Recently, dielectric structures (called photonic crystals) have been fabricated which exhibit photonic band structures. These structures have been created [10, 11] by setting an array of dielectric balls, drilling cylindrical holes in dielectric media or by stacking layers of periodic dielectric media. We expect that with the advancing interest in photonic crystals which yield large photonic band gaps, means will become available to fabricate photonic crystals based on our discussions above. In the context of illustrating the wide variety of possible photonic crystal geometries, we would like to point out some recent very nice work on layered [12] and spherical ball systems in A7 geometries [13]. These too are possible structures for future fabrication of photonic crystals.

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References


Appendix C

Copy of the Program Used to Compute the Transverse Correlation Length of Two-Dimensional Randomly Rough Surfaces
C .. External Subroutine ..
EXTERNAL setall
C .. External Function ..
REAL snorm
EXTERNAL snorm
dimension zp(140,140)
dimension cpp(140)
dimension cpl(140),cp2(140)
dimension cpo(140)
dimension z(140,140)
dimension xx(560,560)
dimension w(420,420)
dimension x(1500),y(1500),x1(1500),y1(1500),x2(1500),y2(1500)
common delta,pi,cl
dimension bout(88203),binp(88203)
integer id,nn,nw,nwl,nw2,dims,nbytes1,nbytes,ni,p,nr
integer type,flag
it=0
ndm=44444
n=140
n4=4*n
do 177 i=1,n
cpo(i)=0.
177 cpo(i)=0.
pi=4.*atan(1.)
delta=0.1
cl=1.0
iseed1=124455578
iseed2=123445565
call setall(iseed1,iseed2)
dx=0.05
n=140
n2=2*n
n3=3*n
call whoami(id,process,host,dims)
nn=2**dims
call split(id,nn,n3,nwl,nw2)
do 1 i=nwl,nw2
  i1=i-3*n/2
6 format(1x,i9)
oxo=dx*i1
do 1 j=1,n3
  jl=j-3*n/2
  yo=dx*jl
call wjp(n,dx,xo,yo,w1)
89 format(1x,e15.8)
w(i,j)=w1
1 continue
if (nn.le.1.0) goto 1221
bout(1)=real(nwl)
bout(2)=real(nw2)
p=2
    do 33 j=nwl,nw2
        do 33 jj=1,n3
            p=p+1
            bout(p)=w(j,jj)
            nbytes=p*4
            nbytes1=(p+n3)*4
        do 11 i=1,nn-1
            nn1=id+i
            nn2=id-i
            if (nn1.gt.(nn-1) ) nn1=nn1-nn
            if (nn2.lt.0) nn2=nn2+nn
            ni=nwrite(bout,nbytes,nn1,type,flag)
            if (ni.eq.0) then
                nr=nread(binp,nbytesl,nn2,type,flag)
            endif
            else
                write(6,55)id,nn1
                stop
            endif
            p=2
            do 22 jj=int(binp(1)),int(binp(2))
                do 22 j=1,n3
                    p=p+1
                    w(jj,j)=binp(p)
            11 continue
        1221 continue
    call split(id,nn,n,nwl,nw2)
    do 11111 i=nwl,nw2
        il=i-n/2
        x(i)=dx*il
        do 11111 j=1,n
            jl=j-n/2
            y(j)=dx*jl
        11111 continue
            bout(1)=real(nwl)
bout(2)=real(nw2)
p=2
    do 333 j=nwl,nw2
        p=p+1
        bout(p)=x(j)
nbytes=p*4
nbytes1=(p+nn)*4
do 211 i=1,nn-1
   nn1=id+i
   nn2=id-i
   if (nn1.gt.(nn-1)) nn1=nn1-nn
   if (nn2.lt.0) nn2=nn2+nn
   ni=nwrite(bout,nbytes,nn1,type,flag)
   if (ni.eq.0) then
      nr=nread(binp,nbytes1,nn2,type,flag)
      nrr=int(int(binp(2))-int(binp(1))+3)*4
      if (nr.ne.nrr) then
         66 format(1x,'node',i9,'calc.bytes :',i9,' read bytes:',i9)
         write(6,66)id,nrr, nr
         stop
      endif
   else
      55 format(1x,'node',i9,' unable to write to',i9)
      write(6,55)id,nnl
      stop
   endif
p=2
do 222 jj=int(binp(1)),int(binp(2))
p=p+l
222 x(jj)=binp(p)
211 continue

75 z(k,kp)=0.
do 76 l=1,50
   write(6,6) l
   do 7 i1=1,n4
      do 7 i2=1,n4
         xx(i1,i2)=snorm()
do 5 k=nwl,nw2
   do 5 kp=1,n
      zp(k,kp)=0.
do 4 j=1,n3
   do 4 jp=1,n3
      zp(k,kp)=zp(k,kp)+delta*w(j,jp)*xx(j+k,jp+kp)
4 continue
5 continue
if (nn.le.1) goto 1220
bout(1)=real(nwl)
bout(2)=real(nw2)
p=2
do 32 j=nwl,nw2
   do 32 jj=1,n
      p=p+1

bout(p)=zp(j, jj)
nbytes=p*4
nbytes1=(p+nn*n)*4
do 10 i=1, nn-1
   nn1=id+i
   nn2=id-i
   if (nn1.gt.(nn-1)) nn1=nn1-nn
   if (nn2.lt.0) nn2=nn2+nn
   ni=nwrite(bout, nbytes, nn1, type, flag)
   if (ni.eq.0) then
      nr=nread(binp, nbytes1, nn2, type, flag)
      nrr=(int((int(binp(2))-int(binp(1))+1)*n)+2)*4
      if (nr.ne.nrr) then
         write(6,66)id, nrr, nr
         stop
      endif
   else
      write(6,55)id, nl
      stop
   endif
   p=2
   do 21 jj=int(binp(1)), int(binp(2))
      do 21 j=1, n
         p=p+l
      21 zp(jj,j)=binp(p)
   10 continue
220 continue
2334 format(1x,f12.4,e15.8)
do 2345 i=1, n
   write(29,2334)x(i), zp(i,55)
2345 continue
stop
call set(dx,n,11,12, zp,x,y,x1,y1,x2,y2, id,nn)
bout(1)=real(11)
do 34 jj=1, 11
   bout(2*jj)=x1(jj)
   bout(2*jj+1)=y1(jj)
34 continue
nbytes=(2*11+1)*4
nbytes1=14000
if (id.ne.0) then
   ni=nwrite(bout, nbytes, 0, type, flag)
else
   do 111 i=1, nn-1
      nr=nread(binp, nbytes1, i, type, flag)
      nrr=(2*int(binp(1))+1)*4
      if (nr.ne.nrr) then
         write(6,66)id, nrr, nr
         stop
      endif
   111 continue
do 112 jj=1,int(binp(1))
   ll=ll+1
   xl(ll)=binp(2*jj)
   yl(ll)=binp(2*jj+1)
112
   continue
endif
bout(1)=real(ll)
   do 43 jj=1,11
      bout(2*jj)=xl(jj)
      bout(2*jj+1)=yl(jj)
   43
nbytes=(2*ll+1)*4
nbytes1=14000
   if (id.eq.0) then
      do 1111 i=1,nn-1
         ni=nwrite(bout,nbytes,i,type,flag)
   1111
   else
      nr=nread(binp,nbytes1,0,type,flag)
      nrr=(2*int(binp(1))+1)*4
      if (nr.ne.nrr) then
         write(6,66)id,nrr,nr
         stop
      endif
      ll=int(binp(1))
   1122
   do 1122 jj=1,ll
      xl(jj)=binp(2*jj)
      yl(jj)=binp(2*jj+1)
   1122
   endif
   bout(1)=real(ll)
   do 234 jj=1,12
      bout(2*jj)=x2(jj)
      bout(2*jj+1)=y2(jj)
   234
nbytes=(2*12+1)*4
nbytes1=14000
   if (id.ne.0) then
      ni=nwrite(bout,nbytes,0,type,flag)
   else
      nr=nread(binp,nbytes1,i,type,flag)
      nrr=(2*int(binp(1))+1)*4
      if (nr.ne.nrr) then
         write(6,66)id,nrr,nr
         stop
      endif
   2111
   do 2112 jj=1,int(binp(1))
      l2=l2+1
      x2(l2)=binp(2*jj)
      y2(l2)=binp(2*jj+1)
   2112
   continue
   endif
bout(1)=real(12)
do 343 jj=1,12
    bout(2*jj)=x2(jj)
    bout(2*jj+1)=y2(jj)
nbytes=(2*12+1)*4
nbytes1=14000
if (id.eq.0) then
    do 21111 i=1,nn-1
       ni=nwrite(bout,nbytes,i,type,flag)
    else
       nr=nread(binp,nbytes1,0,type,flag)
       nrr=(2*int(binp(1))+1)*4
       if (nr.ne.nrr) then
          write(6,66)id,nrr,nr
          stop
       endif
       l2=int(binp(1))
       do 3112 jj=1,12
          x2(jj)=binp(2*jj)
          y2(jj)=binp(2*jj+1)
       endif
       call pair(11,dx,n,x1,y1,cpp,id,nn)
       call pair(12,dx,n,x2,y2,cp1,id,nn)
       call pairl(11,12,dx,n,xl,yl,x2,y2,cp2,id,nn)
76    continue
18    format(1x,4el5.8)
totl=0.
tot2=0.
tot=0.
tot=0.
tot=0.
tot=0.
tot=2=0.
call split(id,nn,n,nwl,nw2)
do 277 i=nwl,nw2
    totl=totl+cp1(i)
    tot2=tot2+cp2(i)
    tot=tot+cpp(i)
    bout(1)=totl
    bout(2)=tot2
    bout(3)=tot
    nbytes=3*4
    nbytes1=3*4
do 1020 i=1,nn-1
    nn1=id+i
    nn2=id-i
    if (nn1.gt.(nn-1)) nn1=nn1-nn
    if (nn2.lt.0) nn2=nn2+nn
    ni=nwrite(bout,nbytes,nn1,type,flag)
    if (ni.eq.0) then
       nr=nread(binp,nbytes1,nn2,type,flag)
       nrr=3*4
if (nr.ne.nrr) then
    write(6,66)id,nrr,nr
    stop
endif
else
    write(6,55)id,nl
    stop
endif
totl=totl+binp(1)
tot2=tot2+binp(2)
tot=tot+binp(3)
1020 continue
    total=total+tot1
tota2=tota2+tot2
    total=total+tot
    do 178 i=nwl,nw2
        cpl(i)=cpl(i)/total
        cp2(i)=cp2(i)/tota2
        cpp(i)=cpp(i)/total
        do 176 i=nwl,nw2
            xi=dx*(i-0.5)
            write(20,18) xi,cpl(i),cp2(i),cpp(i)
        176        stop
    178 end
subroutine wjp(n,dx,x,y,w)
common delta,pi,cl
real q,r,kl,k2,ksp,xl,tm
xl=0.6127
    tm=10.
e=cmplx(-17.2,0.497)
ksp=(2*pi/xl)*real(sqrt(e/(e+1)))
k1=ksp*(1-sin(pi*tm/180.))
k2=ksp*(1+sin(pi*tm/180.))
r=sqrt(x*x+y*y)
call integ(r,0.1,q,kl,k2)
w=2*dx*sqrt(pi)*cl*q/sqrt(k2*k2-kl*kl)
    return
end
Subroutine
set(dx,n,11,12,z,x,y,x1,y1,x2,y2,id,nn)
dimension z(140,140)
dimension x(1500),y(1500)
dimension x1(1500),y1(1500),x2(1500),y2(1500)
integer id,nn,nwl,nw2
    do 100 i=1,n
        x1(i)=0.
y1(i)=0.
x2(i)=0.
y2(i)=0.
100 continue
ll=0
l2=0
n1ll=n-1
n22=n-2
call split(id,nn,n22,nw1,nw2)

nw1=nw1+1
nw2=nw2+1
do 1 i=nw1,nw2
do 1 j=2,n1ll
  im=i-1
  if(im.eq.0) im=n
  ip=i+1
  if(ip.eq.n+1) ip=1
  jp=j+1
  if(jp.eq.n+1) jp=1
  jm=j-1
  if(jm.eq.0) jm=n
    a=z(i,j)
    ap=z(ip,j)
    am=z(im,j)
    bp=z(i,jp)
    bm=z(i,jm)
    cp=z(ip,jp)
    cm=z(im,jm)
    dp=z(ip,jm)
    dm=z(im,jp)
    if(a.lt.ap.and.a.lt.am) go to 200
    if(a.gt.ap.and.a.gt.am) go to 101
    go to 1
 200  if(a.ge.bp) go to 1
    if(a.ge.bm) go to 1
    if(a.ge.cp) go to 1
    if(a.ge.cm) go to 1
    if(a.ge.dp) go to 1
    if(a.ge.dm) go to 1
    ll=ll+1
    xl(ll)=x(i)
    yl(ll)=y(j)
    go to 1
101  if(a.le.bp) go to 1
    if(a.le.bm) go to 1
    if(a.le.cp) go to 1
    if(a.le.cm) go to 1
    if(a.le.dp) go to 1
    if(a.le.dm) go to 1
    l2=l2+1
    x2(l2)=x(i)
    y2(l2)=y(j)
1  continue
return


end

subroutine pair(l,dx,n,x,y,c,id,nn)
dimension x(1500),y(1500)
dimension xp(1500),yp(1500)
dimension z(1500)
dimension c(140),cc(140)
integer
nn, id, nbytes, nbytes1, type, k, bout, binp, nw1, nw2

  do 55 i=1,n
    cc(i)=0.
    if(l.gt.1500) stop
    if(l.eq.0) go to 8
    do 111 i=1,l
      xp(i)=x(i)
      yp(i)=y(i)
      xp(i+1)=x(i)+n*dx
      yp(i+1)=y(i)
      xp(i+2*l)=x(i)-n*dx
      yp(i+2*l)=y(i)
      xp(i+3*l)=x(i)
      yp(i+3*l)=y(i)+n*dx
      xp(i+4*l)=x(i)
      yp(i+4*l)=y(i)+n*dx
      xp(i+5*l)=x(i)
      yp(i+5*l)=y(i)
      xp(i+6*l)=x(i)
      yp(i+6*l)=y(i)-n*dx
      xp(i+7*l)=x(i)
      yp(i+7*l)=y(i)+n*dx
      xp(i+8*l)=x(i)
      yp(i+8*l)=y(i)-n*dx
    111 continue

    l8=l
    call split(id,nn,1,nwl,nw2)
    do 1 i=nwl,nw2
      zzttt=100000000.
      k=0
      do 222 j=1,l8
        if(i.eq.j) go to 222
        a1=xp(i)-xp(j)
        a2=yp(i)-yp(j)
        k=k+1
        zt=sqrt(a1*a1+a2*a2)
        if(zt.lt.zztttt) zztttt=zt
      222 continue
      z(i)=zztttt
    1 continue
    if(k.eq.0) go to 8
    nm=n-4
    do 2 i=nw1,nw2

do 2 j=1,nm
xl=dx*(j-1)
xpl=dx*j
zzttt=z(i)
if(zzttt.gt.xl.and.zzztt.lt.xpl) then
   c(j)=c(j)+1
   cc(j)=cc(j)+1
endif
2 continue
8 continue
call back3(nn,id,c,cc,n)
return
end
subroutine pairl(ll,12,dx,n,xl,yl,x2,y2,c,id,nn)
dimension xl(1500),yl(1500),x2(1500),y2(1500)
dimension z(1500),c(140),cc(140)
integer
nn, id, nbytes, nbytes1, type, k, bout, binp, nw1, nw2
do 55 i=1,n
cc(i)=0.
if(ll.gt.1500.or.12.gt.1500) stop
if(ll.eq.0) go to 8
if(12.eq.0) go to 8
call split(id,nn,ll,nw1,nw2)
do 1 i=nw1,nw2
zzttt=100000000.
k=0
do 222 j=1,12
al=xl(i)-x2(j)
a2=yl(i)-y2(j)
k=k+1
zt=sqrt(al*al+a2*a2)
if(zt.lt.zzttt) zzttt=zt
222 continue
z(i)=zzttt
1 continue
if(k.eq.0) go to 8
nm=n-4
do 2 i=nw1,nw2
2 do 2 j=1,nm
xl=dx*(j-1)
xp=dx*j
zz=z(i)
if (zz.gt.xl.and.zz.lt.xp) then
   c(j)=c(j)+1
   cc(j)=cc(j)+1
endif
2 continue
8 continue
call back3(nn,id,c,cc,nm)
return
end
subroutine split(id, nn, nw, nw1, nw2)
integer id, nn, nw, nw1, nw2, p, q, r
p = id
q = nw/nn
r = nw - q*nn
if (p<.lt.r) then
   nw1 = p*(q+1)
   nw2 = nw1 + q
else
   nw1 = r*(q+1) + (p-r)*q
   nw2 = nw1 + q-1
endif
nw1 = nw1 + 1
nw2 = nw2 + 1
return
end
subroutine back3(nn, id, gath, gathl, n)
dimension
bout(140), gath(140), gathl(140)
integer nn, id, nbytes, ni, p, nr, nbytes1
   do 3 jj = 1, n
3   bout(jj) = gathl(jj)
nbytes = n*4
nbytes1 = n*4
   do 1 i = 1, nn-1
   n1 = id + i
   n2 = id - i
   if (n1.gt.(nn-1)) n1 = n1 - nn
   if (n2.lt.0) n2 = n2 + nn
   ni = nwrite(bout, nbytes, n1, type, flag)
   if (ni.eq.0) then
      nr = nread(binp, nbytes1, n2, type, flag)
      nrr = n*4
      if (nr.ne.nrr) then
         format(1x, 'node', i9, 'calc. bytes :', i9, 'read bytes :', i9)
         write(6, 6) id, nrr, nr
         stop
      endif
   else
      format(1x, 'node', i9, ' unable to write to', i9)
      write(6, 5) id, nl
      stop
   endif
   do 2 j = 1, n
2   gath(j) = gath(j) + binp(j)
   continue
return
end
subroutine bess0(x,b)
real x,b
if (abs(x).ge.3) go to 2
y=x/3 
y2=y*y
y4=y2*y2
y6=y4*y2
y8=y6*y2
y10=y8*y2
y12=y10*y2
b=1.-2.2499997*y2+1.2656208*y4-0.3163866*y6
b=b+0.0444479*y8-0.0039444*y10+0.00021*y12
return
2
y=abs(x)
z=3./y
z2=z*z
z3=z2*z
z4=z2*z2
z5=z4*z
z6=z5*z
b=0.79788456-0.00000077*z-0.0055274*z2
b=b-0.00009512*z3+0.00137237*z4
b=b-0.00072805*z5+0.00014476*z6
th=y-0.78539816-0.04166397*z-0.00003954*z2
th=th+0.00262573*z3-0.00054125*z4-0.0002933*z5
th=th+0.00013558*z6
b=b*cos(th)/sqrt(y)
return
end
subroutine kbess0(ka, k0, kl, k2)
real ka,k0,t,i0,kl,k2,kp1,kp2
kp1=0.
kp2=0.
if (ka.ge.kl) kp1=1.
if (ka.le.k2) kp2=1.
k0=kp1*kp2
continue
return
end
subroutine integ(r,pr,qt,k1,k2)
common delta,pi,cl
real r,pr,xpqr,qt,dk,j01,k01,t0,x11,x21
real x12,x22,x13,x14,x23,x24,j02,j03,j04
real k02,k03,k04,p,xpqr0,k1,k2
integer*2 k
qt=0.
qt0=0.
xpqr0=0.
k=0.
ak=0.
2    continue
dk=0.001
if (k.gt.500) dk=0.01
ak=ak+dk
k=k+1
x14=ak*cl
x24=ak*r
call bess0(x24,j04)
call kbess0(x14,k04,k1,k2)
qt=qt+ak*dk*j04*sqrt(k04)
if (k.le.2000) go to 2
1234 format(1x,i9)
return
end
Appendix D

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The Transverse Correlation Length for Randomly Rough Surfaces: Two-Dimensional Roughness

S. Simeonov, A. R. McGurn and A.A. Maradudin

Department of Physics, Western Michigan University, Kalamazoo, MI 49008 USA

Department of Physics and Astronomy, University of California, Irvine, CA 92697 USA

ABSTRACT

A numerical algorithm is used to generate two-dimensional surfaces defined by \( z_3 = \zeta(x) \), with \( x = (x_1, x_2) \), where \( \zeta(x) \) is a single-valued function of \( x \) that constitutes a zero-mean, stationary, isotropic, Gaussian random process defined by the properties \( \langle \zeta(x) \rangle = 0 \), \( \langle \zeta(x)\zeta(x') \rangle = \sigma^2 W(|x-x'|) \), and \( \sigma^2 = \langle \zeta(x)\zeta(x) \rangle \). The angle brackets here denote an average over the ensemble of realizations of the surface profile function \( \zeta(x) \). The results are used to compute the probability density \( P_2(x)(P_2(x)) \) that the nearest maximum (minimum) to a given maximum (minimum) is at a distance \( x \) from the latter, and the probability density \( P_3(x) \) that the nearest minimum to a given maximum is at a distance \( x \). Results are presented for random surfaces defined by surface height autocorrelation functions \( W(|x|) = \exp(-\epsilon^2 |x|^2), a^2/(\epsilon^2 + a^2), \) and \( 2[(k_x^2-k_y^2)|x|^2]^{-1/2}[J_1(k_x k_y x) - k_x k_y J_1(k_x k_y)] \), where \( J_1(z) \) is a Bessel function. Results are also presented for a novel type of one-dimensional random surface used in recent experimental studies of enhanced backscattering.

Keywords: surface roughness, surface profile, disorder

1. INTRODUCTION

Many theories of the properties of two-dimensional randomly rough surfaces assume that the profile function \( \zeta(x, z_3) \equiv \zeta(x) \) that defines the surface through the equation \( z_3 = \zeta(x) \) is a single-valued function of \( \zeta(x) \) that constitutes a zero-mean, stationary, isotropic, Gaussian random process defined by the properties

\[
\begin{align*}
\langle \zeta(x) \rangle &= 0, \\
\langle \zeta(x)\zeta(x') \rangle &= \sigma^2 W(|x-x'|).
\end{align*}
\]

The angle brackets here denote an average over the ensemble of realizations of \( \zeta(x) \), and \( \sigma = \langle \zeta^2(x) \rangle^{1/2} \) is the rms height of the surface. The ensemble averages of products of larger numbers of surface profile functions are then given by

\[
\langle \zeta(x_1) \zeta(x_2) \zeta(x_{2n+1}) \rangle = 0
\]
\[ (\zeta_1, \ldots, \zeta_{2k}) = \sum_{\pi} (C(\zeta_{\pi(1)} \zeta_{\pi(2)}) \cdots C(\zeta_{\pi(2k-1)} \zeta_{\pi(2k)})) \]  
\[ \text{where } \sum_{\pi} \text{ is the sum over different permutations of pairs from the sequence } 1, 2, \ldots, 2k. \]

The assumption that a random surface is defined by a Gaussian random process is particularly useful in multiple-scattering theories of the scattering of volume waves from or the propagation of surface waves along such surfaces, because Eqs. (2) constitute a Wick's theorem for the calculation of averages of products of surface profile functions. This in turn makes possible a Feynman diagrammatic treatment of small-amplitude perturbation theory for, e.g., the scattering of electromagnetic waves from a random surface, in which the scattering amplitude and the scattered intensity are expanded in powers of the surface profile function and then averaged over the ensemble of realizations of \( \zeta(x) \). Aside from these theoretical considerations, experimental techniques for generating two-dimensional random surfaces possessing Gaussian statistics are now available. For these reasons it is of interest to investigate the statistical properties exhibited by such surfaces to gain insight into the general topography of randomly rough surfaces.

2. THEORY

Recently Maradudin and Michel presented a study of the statistical properties of one-dimensional randomly rough surfaces defined by \( z_3 = \zeta(x_1) \), where \( \zeta(x_1) \) was assumed to be a zero-mean, stationary, Gaussian random process. A central result of this study was the determination, by means of computer simulations, of the probability density \( p(x_1) \) defined such that if the surface possesses a maximum at \( x_1 = 0 \), the nearest minimum to it lies in the interval \( (x_1, z_1 + dz_1) \) with probability \( p(x_1)dz_1 \). This probability density was computed for several different forms of the surface height autocorrelation function \( W(|z_1|) = \langle \zeta(x_1)\zeta(0) \rangle / \langle \zeta^2(x_1) \rangle \). Physical features of these forms of \( W(|z_1|) \) were related to properties of the resulting probability density functions \( p(x_1) \).

In this paper we extend the simulation calculations of Maradudin and Michel to determine three probability density functions \( P_1(x), P_2(x), \) and \( P_3(x) \) for a two-dimensional randomly rough surface. The probability density function \( P_1(x)(P_2(x)) \) is defined such that if the surface has a maximum (minimum) at the origin, \( x_1 = x_2 = 0 \), the probability that the nearest maximum (minimum) to it lies a distance between \( z \) and \( z + dz \) away from it in the \( x_1, x_2 \)-plane is \( P_1(x)dz \) (\( P_2(x)dz \)). The probability density function \( P_3(x) \) is defined such that if the surface has a maximum at \( x_1 = x_2 = 0 \), the probability that the nearest minimum to it lies a distance between \( z \) and \( z + dz \) away from it in the \( x_1, x_2 \)-plane is \( P_3(z)dz \). Because the two-dimensional surfaces for which these functions are calculated are assumed to be isotropic, \( P_j(x)(j = 1, 2, 3) \) is a function of \( x_3 \) and \( x_2 \) only through the combination \( z = (x_1^2 + x_2^2)^{3} \), and we have indicated this in our notation. In what follows we will be concerned with the functions \( P_j(x)(j = 1, 2, 3) \).

We also note that from symmetry considerations the functions \( P_1(x) \) and \( P_3(x) \) are expected to be identical. The degree to which this requirement is satisfied by our numerical results is a measure of their accuracy.
A two-dimensional surface defined by \( z_2 = \zeta(z_1) \), where \( \zeta(z_1) \) is a single-valued function of \( z_1 \) and constitutes a zero-mean, stationary, isotropic, Gaussian random process can be generated numerically in the following way. The \( z_1 \)- and \( z_2 \)-axes are discretized into segments of length \( \Delta z \) so that a mesh is formed in the \( z_1, z_2 \)-plane. The points of this mesh are given by the vectors \( \vec{z}(m, n) = (m \Delta z, n \Delta z) \) with \( m, n = 0, \pm 1, \pm 2, \ldots \). With each site \( m, n \) of this mesh we associate an independent, zero-mean, Gaussianly distributed random number \( X_{m, n} \) with a standard deviation of unity, so that

\[
X_{m, n} = 0 \quad \text{(3a)}
\]
\[
X_{m, n} X_{m', n'} = \delta_{mn} \delta_{mn'} \quad \text{(3b)}
\]

The surface profile function at the point \( \vec{z}(m, n) \) is then written in the form

\[
\zeta(\vec{z}(m, n)) = \sigma \sum_{\ell} W_{\ell, \ell} X_{m+\ell, n-\ell} \quad \text{(4)}
\]

where the weight \( W_{m, n} \) is given by

\[
W_{m, n} = \Delta z \int \frac{d^2 \vec{q}}{(2\pi)^2} g^2(|\vec{q}|) e^{i\vec{q}\cdot \vec{z}(m, n)} \quad \text{(5)}
\]

and \( g(|\vec{q}|) \) is the power spectrum of the surface roughness.

\[
g(|\vec{q}|) = \int d^2 \vec{z} W(|\vec{z}|) e^{-i\vec{q}\cdot \vec{z}} \quad \text{(6)}
\]

The generating functional of the random process \( \zeta(\vec{z}) \) is defined by

\[
\Phi[\zeta] = \exp \left\{ \int d^2 \vec{z} \zeta(\vec{z}) \right\} \quad \text{(7)}
\]

With the aid of the result that for any reasonable function \( f(\vec{z}) \)

\[
\sum_{m, n} f(\vec{z}(m, n)) = \frac{1}{\Delta z^2} \int f(\vec{z}) d^2 \vec{z} \quad \text{(8)}
\]

in the limit as \( \Delta z \to 0 \) and the assumption that the \( \{X_{m, n}\} \) are independent, zero-mean, Gaussianly distributed random numbers with a standard deviation of unity, we find that

\[
\Phi[\zeta] = \exp \left\{ -\frac{1}{2} \sigma^2 \int d^2 \vec{z} d^2 \vec{z}' \zeta(\vec{z}) W(|\vec{z} - \vec{z}'|) \zeta(\vec{z}') \right\} \quad \text{(9)}
\]

which is the generating functional for a Gaussian random process defined by Eqs. (1).^4

3. RESULTS

We have used the algorithm defined by Eqs. (3)-(6) to generate a single Gaussian random surface whose profile function satisfies Eqs. (1). The position of each maximum on it was determined, as well as the distances to its nearest maxima and minima. Similarly, the position of each minimum on the surface was determined, together with
the distances to its nearest minima and maxima. Histograms giving the number of nearest maxima as a function of distance from a given maximum, the number of nearest minima as a function of distance from a given minimum, and the number of nearest minima as a function of the distance from a given maximum, were constructed. These calculations were repeated for \( N \) different realizations of the surface, all with the same statistical properties, and the histograms obtained were averaged over the results for these realizations. Suitably normalized, they provide the functions \( P_1(x) \), \( P_2(x) \), and \( P_3(x) \). In the results presented below we used \( N = 6000 \), \( N = 4000 \), and \( N = 1200 \) different surfaces to generate the distributions plotted in Figs. 1, 2, 3 respectively.

These calculations were carried out for two-dimensional random surfaces generated on the basis of three different forms of the surface height autocorrelation function \( W(r) \).

\[
W(r) = \exp(-x^2/a^2) \quad \text{(10a)}
\]

\[
W(r) = a^2 (x^2 - a^2) \quad \text{(10b)}
\]

\[
W(r) = \frac{2}{k_1^2 - k_2^2} \left[ k_2 J_1(k_2 x) - k_1 J_1(k_1 x) \right] \quad \text{(10c)}
\]

where \( J_1(z) \) is a Bessel function. The random surface characterized by the surface height autocorrelation function \( W(r) \) has recently been proposed as one that should be of interest in studies of the enhanced backscattering of light from two-dimensional randomly rough surfaces caused by the surface plasmon polariton mechanism. The values of the wave numbers \( k_1 \) and \( k_2 \) entering Eq. (10c) are given by

\[
k_1 = k_{pp}(\omega) - \frac{2\pi}{c} \sin \theta_{max} \quad \text{(11a)}
\]

\[
k_2 = k_{pp}(\omega) - \frac{2\pi}{c} \sin \theta_{max} \quad \text{(11b)}
\]

where \( k_{pp}(\omega) = (\omega/c) \text{Re} [\varepsilon(\omega)/\varepsilon(\omega) - 1] \) is the wave number of the surface plasmon polariton whose frequency equals that of the incident light, supported by the vacuum-metal interface in the absence of the random roughness.

The power spectra \( g_1(|\eta|) \) corresponding to the autocorrelation functions (10) are given by

\[
g_1(|\eta|) = \frac{\pi a^2 \exp(-a^2 |\eta|^2/4)}{12a}
\]

\[
g_2(|\eta|) = 2\pi a^2 K_0(|\eta|) \quad \text{(12b)}
\]

\[
g_3(|\eta|) = \frac{4\pi}{k_2^2 - k_1^2} \theta(q - k_1) \theta(k_2 - q) \quad \text{(12c)}
\]

respectively, where \( K_0(|\eta|) \) is a modified Bessel function, and \( \theta(z) \) is the Heaviside unit step function.

In obtaining the results presented below for the surfaces defined by Eqs. (10a,b) and (12a,b) we have measured all lengths in units of the characteristic length \( a \), appearing in these expressions, and have taken \( \Delta z = 0.05a \). The functions \( P_1(x) \), \( P_2(x) \), and \( P_3(x) \) were obtained by considering an \( L \times L \) portion of the \( x_1 x_2 \)-plane, with \( L = 7a \). In the case of the surface defined by Eqs. (10c) and (12c), in which no characteristic length appears explicitly, we have measured all lengths in units of \( b = (2k_1(k_2 - k_1))^{-1/2} \), and have taken \( \Delta z = 0.55b \). The functions \( P_1(x) \), \( P_2(x) \), and \( P_3(x) \) were obtained by considering an \( L \times L \) portion of the \( x_1 x_2 \)-plane with \( L = 7.7b \).
In Fig. 1 we present results for the probability density $P_1(z)$, $P_2(z)$, and $P_3(z)$ for a random surface characterized by the height autocorrelation function $C_x$. As we have noted earlier, the results for $P_1(z)$ and $P_2(z)$ should coincide, and we see from Figs. 1a and 1b that they are in fact in good agreement. The maxima of $P_1(z)$, $P_2(z)$, and $P_3(z)$, which give the most probable values of the corresponding separations, occur at $z = 1.675a$, $1.675a$, and $1.225a$, respectively. The average value of the distance $D_1 = D_2$ from a given maximum (minimum) to its nearest maximum (minimum) is given by

$$D_1 = \int_0^\infty dz x P_1(z).$$

For the random surface defined by Eqs. (10a) and (12a) these distances are $1.730a$, $1.730a$, and $1.400a$, respectively.
Figure 2. The initial (dashed curve) and calculated (solid curve) surface height autocorrelation functions for the two-dimensional random surface defined by Eq. (10a).

As a check on the accuracy of the ensemble of computer generated surfaces as a representation of a zero-mean Gaussian random process characterized by the height autocorrelation function $W(|z|)$ given by Eq. (10a), we used this ensemble of random surfaces to compute $W(|z|)$. In Fig. 2 we present a plot of $W(|z|)$ as a function of $z$ computed from the numerically generated surfaces (solid curve) and the function $W(|z|)$ used as the basis for their generation (dashed curve). The noise in the former curve decreases as $1/\sqrt{N}$ where $N$ is the number of generated surfaces used in computing $W(|z|)$. The result displayed in Fig. 2 was obtained from an ensemble of $N = 900$ surfaces.

The results for $P_1(z)$, $P_2(z)$, and $P_3(z)$ obtained for a random surface characterized by the surface height correlation function $W(|z|)$ given by Eq. (10b) are presented in Figs. 3a, 3b, and 3c, respectively. The maxima of these functions occur at $z = 1.025a$, $1.025a$, and $0.925a$, respectively. The values of $D_i z_j$ for this surface are $1.112a$, $1.088a$, and $0.964a$, respectively. For comparison, we plot in Fig. 4 $W(|z|)$ computed from the numerically generated surfaces (solid curve) and the function $W(|z|)$ used as the basis for their generation (dashed curve). To obtain the numerical results presented in Fig. 4 1200 numerically generated surfaces were used. Apart from the noise in the result for $W(|z|)$ computed from the numerically generated surfaces, it goes to zero with increasing $z$ more rapidly than the function $W(|z|)$ used as the basis for the generation of those surfaces, which is cut off in range by the limited size of the simulation region in the $z_1 z_2$-plane.

From the results presented in Figs. 1 and 3 we see that $P_i(z)$ as functions of $z$ exhibit maxima for $z$ of the order...
Figure 3. The probability density function \( p_{1}(x) \), \( p_{2}(x) \), and \( p_{3}(x) \) for the two-dimensional random surface defined by Eq. (10b).

For a. However, the values of \( x \) at which the maxima of \( P_{j}(x) \) computed on the basis of the Lorentzian height autocorrelation function (10b) occur are smaller than the values of \( x \) at which the maxima of the corresponding \( P_{j}(x) \) computed on the basis of the Gaussian autocorrelation function (10a) occur. For both choices of the surface height autocorrelation function the maximum in \( P_{3}(x) \) occurs at a smaller value of \( x \) than do the maxima in \( P_{1}(x) \) and \( P_{2}(x) \). The same can be said of the values of \( \langle D_{1,2,3} \rangle \) for these two surfaces.

In Figs. 5a, 5b, and 5c we present results for the probability densities \( P_{1}(x) \), \( P_{2}(x) \), and \( P_{3}(x) \), respectively, calculated for a random surface characterized by the surface height autocorrelation function (10c). In obtaining these results we assumed the values \( \lambda = 0.9 \text{nm} \), \( \epsilon_{\infty} = -7.7 - i0.24 \), and \( \delta_{\text{max}} = 10^{6} \) in calculating the values of \( x_{1} \) and \( k_{3} \) (Eqs. (11)) entering its definition. This value of the dielectric function is that of a silver surface at the wavelength quoted. The maxima of \( P_{1}(x) \), \( P_{2}(x) \), and \( P_{3}(x) \) occur at \( x = 0.3256 \), 0.3256, and 0.2256, respectively. The values of \( \langle D_{1,2,3} \rangle \) for this surface are found to be 0.3686, 0.3686, and 0.2486, respectively.

In Fig. 6 we compare the power spectrum \( g(\langle q \rangle) \) calculated from an ensemble of 600 random surfaces (solid curve) with the function \( g(|q|) \) used in generating that ensemble (dashed curve). The "wings" present in the results of the
Figure 4. The initial (dashed curve) and calculated (solid curve) surface height autocorrelation function for the two-dimensional random surface defined by Eq. (10b).

The simulation decrease with increasing \( L \) and are a consequence of the finite size of the region in the \( z_1 \) \( z_2 \)-plane used in the generation of the random surfaces.

In addition to the results presented above for the probability density functions \( P_1(x_1), P_2(x_1), \) and \( P_3(x_2) \), we now present the probability density function \( p(x_1) \), which is the probability that the nearest minimum to a given maximum is at a distance \( z \) from the latter. For a one-dimensional random surface that has been of interest recently in connection with experimental studies of the enhanced backscattering of light from one-dimensional random surfaces caused by the surface plasmon polariton mechanism. This surface is characterized by the surface height autocorrelation function

\[
W_l(x_1) = \frac{1}{k_2 - k_1} \left( \frac{\sin k_2 \xi_1}{\xi_1} - \frac{\sin k_1 \xi_1}{\xi_1} \right),
\]

whose power spectrum is

\[
\phi(\eta) = \frac{\pi}{k_2 - k_1} \theta(\eta - k_1) \theta(k_2 - \eta) \theta(k_2 - \eta - k_1) \theta(k_2 - \eta - k_1).
\]

The values of \( k_1 \) and \( k_2 \) are given by Eqs. (11).

The manner in which a one-dimensional surface profile function \( \xi(x_1) \) that constitutes a zero-mean, stationary Gaussian random process, can be generated numerically from a given surface height autocorrelation function \( W_l(x_1) \) is described, e.g. in Refs. 11 and 12. Methods for fabricating such surfaces in the laboratory are presented in Refs. 13.
Figure 5. The probability density function (a) $p_z(x)$, (b) $p_{xz}(z)$, and (c) $p_{x^2}(x)$ for the two-dimensional random surface defined by Eq. (10c).

and 14. In the calculations whose results are displayed in Figs. 7 and 8, we assumed that $\lambda = 512.7 \text{nm}$, $\phi_{\text{max}} = -9 - i1.29$, and $\gamma_{\text{max}} = 13.3^\circ$. These are the parameters that characterize the gold surface studied experimentally in Ref. 8.

The probability density function $p(x)$ for this surface was calculated by the approach used by Maradudin and Michel. The result is plotted in Fig. 7. It is seen to be sharply peaked about $\Delta k \approx \Delta k = 0.69$, and to have a full width at half-maximum of 0.1 units of $(\Delta k/2)^{-1}$. The average distance from a given maximum to its nearest minimum for these surfaces was found to be 0.612 in units of $(\Delta k/2)^{-1}$. As a check on this result, we can obtain an estimate of the value of $x$ at which the peak in $p(x)$ occurs if we consider that the power spectrum of the random surface, Eq. (15), is that of an almost periodic surface whose periodicity is defined by the wavenumber $k_{\text{av}} = \frac{1}{2}(k_1 + k_2)$. The distance between a maximum and its nearest minimum on such a surface, $\Delta x$, is given by $k_{\text{av}} \Delta x = \pi$. Consequently, we find that $\frac{1}{2} \Delta k \Delta x = \frac{1}{2} \Delta k/k_{\text{av}} = 0.69$, which is in reasonable agreement with the value 0.6 obtained from Fig. 7. In addition, a good estimate of the average distance between a given maximum and its nearest minimum on a one-dimensional random surface is provided by the reciprocal of the density of zeros $(d)$ of
Figure 6. The initial (dashed curve) and calculated (solid curve) power spectra for the two-dimensional random surface defined by Eq. (10c).

Figure 7. The probability density function $p(x)$ for the one-dimensional random surface defined by Eq. (14).
Figure 8. The initial (dashed curve) and calculated (solid curve) power spectra for the one-dimensional random surface defined by Eq. (14).

As an additional check on our numerical work, we present in Fig. 8 a plot of $g(k)$ as a function of $2k/(k_0-k)$ computed from numerically generated realizations of the surface defined by Eqs. (14)-(15), together with a plot of the power spectrum (15) used as input to these calculations. Good agreement is found between these two results for $g(k)$.

4. CONCLUSIONS

In conclusion, a method for generating numerically a two-dimensional, zero-mean, stationary, isotropic Gaussian random surface, defined by a specified surface height correlation function, or power spectrum, has been used to generate an ensemble of such surfaces for three different forms for the height autocorrelation function. From these results the probability density $P_1(z)/P_2(z)$ for finding the nearest maximum (minimum) to a given maximum (minimum) at a distance $z$ from the latter, as well as the probability density $P_3(z)$ for finding the nearest minimum to a given maximum at a distance $z$ from the latter, were calculated. The maxima of these functions are found to occur at values of $z$ that are of the order of the transverse correlation length $\sigma$ of the surface roughness for surfaces defined by the Gaussian and Lorentzian surface height autocorrelation functions (10a) and (10b) respectively. A determination of the probability density function $p(z)$ for a one-dimensional random surface defined by the West-O'Donnell power spectrum (15) was also carried out. The position of its maximum was explained by regarding this surface as almost periodic.
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Appendix E

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Determination of surface profile statistics from electromagnetic scattering data

V. Malyshekin, S. Simeonov, and A. R. McGurn

Department of Physics. Western Michigan University. Kalamazoo. Michigan 49008

A. A. Maradudin

Department of Physics and Astronomy and Institute for Surface and Interface Science.
University of California. Irvine. Irvine. California 92697

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A new reverse Monte Carlo method for the determination of the surface profile statistics from differential reflection data was recently developed and applied to the atomic arrangement in these materials. In this Letter we present a new application of RMC ideas, namely, the determination of the power spectrum of a randomly rough surface from the differential reflection coefficient of electromagnetic radiation scattered from such a surface. E.g., from far-field scattering from such a surface, i.e., from far-field experimental data.

We consider a randomly rough surface defined by \( x_2 = (x_2, \alpha, \beta) \). The surface profile function is assumed to be a single-valued function of \( x_2 \) that is differentiable as many times as is necessary and that constitutes a stationary, zero-mean, isotropic, Gaussian random process defined by \( \langle \gamma(x_2) \gamma(x_2') \rangle = \delta^2 W(x_2 - x_2') \). The angle brackets denote an average over the ensemble of realizations of the surface profile function, and \( \delta = \langle \gamma^2(x_2) \rangle^{1/2} \) is the rms height of the surface. The power spectrum of the surface roughness is defined as \( g_{kk}(k) = \int \int d^2 x_2 W(x_2) \exp(-i k \cdot x_2) \), where \( k_4 = (k_1, k_2, 0) \).

The contribution to the mean differential reflection coefficient (mdrc) from the diffuse component of the light scattered from such surfaces depends explicitly on \( g_{kk}(k) \) in those cases when the roughness is weak enough that the mdrc can be calculated perturbatively, with the necessary ensemble averages evaluated analytically.\(^2\)\(^3\) It depends implicitly on \( g_{kk}(k) \) when the roughness is strong enough that a computer simulation approach to its evaluation is required.\(^4\)\(^5\)

The RMC method when applied to scattering data from either type of surface works as follows. Let \( [dR_{\alpha, \beta}(\Omega, \Omega_\alpha, \Omega_\beta)/d\Omega_\alpha]_{\exp} \) be the experimental data for the contribution to the mdrc from the diffuse component of the scattered electromagnetic waves when electromagnetic waves of polarization \( \alpha \) and angles of incidence \( \Omega_\alpha \) are scattered into waves of polarization \( \beta \) and scattering angles \( \Omega_\beta \). Let \( g_0(k_4) \) be an initial guess at the power spectrum, and let \( [dR_{\alpha, \beta}(\Omega, \Omega_\alpha, \Omega_\beta)/d\Omega_\alpha]_{\exp} \) be the contribution to the mdrc computed by theory or computer simulation from \( g_0(k_4) \). Next compute

\[
\begin{align*}
\rho_0 &= \sum \sum \int d\Omega_\alpha [\sigma(\Omega, \Omega_\alpha)\Omega_\beta]|^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 - \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp} \\
\end{align*}
\]

where \( [\sigma(\Omega, \Omega_\alpha, \Omega_\beta)]^2 \) is the variance of the experimental data about their mean. The sum on \( \Omega_\alpha \) allows for the use of scattering data from more than one angle of incidence. The exact power spectrum \( g_0(k_4) \) gives \( \rho_0 = 0 \) when it is substituted into the RMC method as a guess.\(^1\) A random change is then made in \( g_0(k_4) \) to create a new guess power spectrum \( g_1(k_4) \), which yields a new differential reflection coefficient \( [dR_{\alpha, \beta}(\Omega, \Omega_\alpha, \Omega_\beta)/d\Omega_\alpha]_{\exp} \), and

\[
\begin{align*}
\rho_1 &= \sum \sum \int d\Omega_\alpha [\sigma(\Omega, \Omega_\alpha)\Omega_\beta]|^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 - \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp}^2 \left\{ \frac{dR_{\alpha, \beta}(\Omega, \Omega_\alpha)}{d\Omega_\alpha} \right\}_{\exp} \\
\end{align*}
\]

If \( \chi_1 < \chi_0 \) then \( g_1(k_4) \) is retained over \( g_0(k_4) \) as a good guess for the power spectrum. If \( \chi_1 \geq \chi_0 \) then \( g_1(k_4) \) is retained over \( g_0(k_4) \) with probability \( p = \exp(-\rho_1 - \rho_0) \). This last step keeps the system from becoming stuck in a local minimum of \( \chi_1 \) and is based on maximum entropy\(^7\) methods, which choose the most probable solution for \( g(k_4) \) consistent with the experimental data. Otherwise, \( g_0(k_4) \) is retained. The above process is repeated until \( [dR_{\alpha, \beta}(\Omega, \Omega_\alpha, \Omega_\beta)/d\Omega_\alpha]_{\exp} \)
agrees with $dR_p(\theta, \phi)/d\Omega$, from theory, i.e., $\gamma_1$ is smaller than its value computed from the experimental error in the mdr. The final guess for $g(k)$ is taken to represent the true power spectrum. In view of the Monte Carlo sampling on which the RMC method is based, we suspect that it converges to the true power spectrum with an error that decreases inversely with the square root of the number of Monte Carlo comparisons used.

Here we apply the method just described to the determination of the power spectrum of weakly rough, one-dimensional, random metal surfaces [i.e., surfaces for which (x,y) is independent of z], for which an analytic expression for the mdr in terms of the power spectrum exists. The expression has been obtained by an infinite-order perturbative calculation in the small-roughness approximation. The plane of incidence is assumed to be the x-z plane, and the incident light is p polarized. In this scattering geometry there is no cross-polarized scattering. The contribution to the mdr from the diffuse component of the scattered light is related to the power spectrum $g(k)$ by

$$g(k, \gamma) / g(k, \gamma)_{\text{diff}} = \frac{\omega}{4\pi c} \cos \gamma \left[ e^{i2\gamma q(k)} - 1 \right],$$

where $q = (\omega/c)\sin\gamma$, $k = (\omega/c)\sin\gamma$, and $\omega(q(k))$ are given by Eqs. (35) and (45) of Ref. 2. $K(q(k))$ in Eq. (3) of Ref. 2 is defined by $K(q(k)) = \delta^2 (\gamma - k) [2(i\omega - i\gamma) / c + \alpha] + i\omega q(k) \gamma$, where $e^{i\omega q(k)}$ is the dielectric function of the metal: $q(k) = \alpha q(k) - \psi(k)$, with $\psi(k)$ the phase of the complex frequency $\omega q(k)$. $\alpha q(k)$ is used to normalize the power spectrum for $g(k)$ and does not affect the RMC calculation of $g(k)$. For $k > 0$, $\alpha q(k) > 0$, and $\Delta_{\gamma}$ in Eqs. (35) and (45) of Ref. 2 is defined by $\Delta_{\gamma} = 2\delta^{3/2} \left[ C_{\gamma} q(k) - (i\omega - i\gamma) \right]^2, \Delta_{\gamma} = 2\delta^{3/2} \left[ C_{\gamma} q(k) - (i\omega - i\gamma) \right]^2$, and $e^{i\omega q(k)} = \Re e e^{i\omega q(k)}$. We have used the theoretical results of Eq. (3) to generate experimental mdr data for the scattering of p-polarized light of wavelength $\lambda = 512 \mu m$ incident at 0°, 10°, and 18° from the normal to the mean surface. The surface was fabricated in a manner that ensured that the surface profile would be Gaussian statistics.

As the surface studied in Ref. 11 is a weakly rough surface, we used in our RMC method the perturbation theory of McGurn et al. to express the differential reflection coefficient in terms of the guessed $g(k)$. In Fig. 2 we present the results in dimensionless units for $g(k)$ versus $kq$ obtained in Ref. 11 by contact profilometry and by our application of the RMC method discussed above. The RMC result for $g(k)$ was obtained by use of the scatter data in Fig. 3 of Ref. 11 for angles of incidence $\theta = 10°, 13°, 15°$. Again, the initial guess for $g(k)$ was taken to be $g(k) = 0$, and 20,000 Monte Carlo comparisons were available. In such cases, by trial and error we

![Fig. 1. Plot of $\gamma k$ versus $kq$. The curves shown are for the experimental power spectrum. The dashed curve $\gamma k = 0.76 \sqrt{\alpha} \exp(-kq^2/\alpha)$ and for the RMC extraction of it (solid curve).](image-url)
choose $r$ small enough to reproduce the published data closely but large enough to allow the maximum entropy component of our computer routine to operate efficiently. In the present case we chose $r(\theta, \leq 90^\circ, \theta, = 10^{-6} \text{rad}^{-1}$ and $r(\theta, \geq 90^\circ, \theta, = 10^{-5} \text{rad}^{-1}$). Scattering data for $\theta, = 10^\circ, 18^\circ$ were necessary for accurate RMC results for $g(\hat{k})$.

Although clearly much can be done to improve the efficiency of the method, we have demonstrated how RMC techniques can be used to extract the power spectrum of a randomly rough surface from measured results for the mdr. light scattered diffusely from randomly rough surfaces. Existing methods for obtaining the power spectrum from diffuse scattering data [see, e.g., Ref. 12] are based on a single-scattering approximation to the mdr., which could not be used in reconstructing the West-O'Donnell power spectrum because it produces surfaces from which single-scattering processes are largely suppressed. The RMC method in the present study is based on a theory that includes the multiple scattering of surface waves. As a result, the power spectrum $g(\hat{k})$ can be obtained for a larger range of $\hat{k}$ than is possible with a single-scattering theory.

In addition, the RMC method contains two important improvements over routines that compute $g(\hat{k})$ by a straightforward minimization of $\gamma$ (Ref. 13): (1) the Monte Carlo component of the RMC offers an efficient way to minimize $\gamma$ approximately and (2) the maximum entropy component of the RMC sorts out from all the local minima of $\gamma$ the most probable solution for $g(\hat{k})$. In this regard, the more scattering data (more experimental points and more angles of incidence) used, the more probable is the agreement of the $g(\hat{k})$ computed by the RMC with the actual $g(\hat{k})$.

It is important along with a study of the convergence of the RMC routine itself to study the change in the computed $g(\hat{k})$ as data from additional angles of incidence are added. Data from two angles of incidence were needed to achieve the accuracy displayed in the figures. The use of data taken at more angles of incidence should improve the computed $g(\hat{k})$.

The method that we have presented is readily generalized to treat surfaces that are defined by surface profile functions that are not Gaussian random processes. One generalization of the RMC method described here that we are currently pursuing is the extraction of deterministic surface profiles from scattering data. Here the differential reflection coefficient is expressed in terms of the surface profile function $\gamma(x)$, and the random guesses in the RMC method are made of $\gamma(x)$ rather than of the power spectrum as in the random surface RMC.

When an analytic result for $\gamma(R \theta, \theta, \theta, \omega)$ is not available, the RMC method can still be used to determine the power spectrum $g(\hat{k})$, at the expense of additional computational effort. For each choice of $g(\hat{k})$ an ensemble of several hundred profiles would have to be generated by a standard method. The results for $\gamma(R \theta, \theta, \omega)$, for each member of the ensemble would have to be averaged, and the result would have to be used in the RMC algorithm.

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*Permanent address, A. F. Ioffe Physical Technical Institute, 194021 St. Petersburg, Russia.

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