Comparison of the Kirchhoff and Rayleigh-Rice diffractions for sinusoidal surfaces

by Tod Forrest Schiff

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Electrical Engineering
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Abstract:
This thesis examines the requirements for reflector scatter measurements (BRDF scans) that are imposed when scatter data is used to calculate reflector surface statistics (roughness and slope). There are many different theories that one can use to perform these calculations. Each theory has advantages and disadvantages, depending on the surface and measurements made. Two theories, Kirchhoff and Rayleigh/Rice, are emphasized since they are the most commonly known and used. Kirchhoffs theory yields better results for rougher surfaces, but fails at larger angles of scatter measurements. The Rayleigh-Rice theory performs best at larger angles, but fails for rougher surfaces. New applications require that rougher surfaces and larger angles are to be measured, and that reliable surface statistics be calculated from the results. This raises the issue of which theory to use. By measuring a known surface (sinusoidal in this case), comparisons can be made between predicted and measured results for the two theories. Techniques to improve the measurement conditions and accuracy of the results are described. The samples appear smoother for both theories if the wavelength of the incident light is increased. Increasing the incident angle improves the results for Rayleigh/Rice on rougher surfaces, but causes problems for Kirchhoff due to the increase in the scatter angle.

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ABSTRACT

This thesis examines the requirements for reflector scatter measurements (BRDF scans) that are imposed when scatter data is used to calculate reflector surface statistics (roughness and slope). There are many different theories that one can use to perform these calculations. Each theory has advantages and disadvantages, depending on the surface and measurements made. Two theories, Kirchhoff and Rayleigh/Rice, are emphasized since they are the most commonly known and used. Kirchhoff's theory yields better results for rougher surfaces, but fails at larger angles of scatter measurements. The Rayleigh-Rice theory performs best at larger angles, but fails for rougher surfaces. New applications require that rougher surfaces and larger angles are to be measured, and that reliable surface statistics be calculated from the results. This raises the issue of which theory to use. By measuring a known surface (sinusoidal in this case), comparisons can be made between predicted and measured results for the two theories. Techniques to improve the measurement conditions and accuracy of the results are described. The samples appear smoother for both theories if the wavelength of the incident light is increased. Increasing the incident angle improves the results for Rayleigh/Rice on rougher surfaces, but causes problems for Kirchhoff due to the increase in the scatter angle.

CHAPTER 1

INTRODUCTION

For centuries man has made use of optics in a variety of instruments. As optics improved, the quality and performance of the instruments have become better. But the optics used, even today, are not perfect and tend to cause distortion in the image that passes through them. Scattering of light occurs that can cause a loss of power, a reduction in resolution, or an increase in the optical noise of a system. The rougher the surface of the optic, the more light that will be scattered from it.

It becomes important to measure this scatter and determine better processes to improve the quality of the optics. If a relationship between the surface and the scattered light were known, one could quantitatively describe the features of the optic, thus giving a basis for fabrication standards. This same technique would find use in the characterization of many other types of materials, as well as optical components.

Scatter can be distributed anywhere in the entire observation sphere centered about the sample. The intensity of light within the scatter sphere is dependent on incident angle and wavelength as well as sample parameters such as orientation, transmittance, reflectance, absorptance, surface finish, etc. The bidirectional distribution reflectance function, BRDF[1,2], is the term commonly used to describe scattered light patterns from reflective samples. Since the BRDF format is a common form of scatter characterization and can be used to quantify surface specifications, it is worthwhile to understand its mathematical expression.

The derivation of BRDF is credited to F. E. Nicodemus[3]. A complete derivation is not given since only an understanding of the parameters is required. Equation (1) is the BRDF expression derived by Nicodemus for describing reflective scattering. Figure 1 shows the defining geometry of the sample and incident beam. The subscript i is used for the incident quantities while the subscript s is for the scattered.

BRDF can be defined in radiometric terms as the scattered surface radiance (watts/m^{2}sr) divided by the incident surface irradiance. The incident irradiance is the light flux (watts) on the surface per unit area of illuminated surface. The scattered radiance is the light flux (watts) scattered per unit solid angle (sr) per unit projected illuminated surface area (A). The projected illuminated surface area is the illuminated surface area, A, multiplied by cosθ_s.

$$\mathrm{BRDF} \equiv \frac{\dfrac{(dP_s/d\Omega_s)}{(A\cos\theta_s)}}{P_i/A} = \frac{dP_s/d\Omega_s}{P_i\cos\theta_s} \approx \frac{P_s/\Omega_s}{P_i\cos\theta_s} \qquad (1)$$

Ω_s - Solid angle defined by the detector aperture

θ_i - Angle of incidence measured from surface normal

θ_s - Angle of detector measured from surface normal

P_i - Incident power irradiating the sample

P_s - Radiant power measured through the detector aperture

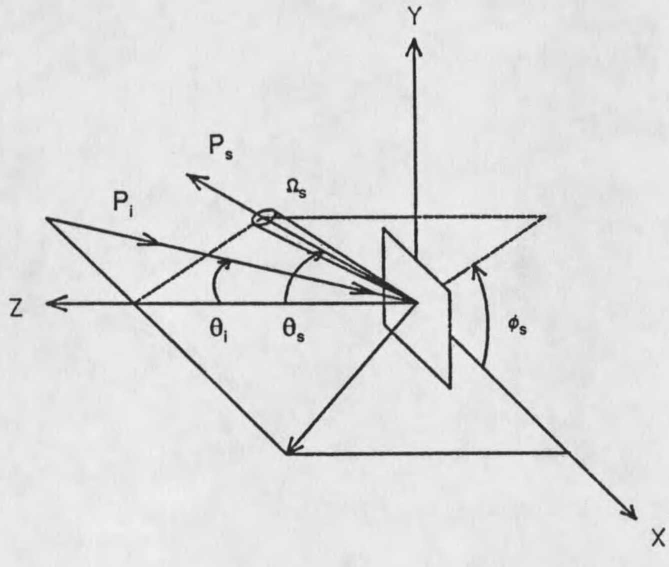


Figure 1. Geometry for the definition of BRDF.

Another useful expression for describing the surface topography of a sample is the power spectral density function (PSD). Characteristics of the surface, such as amplitude and slope, can be derived from the PSD. The conversion of the bidirectional reflectance distribution function (BRDF) into the reflective surface power spectral density (PSD) may be accomplished via several diffraction theories[4-10] providing that the sample has the following properties;

1) It must be a front surface reflector meaning that the scatter is due only to the surface and not to sub-surface or bulk scattering.
2) The sample must also be clean, implying that the scatter is not due to surface contaminants.
3) The surface must be smooth.

The first two criteria are necessary to assure that the scatter signal is dominated by surface topography. The third requirement, and the one that is the focus of this thesis, is a result of the diffraction theories that are used to convert the BRDF to surface topography information (ie: the PSD, rms roughness, slope, etc.). A "smooth surface" may be loosely defined as one for which the rms roughness is much less than a wavelength of the incident light (i.e. $\sigma << \lambda$, where $\sigma = .707a$; see Equation (2)). This means that for visible light, surfaces are restricted to those of mirror-like quality. But there are also industrial processes, involving surfaces that are considered much rougher than mirrors, for which a non-contact roughness measurement is desirable.[12] The work reported here examines how accurately two of the diffraction theories behave for various degrees of sample surface roughness, as well as measurement techniques that can be used to make the sample appear "smooth" so that each theory holds.

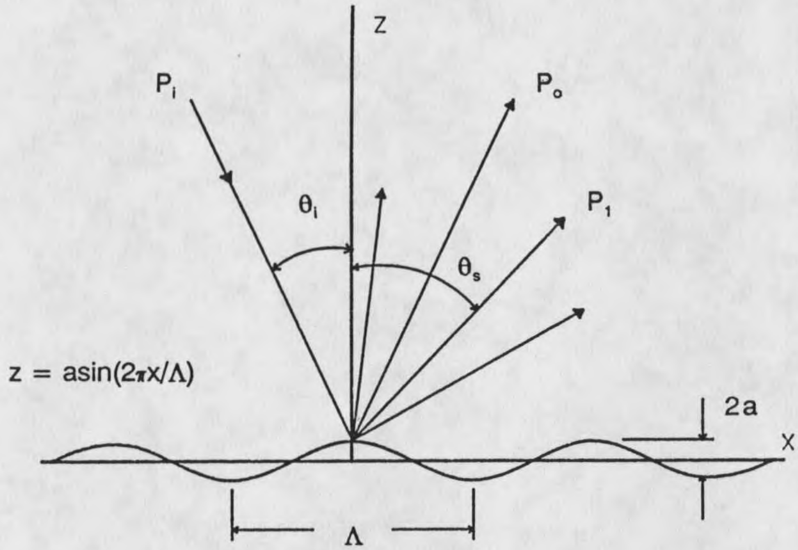
A sample's smoothness is generally stated in terms of the Rayleigh criterion;[4]

$$(4\pi a/\lambda)\cos\theta_i << 1 \qquad (2)$$

a - surface peak amplitude

λ - wavelength of incident light

Figure 2 shows the sample geometry for the parameters of Equation 2 as related to a sinusoidal grating surface with amplitude a and line spacing Λ.



P_1 - power in diffracted first order

P_o - power in diffracted zeroth order

Λ - sinusoidal surface spatial wavelength

Figure 2. Diffraction from a sinusoidal grating surface.

The relationship between the incident light angle and the scattered light angle is commonly known as the grating equation. This expression, shown as Equation (3) below, yields accurate information independently of how rough a surface is. The location of the diffracted orders can be found if the angle of incidence, as well as the light wavelength and surface spatial wavelength, are known.

$$\sin(\theta_s) = \sin(\theta_i) + m\lambda/\Lambda \quad , \quad m = +/- \ 1,2,3,... \qquad (3)$$

m - diffracted order

According to Equation (2) there are two ways to make reflectors appear smoother. The first is to increase θ_i, thus causing $\cos\theta_i$ to get smaller. The second is to increase the wavelength (λ) of the incident light. Because the wavelength increases by over an order from mid-visible (.633 μm) to mid-IR (10.6 μm) and because $\cos\theta_i$ decreases by an order as the incident angle is changed from zero to eighty four degrees, it should be possible to extend the measurement technique to surfaces that are far from optically smooth (i.e. larger amplitudes; see Equation 2) by varying one or both of these. Several questions arise. First of all, what is meant by "much less than" when referring to the smooth surface limit in Equation (2), and is it different depending on the diffraction theory used? Which diffraction theory is best at converting scatter data to surface statistics? Is it more effective to increase the incident angle or the wavelength to make a surface appear smoother? Do these improvements depend on the theory used? These are questions that will be addressed in this thesis.

The approach to answering these questions was to first compare two different theories that are used to convert scatter measurements into surface statistics and determine how they behaved for different conditions. This was done using sinusoidal gratings of varying amplitude and spatial wavelength for which the surface statistics are known. Care was used in handling the samples so they remained clean, front surface reflectors. Comparisons are given for each that describe theoretically how the results obtained correlate to the actual parameters for various incident angles and wavelengths.

The next section gives a basic description of the experiment and the equipment used. A complete listing of the measured results is presented. The experimental results are then compared to the expected results using various techniques including graphical presentations. Finally, conclusions stemming from these comparisons are presented and the previous questions answered.

CHAPTER 2

DIFFRACTION THEORIES

Two of the theories that can be used to convert BRDF measurements into surface statistics are the Rayleigh/Rice Vector Perturbation Theory and the Kirchhoff Scaler Theory. For small angles of incidence and scatter, both theories give essentially the same results. This can be demonstrated after each theory's mathematical expression is given. It should be noted that there are several other approaches that could be used for extracting surface statistics from BRDF measurements, but the two studied here are the most common.

Rayleigh/Rice Vector Perturbation Theory

This theory[5-7] takes polarization of the incident and scattered light into account. For s polarization used in this experiment (polarization vector normal to the plane defined by the surface normal and propagation direction), the theory states that the power in the diffracted first order divided by the power in the diffracted zeroth order is given by Equation (4) below. This expression is commonly refered to as the grating efficiency. The reflectance of the sample has been assumed to be one, thus implying that all of the incident light power (P_i) is reflected off the surface.

$$\rho_r(\theta_i) = P_1/P_o = (2\pi a/\lambda)^2 \cos\theta_i \cos\theta_s \qquad (4)$$

ρ_r - grating efficiency for Rayleigh/Rice

This theory was developed on the basis of the boundary conditions for a perfectly conducting surface. The power spectrum of a smooth surface was used yielding an exact function for the scattering based on different polarizations. Excellent agreement with experimental data has been reported for this theory at visible wavelengths on smooth surfaces.[8-10]

Since the theory was developed assuming that the surface is "smooth", it would be expected that the theory would not hold true for "rough" surfaces. The following has been used for the criterion of smoothness;[11]

$$\frac{a_{mr}}{\lambda} \leq \frac{.05}{\pi(\cos\theta_i)} \qquad (5)$$

a_{mr} - maximum surface amplitude (Rayleigh/Rice)

Equation (5) can be used to find the maximum surface amplitude that can be measured accurately using this theory. For surfaces with larger amplitudes (roughness), the obtained results would be expected to be in error.

Notice that Equation (5) does not contain the scattering angle as a factor. Since no assumptions were made regarding this angle in the development of the theory,[5-7,11] there is no reason it should appear. Therefore, one might anticipate the Rayleigh/Rice method of calculating surface statistics to give results that are precise and independent of the scattering angle being measured (assuming the surface is smooth).

Kirchhoff Scalar Theory

This theory was developed from a scalar analysis that does not take into account the polarity of the light[4]. Results are given in terms of Bessel functions of the first kind. These can be simplified if the sample is assumed to be "smooth". Both cases are shown below in the expression for the grating efficiency.

$$\rho_b(\theta_i) = P_1/P_0 = \frac{[\ (1 + \cos\theta_i + \theta_s) \qquad J_1(s)]^2}{[(\cos\theta_i + \cos\theta_s\cos\theta_i) \quad J_0(s)]^2} \tag{6}$$

$$s = (2\pi a/\lambda)(\cos\theta_i + \cos\theta_s)$$

If the assumption is made that $s \leq 0.5$, then $J_1(s)/J_0(s) \approx s/2$. Equation (7) is a result of this assumption and provides a limitation on the maximum surface amplitude. The grating efficiency in Equation (6) can then be simplified to Equation (8). The maximum amplitude for the Kirchhoff theory is seen to be greater than that for the Rayleigh/Rice theory.

$$\frac{a_{mk}}{\lambda} \leq \frac{.25}{\pi(\cos\theta_i + \cos\theta_s)} \tag{7}$$

a_{mk} - maximum surface amplitude (Kirchhoff)

$$\rho_b(\theta_i) = (2\pi a/\lambda)^2 \frac{[1 + \cos(\theta_i + \theta_s)]^2}{[2\cos\theta_i]^2} \tag{8}$$

This theory was developed by doing an evaluation of the Kirchhoff diffraction integral, which is inadequate at high scattering angles.[4] It has been shown that the Kirchhoff diffraction theory fails when the relationship shown in Equation (9) cannot be met;[11]

$$\frac{a_{mk}}{\lambda} \leq \frac{.025}{\pi(\tan^2\theta_s)} \tag{9}$$

It would be expected that poor results would be obtained for high scattering angles and high frequency roughness (small spatial wavelength, which yields large scattering angles, as shown by Equation (3)). A surface that may appear smooth via Equation (7) could be in violation of Equation (9) if θ_s is too large. But if the scattering angle is small, Kirchhoff should give better results than Rayleigh/Rice for slightly rougher surfaces.

Comparison of Theories

Figure 3 contrasts the expected accuracy of the two theoretical expressions with respect to the scattering angle (θ_s) and the amplitude/wavelength ratio (a/λ). Each of the limiting relationships for the two theories are plotted and the regions of acceptable measurements are indicated. For Rayleigh/Rice, the $\cos\theta_i$ term is combined with a_{mr} and this new factor $a_{mr}(\cos\theta_i)$ is divided by the wavelength and plotted against θ_s.

The Kirchhoff conditional Equation (7) has both the incident angle and the scattering angle as factors. This equation only becomes important at small angles of scatter, since Equation (9) is the limiting factor for higher scattering angles. Thus, the $\cos\theta_s$ term is approximately one when the scattering angle is small. By combining this term with a_{mk}, a new factor $a_{mk}(\cos\theta_i + 1)$ is divided by the wavelength, λ. This expression, and Equation (9), when plotted against θ_s, can be used to find the acceptable Kirchhoff region on Figure 3.

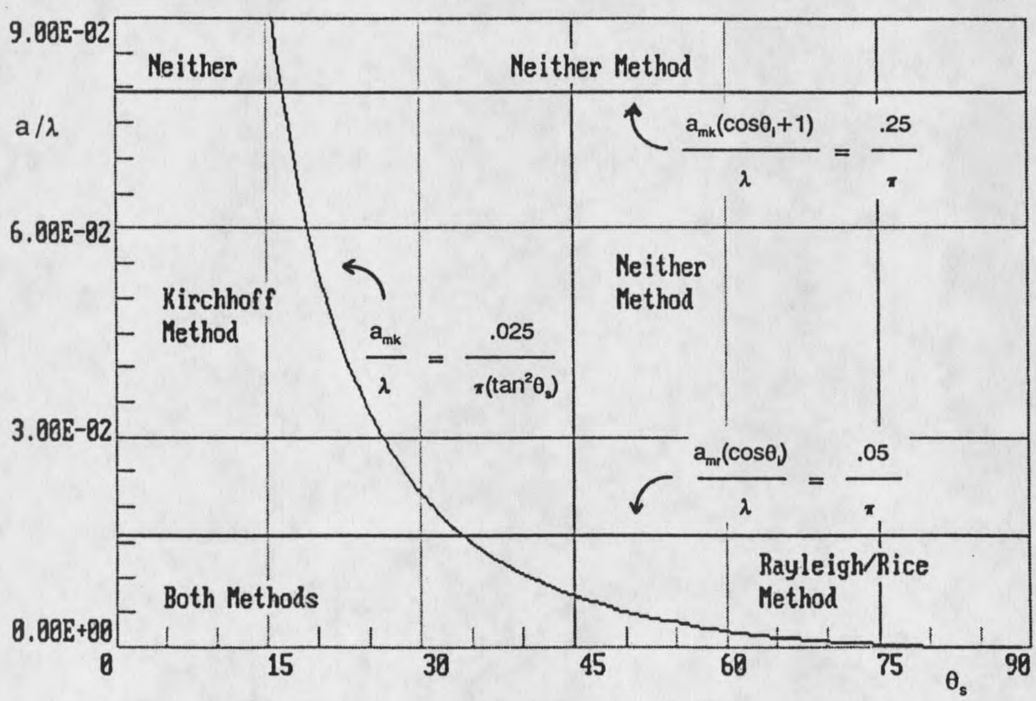


Figure 3. Comparison of theoretical models for increase in amplitude and scatter angle.

Figure 3 gives a visual comparison on how the two theories relate to each other. If the incident angle is known, this plot can be used to find the acceptable range of amplitudes and scattering angles for each theory.

One of the objectives of this work was to find ways to make a surface appear smoother and extend the roughness values allowed for calculation. By increasing the incident angle, both Equations (7) and (9) indicate that a larger surface amplitude can be measured for both theories. But increasing the incident angle also causes the scatter angle to increase, as noted by Equation (3). For the Rayleigh/Rice theory, this does not pose a problem, so it might be expected that an increased angle of incidence will yield more accurate results for rougher surfaces. The Kirchhoff theory, on the other hand, gives poor results if the scatter angle is too large, thus implying that an increase in θ_i could produce information even more inaccurate. This can be seen in Figure 3, which shows an increasing θ_s to have the predominate effect of limiting the maximum amplitude attainable with the Kirchhoff method.

Another way of improving the largest surface amplitude that can be measured is to increase the wavelength of the incident light. This factor appears in all of the equations and is not restricted by any assumptions for either theory. By using a wavelength in the mid-infrared (10.6 μm for a CO_2 laser) instead of a visible wavelength (.633 μm for a HeNe laser), one should be able to measure accurately amplitudes seventeen times rougher.

CHAPTER 3

EXPERIMENTAL DESCRIPTION

The BRDF and grating efficiency measurements were done using a TMA CASI™ Scatterometer[13] as shown in Figure 4. Measurements were made at wavelengths of .6328, 1.06, 3.39, and 10.6 μm. A power meter was also used to measure the zero and first diffracted orders of the sinusoidal gratings for the higher power laser wavelengths.

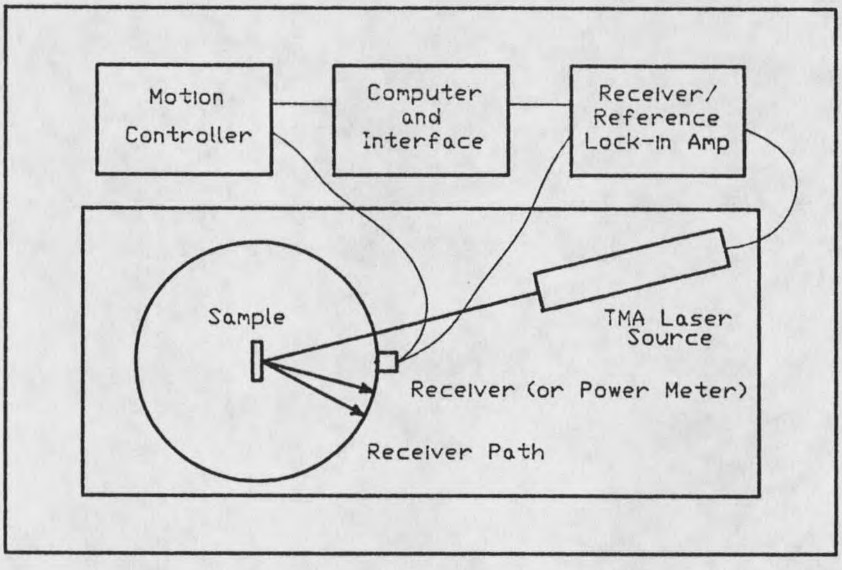


Figure 4. Block diagram of a scatterometer.

For the weaker powered laser (3.39 μm), the BRDF scan was used to determine the power in the diffracted orders. This information is obtainable with the analysis software on the instrument. Figure 5 shows a typical diffraction grating BRDF scan for wavelengths of .633, 3.39, and 10.6 μm. The incident angle was 20 degrees, and the horizontal axis is the measure of the scatter angle with respect to the diffracted first order. By adding $\theta_i = 20°$ to this angle, one can find the value for θ_s.