**EXPERIMENTAL VALIDATION OF THE GENERALIZED HARVEY-SHACK SURFACE
SCATTER THEORY**

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requirements for the degree of
Master of Science

By

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ABSTRACT

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The Generalized Harvey-Shack (GHS) surface scatter theory claims to predict the scatter from rough surfaces over a wide domain of validity but has not been widely implemented or tested. The focus of this research is to provide a documented implementation and experimental validation of the GHS theory for the prediction of the bidirectional reflectance distribution function (BRDF) from real rough surfaces. First, the GHS theory was developed for the MATLAB[®] software and the details of its implementation and application to experimental comparison are discussed. Next, a BRDF measurement system was designed, built, and validated. The BRDF of the Spectralon reflectance standard was measured with high agreement. Sample surfaces were characterized via atomic force microscopy as inputs to the GHS theory. The BRDF of each surface was then measured and simulated with the assumption of Gaussian autocovariance. When this assumption held, the GHS theory predictions matched well with experimental results.

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“For from him and through him and to him are all things.

To him be glory forever. Amen.”

- Romans 11:36

Chapter 1

Introduction

1.1 Motivation

The scattering of light off of surfaces is important to human vision, photography, computer graphics, and many other aspects of life and science. The ability to understand and model the behavior of this scattered light provides countless advantages. Photographers seek to vary the light profiles of landscapes or objects and often use diffusers or perspectives to change the effect of scattered light. Computer graphics designers must model and simulate the reflection of light off of everyday surfaces to emulate the appearance of real-life objects in computer-generated graphics. Optical engineers must account for stray light scatter when designing high-fidelity optical systems such as ultraviolet telescopes. The measurement of light scatter often requires high-precision equipment and long measurement times that regularly prove infeasible for the application. If, however, one were able to model the scatter of light off of surfaces, some of the aforementioned challenges encountered could be handled efficiently.

Though the need for modeling surface scatter is high, the ability to accurately predict it is scarce. Many of the existing surface scatter models require empirical parameterization or only work for a small domain of validity. An exhaustive survey of approximate scattering wave theories from random rough surfaces was done in 2004 and concluded that there was no universal method to be preferred systematically and that there is still room for improvement [10].

One particular model developed in 2006, the Generalized Harvey-Shack (GHS) model, uses a linear systems approach to model light scattering from surfaces that does not impose limitations on the domain of validity and claims accuracy over virtually all surface roughness scales and wavelengths. The current literature, however, features a scarce amount of comparison between GHS prediction and experimental results. Current validations feature numerical simulation comparisons or limited surfaces and wavelengths. Furthermore, there are very few documented implementations of the GHS model outside of the research group responsible for its formulation. Therefore, this research seeks to provide the field with comparison between the GHS model and surface scatter measurements, namely bidirectional reflectance distribution function (*BRDF*) measurements. Additionally, this research provides an example implementation of the GHS model aimed at supplying future scientists with documentation and lessons learned.

1.2 Background

Surface scatter theory describes the interaction of an incident electromagnetic wave with an arbitrarily rough surface and the resulting distribution of the reflected (and/or transmitted) wave. A “rough” surface in this context encompasses any reflective boundary whose variation in surface height is on the order of the wavelength of incident light. This height variation may be deterministic, such as the diffraction grating on the left in Figure 1.1, or statistically random like many manufactured surfaces as pictured on the right in Figure 1.1. The most commonly used statistical description of surface roughness is the autocovariance (ACV) function which generally describes the separation of surface features by calculating the covariance of the surface profile, h , with itself. The “correlation length”, l , then describes the spacing of surface features, while the root-mean-square (rms) roughness, σ_s , describes the height of surface features. The ACV and its Fourier transform pair, the power spectral density (PSD), provide the statistical representation of surface roughness used in many surface scatter theories.

The study of scattering off of rough surfaces began in the field of acoustics by Lord Rayleigh in the 19th century. In 1951, Rice applied Rayleigh’s vector perturbation theory to the study of radar scatter from the sea and developed what is now referred to as the Rayleigh-Rice vector perturbation theory [11]. This theory considered the surface roughness to be a small perturbation to a perfectly

Figure 1.1: Deterministic [1] and Statistically Random Rough Surfaces [2]

smooth surface and was therefore only viable in calculations for smooth surfaces.

Later, the Kirchhoff approximation (KA) was employed by many and formalized by Beckmann to characterize the scattering off of rougher surfaces. Instead of solving rigorous boundary conditions like in the Rayleigh-Rice formulation, the Beckmann-Kirchhoff (BK) model assumes that the radii of curvature of the surface roughness are much larger than the wavelength [12]. The accuracy of the Beckmann-Kirchhoff approximation is limited to only moderate angles of incidence and to surfaces with Gaussian ACV functions [2]. Thus, the two classical diffraction approaches, Rayleigh-Rice and Beckmann-Kirchhoff, are complementary but not all-inclusive.

In 1976, Harvey and Shack developed a linear systems formulation of surface scatter that described scattering by a surface transfer function for surfaces with Gaussian ACV and for small incident and scattering angles [13]. This theory was then modified to allow for larger incident (but not scattering) angles and moderately rough surfaces [14]. Finally, this formulation was adjusted to give way to the Generalized Harvey-Shack (GHS) model that applies to arbitrary incident and scattering angles and rough surfaces given by arbitrary roughness statistics [2]. This model, though computationally intensive, produces accurate results over the largest domain of validity.

This new GHS model thus seems to combine the advantages of the classical Rayleigh-Rice and Beckmann-Kirchhoff theories without the disadvantages of either [15]. Since its inception in 2006, however, nearly all of the literature that discusses or uses the GHS model is from of the same research group that developed the model. Thus, there is a significant lack of experimental verification and implementation examples. The few examples of experimental validation mostly include surfaces with Gaussian ACV and polished smooth surfaces. Documented usage of the GHS model is just as rare as experimental validation. Outside of the research group associated with

its invention the GHS model has only been implemented a handful of times, all without helpful detail. This research therefore intends to provide a new source of experimental comparison for, and documented implementation of, the GHS model.

1.3 Statement of Objective

The objectives of this research were threefold:

1. To implement the GHS theory for arbitrary inputs and provide a documented implementation to the field.
2. To design, build, and execute a surface scatter measurement system.
3. To provide a comparison between the GHS theory and experimental results, using real surfaces with characterized roughness.

First, the GHS model was implemented in the MATLAB[®] software. The details of this implementation are discussed, along with explanations of physical meaning of the algorithm design. These explanations are not explicitly stated in the literature and are therefore recognized and discussed in this research.

Additionally, a surface scatter measurement system was designed, built, and used for the collection of the $BRDF$ of several different surfaces with varying roughness. Though this system is able to collect out-of-plane scatter, only in-plane measurements are performed in this research due to time constraints. Initially, these measurements were to be performed at three wavelengths spanning the visible spectrum. However, due to time and funding constraints, only one wavelength was used. Design choices and capabilities and limitations are discussed.

Finally, surface profilometry measurements were conducted of the sample surfaces in order to obtain surface roughness parameters. These parameters are then used in the GHS model to predict $BRDF$. These GHS results are then compared to experimental $BRDF$ results with analysis on the applicability of the GHS model.

Chapter 2

Theory and Literature Review

Before discussing the implementation of the GHS model, development of a surface scatter measurement system, and presenting results, the theoretical background and a review of relevant literature are presented. This section primarily focuses on the development of the GHS model, its foundation in scalar diffraction theory, and the relevant examples of the GHS in literature. This section also includes a discussion and review of surface scatter, namely the bidirectional reflectance distribution function ($BRDF$), and the standards and best practices associated with surface scatter measurement.

2.1 Surface Scatter Theory

The two classical approaches discussed in Section 1.2, Rayleigh-Rice and Beckmann-Kirchhoff, make up the foundation of the so-called diffraction approach to surface scatter theory. These differ from the microfacet approaches to surface scatter theory which are often used in computer graphics in order to obtain realistic rendering of surfaces [16]. The microfacet models often require experimental parametric fitting and aren't easily deduced from surface profile parameters. In microfacet scatter theories, geometrical optics is assumed as opposed to the physical optics employed in diffraction scatter theories. The surface is described as having individual facets with randomly-distributed surface normals [17]. The $BRDF$ is then often calculated from a microfacet distribution, the Fresnel reflection, and a geometric attenuation factor that expresses the ratio of light that is not occluded

by the surface due to shadowing [18]. In general, diffraction approaches to surface scatter theory provide a potentially more rigorous solution, but often require computationally intensive implementation [19].

2.1.1 Fundamentals of Scalar Diffraction Theory

Before describing the details of the GHS model, the underlying physical theory is discussed. The Original, Modified, and Generalized Harvey-Shack models all have their basis in scalar diffraction theory, particularly the angular spectrum of plane waves. Thus, the needed fundamentals of scalar diffraction theory are discussed here before the linear systems treatment of scalar diffraction theory. The following is largely from Goodman, [3], and Krywonos' dissertation, [2]. This section is intended provide details that are sufficient to shed light on the development of the GHS model.

The discovery of the diffraction phenomenon is generally credited to Francesco Grimaldi in 1665. Grimaldi, when illuminating an aperture in an opaque screen with a point source, did not observe a shadow with sharp borders in the observation plane. Instead, he noticed that the transition from light to shadow was gradual rather than sharp. Christian Huygens, in 1678, expressed the idea that if every point on the wavefront of a disturbance were considered to be a source of a secondary spherical disturbance, then the wavefront at some later time could be found by constructing the envelope of the secondary disturbance. Later, in 1704, Thomas Young furthered the theory of light as a wave by introducing interference, stating that it was possible that "light could be added to light and produce darkness" [3]. Finally, Fresnel used the work of Huygens and Young to produce a calculation of the distribution of light in diffraction patterns in 1818. Fresnel extended Huygens' work to allow for mutual interference of the wavelets by making some arbitrary assumptions about their amplitudes and phases. Fresnel, when presenting his work to a committee, was challenged by the great mathematician Poisson, who marked its absurdity in predicting a bright spot at the center of a shadow of an opaque disk. Arago, the chairman, performed the experiment and confirmed Fresnel's findings. The effect has since been known as "Poisson's spot" [3].

After Maxwell formulated his equations, identifying light as an electromagnetic wave, the ideas of Huygens and Fresnel received firmer mathematical rigor by Gustav Kirchhoff. Kirchhoff showed that the amplitudes and phases ascribed to the secondary sources by Fresnel were logical consequences of the wave nature of light. He showed this by choosing a Green's function that satisfied

the differential wave equation. However, Kirchhoff accomplished this by making two assumptions about the boundary values of the light incident on a surface that were later proved to be inconsistent with each other. In 1896, Sommerfeld eliminated the need for Kirchhoff's boundary conditions, formulating the Rayleigh-Sommerfeld diffraction theory. This theory is a rigorous treatment of *scalar* diffraction in that it ignores the fact that the components of the electric and magnetic fields are coupled through Maxwell's equations.

The Rayleigh-Sommerfeld diffraction formula is valid throughout the entire observation space and is given by:

$$U_2(x_2, y_2) = \frac{1}{i\lambda} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_1(x_1, y_1) \frac{\exp ikl}{l} \cos(\vec{n}, \vec{l}) dx_1 dy_1 \quad (2.1)$$

where $U_1(x_1, y_1)$ is the complex field distribution emerging from the diffracting aperture, Σ , and $U_2(x_2, y_2)$ is the complex field distribution in the observation region, while

$$l = \sqrt{z^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2}$$

is the distance from an arbitrary point in the diffracting aperture to an arbitrary point in the observation plane as shown in Figure 2.1 [2].

Figure 2.1: Geometry of the Rayleigh-Sommerfeld Diffraction Integral from [2]

Because the Rayleigh-Sommerfeld diffraction integral is difficult to solve in closed form, approximations are often made to allow for the simple calculation of certain diffraction patterns. The famous Fresnel approximation is obtained by employing a binomial expansion of the distance, l , in the Rayleigh-Sommerfeld integral of Equation 2.1 and only retaining the first two terms of the expansion in the exponent while also substituting z for l in the denominator. The resulting Fresnel approximation for the complex field distribution in the observation plane, using Krywonos' notation

[2], is:

$$U_2(x_2, y_2) = \frac{\exp(ikz)}{i\lambda z} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_1(x_1, y_1) \exp \left\{ \frac{ik}{2z} [(x_2 - x_1)^2 + (y_2 - y_1)^2] \right\} dx_1 dy_1. \quad (2.2)$$

Equation 2.2 is valid when the *Fresnel criterion* is met:

$$z^2 \gg \frac{\pi}{4\lambda} [(x_2 - x_1)^2 + (y_2 - y_1)^2]_{max}. \quad (2.3)$$

Additionally, Equation 2.2 can easily be seen as a convolution integral of the form:

$$U_2(x_2, y_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_1(x_1, y_1) h(x_2 - x_1, y_2 - y_1) dx_1 dy_1, \quad (2.4)$$

where the convolution kernel, or impulse response from linear systems, is:

$$h(x, y) = \frac{\exp(ikz)}{i\lambda z} \exp \left[\frac{ik}{2z} (x^2 + y^2) \right]. \quad (2.5)$$

This provides an appropriate segue into the basis of the GHS theory, a linear systems treatment of scalar diffraction theory in which the diffraction process is formulated in a way that resembles linear, invariant systems.

2.1.2 Linear Systems Treatment of Scalar Diffraction Theory

2.1.2.1 The Angular Spectrum of Plane Waves

This linear systems treatment of scalar diffraction theory is commonly referred to as “The Angular Spectrum of Plane Waves” [3]. In this formulation, the complex field distribution of a monochromatic disturbance is Fourier-analyzed across any plane. The resulting spatial components can thus be identified as plane waves traveling in different directions. The field amplitude at any point can then be calculated by adding the superposition of all of these plane waves, taking in account phase shifts [3].

Let the monochromatic complex field distribution in the plane P_0 be given by $U_0(\hat{x}, \hat{y}, 0)$, where the plane P_0 is at $z = 0$, as shown in Figure 2.2. Note that a scaled coordinate system is used in which $\hat{x} = x/\lambda$, $\hat{y} = y/\lambda$, $\hat{z} = z/\lambda$. When calculating the resulting field, $U(\hat{x}, \hat{y}, \hat{z})$, that appears across a second parallel plane a distance z from the first plane, it is assumed that this resultant field is only due to U_0 .

Across plane P_0 , the function U_0 has a two-dimensional Fourier transform pairing given by:

$$A_0(f_x, f_y; 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(x, y, 0) \exp [-i2\pi(f_x \hat{x} + f_y \hat{y})] d\hat{x} d\hat{y}, \quad (2.6)$$

Figure 2.2: Geometry of Propagation from plane P_0 to Plane P from [2]

$$U_0(\hat{x}, \hat{y}, 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_0(f_x, f_y, 0) \exp [i2\pi(f_x \hat{x} + f_y \hat{y})] df_x df_y, \quad (2.7)$$

where f_x and f_y are the spatial frequencies associated with x and y , respectively. Introducing the direction cosines, α , β , and γ as

$$\alpha = \lambda f_x, \quad \beta = \lambda f_y, \quad \gamma = \sqrt{1 - (\lambda f_x)^2 - (\lambda f_y)^2}, \quad (2.8)$$

yields

$$A_0(\alpha, \beta; 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(\hat{x}, \hat{y}, 0) \exp [-i2\pi(\alpha \hat{x} + \beta \hat{y})] d\hat{x} d\hat{y}, \quad (2.9)$$

$$U_0(\hat{x}, \hat{y}, 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_0(\alpha, \beta; 0) \exp [i2\pi(\alpha \hat{x} + \beta \hat{y})] d\alpha d\beta. \quad (2.10)$$

These direction cosines formulate the angle between each Cartesian axis and an arbitrary vector in space, as illustrated in Figure 2.3. Direction cosines are used extensively in the GHS model. In the same way as above, the complex field amplitude and its Fourier pair in the plane P are:

$$A(\alpha, \beta; \hat{z}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(\hat{x}, \hat{y}, \hat{z}) \exp [-i2\pi(\alpha \hat{x} + \beta \hat{y})] d\hat{x} d\hat{y}, \quad (2.11)$$

$$U(\hat{x}, \hat{y}, \hat{z}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A(\alpha, \beta; \hat{z}) \exp [i2\pi(\alpha \hat{x} + \beta \hat{y})] d\alpha d\beta. \quad (2.12)$$

$A_0(\alpha, \beta; 0)$ and $A(\alpha, \beta; \hat{z})$ are referred to as the *angular spectrum* of $U_0(\hat{x}, \hat{y}, 0)$ and $U(\hat{x}, \hat{y}, \hat{z})$ respectively. Because U must satisfy the Helmholtz equation in the scaled coordinate system,

$$[\hat{\nabla}^2 + (2\pi)^2]U(\hat{x}, \hat{y}, \hat{z}) = 0, \quad (2.13)$$

A must satisfy the differential equation

$$\frac{d^2}{d\hat{z}^2} A(\alpha, \beta; \hat{z}) + (2\pi)^2 \gamma^2 A(\alpha, \beta; \hat{z}) = 0, \quad (2.14)$$

where

$$\gamma = \sqrt{1 - \alpha^2 - \beta^2}. \quad (2.15)$$

Figure 2.3: Illustration of Direction Cosines from [3]

Thus, the angular spectrum in plane P_0 can be shown to be related to the angular spectrum in plane P by

$$A(\alpha, \beta; \hat{z}) = A(\alpha, \beta; 0) \exp(i2\pi\gamma\hat{z}). \quad (2.16)$$

The linear systems notion of the transfer function allows the simple expression of this relation to give the transfer function for free space propagation as

$$H(\alpha, \beta, \hat{z}) = \frac{A(\alpha, \beta; \hat{z})}{A(\alpha, \beta; 0)} = \exp(i2\pi\gamma\hat{z}). \quad (2.17)$$

This result shows that when

$$\alpha^2 + \beta^2 \leq 1,$$

the corresponding part of the optical disturbance will propagate and each component will proceed at its given angle, producing relative phase delays. However, when

$$\alpha^2 + \beta^2 > 1,$$

the associated components of the angular spectrum will rapidly attenuate during propagation. These are called *evanescent waves* and are analogous to waves produced in a waveguide below the cutoff frequency. Thus, the only portion of the angular spectrum that contributes to the optical disturbance in plane P are those whose direction cosines fall within the (α, β) unit circle, as depicted in Figure 2.4.

Figure 2.4: Unit Circle in Direction Cosine Space from [2]

2.1.2.2 Harvey-Shack Surface Scatter Theory

When calculating the Fresnel diffraction formula of Equation 2.2, some restriction on the distance from the aperture is required. A similar, but more stringent approximation, is the Fraunhofer approximation that, when satisfied, produces greatly simplified computation in the *far field*. Both of these approximations put severe restrictions on both the size of the aperture and the region over which the calculations are valid. These calculations are invalid in the *near field* and anywhere outside the *paraxial* region.

To avoid these restrictions, all of the terms in the expansion of l in Equation 2.1 must be retained. Harvey showed that this may be done by writing the Rayleigh-Sommerfeld diffraction integral, given in Equation 2.1, as a Fourier transform [20]. When the observation plane is a hemisphere, this new formulation is given by [2]

$$U(\alpha, \beta; \hat{r}) = \gamma \frac{\exp(i2\pi\hat{r})}{i\hat{r}} \mathcal{F}\{U_0(\hat{x}, \hat{y}, 0)\}, \quad (2.18)$$

where

$$\hat{r}^2 = \hat{x}^2 + \hat{y}^2 + \hat{z}^2,$$

and $U_0(\hat{x}, \hat{y}, 0)$ is the complex field distribution emanating from the aperture.

If light is incident upon the diffracting aperture at an angle θ_i , as in Figure 2.5, then applying

the shift theorem of Fourier transform theory yields

$$U(\alpha, \beta - \beta_0; \hat{r}) = \gamma \frac{\exp(i2\pi\hat{r})}{i\hat{r}} \mathcal{F}\{U'_0(\hat{x}, \hat{y}, 0) \exp(i2\pi\beta_0\hat{y})\}, \quad (2.19)$$

where

$$U'_0(\hat{x}, \hat{y}, 0) = \sqrt{\gamma_i} U_0(\hat{x}, \hat{y}, 0), \quad (2.20)$$

β is the direction cosine of the position vector of the observation point, and β_0 is the direction cosine of the undiffracted beam.

Figure 2.5: Converging Incident Beam Striking an Aperture at an Arbitrary Angle from [2]

Using Parseval's theorem and Equation 2.18, the total radiant power reflected from a surface can be written as

$$P = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\hat{r}^2}{\gamma^2} |U(\alpha, \beta; \hat{r})|^2 d\alpha d\beta = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |U_0(\hat{x}, \hat{y}, 0)|^2 d\hat{x} d\hat{y}. \quad (2.21)$$

Intensity (I), defined as power per solid angle ($dP/d\omega$), may then be defined as

$$I(\alpha, \beta) = \frac{dP}{d\omega} = \frac{\hat{r}^2}{\gamma} |U(\alpha, \beta; \hat{r})|^2 = \gamma \left| \mathcal{F}\{U_0(\hat{x}, \hat{y}, 0)\} \right|^2, \quad (2.22)$$

where the substitution has been made for $d\omega = d\alpha d\beta / \gamma$.

Using the autocorrelation theorem of Fourier transform theory, the above equation is equivalent to [2]

$$I(\alpha, \beta) = \gamma \mathcal{F} \left\{ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(\hat{x}', \hat{y}', 0) U_0^*(\hat{x}' - \hat{x}, \hat{y}' - \hat{y}, 0) d\hat{x}' d\hat{y}' \right\}. \quad (2.23)$$

Harvey then developed an analytical expression for the surface transfer function by following the transfer function procedure of image formation. The effective transfer function of the scattering system is defined as the normalized autocorrelation of the pupil function

$$H_{eff}(\hat{x}, \hat{y}, 0) = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(\hat{x}', \hat{y}', 0) U_0^*(\hat{x}' - \hat{x}, \hat{y}' - \hat{y}, 0) d\hat{x}' d\hat{y}'}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |U_0(\hat{x}, \hat{y}, 0)|^2 d\hat{x} d\hat{y}}. \quad (2.24)$$

The effective *angle* spread function, analogous to the *point* spread function, is then defined as the Fourier transform of this effective transfer function [2]

$$ASF(\alpha, \beta) = \mathcal{F}\{H_{eff}(\hat{x}, \hat{y}, 0)\}. \quad (2.25)$$

Substituting the equations for intensity and power yields the expression for the angle spread function in terms of the radiant intensity of the scattered light

$$ASF(\alpha, \beta) = \frac{1}{\gamma P} I(\alpha, \beta) \quad (2.26)$$

Original Harvey-Shack Formulation

Harvey then makes a series of expansions of the pupil function in Equation 2.24, describing the random phase variance introduced by reflection from the scattering surface (at normal incident) as

$$\phi(\hat{x}, \hat{y}; 0) = (2\pi/\lambda) OPD = 4\pi \hat{h}(\hat{x}, \hat{y}; 0), \quad (2.27)$$

where OPD is the optical path difference, and $\hat{h}(\hat{x}, \hat{y})$ is the surface height distribution scaled by the wavelength. Harvey then goes on to make some statistical assumptions about $\hat{h}(\hat{x}, \hat{y})$ that include Gaussian distribution and local stationarity. After applying these assumptions and taking the expected value, Harvey arrives at the surface transfer function formulated as

$$H_s(\hat{x}, \hat{y}) = \exp \left\{ - (4\pi \hat{\sigma}_s)^2 \left[1 - \frac{C_s(\hat{x}, \hat{y})}{\sigma_s^2} \right] \right\}, \quad (2.28)$$

where $C_s(\hat{x}, \hat{y})$ is the two-dimensional autocovariance function of the surface and σ_s^2 is the variance of the surface height distribution function. The distribution of scattered light, given by the angle spread function, is the Fourier transform of Equation 2.28.

The transfer function of Equation 2.28 can be written in the form of

$$H_s(\hat{x}, \hat{y}) = A + B G(\hat{x}, \hat{y}), \quad (2.29)$$

where

$$A = \exp \left[- (4\pi \hat{\sigma}_s)^2 \right], \quad (2.30)$$

$$B = 1 - \exp \left[- (4\pi \hat{\sigma}_s)^2 \right], \quad (2.31)$$

and

$$G(\hat{x}, \hat{y}) = \frac{\exp \left[(4\pi)^2 \hat{C}(\hat{x}, \hat{y}) \right] - 1}{\exp \left(4\pi \hat{\sigma}_s \right)^2 - 1}. \quad (2.32)$$

Equation 2.29 formulates the surface transfer function as two separate components. The corresponding angle spread function can then be written as the sum of the Fourier transforms of the two individual components of the transfer function:

$$ASF(\alpha, \beta) = \mathcal{F}\{A + BG(\hat{x}, \hat{y})\} = A\delta(\alpha, \beta) + S(\alpha, \beta), \quad (2.33)$$

where

$$S(\alpha, \beta) = B \mathcal{F}\{G(\hat{x}, \hat{y})\}. \quad (2.34)$$

Thus the scattering surface reflects incident light as a specularly reflected beam of diminished intensity surrounded by diffusely scattered light. Because $A + B = 1$, the value of the surface transfer function is unity at the origin. The central ordinate theorem of Fourier transform theory thus requires that the angle spread function have unit volume. From Equation 2.34, it is clear that A and B correspond to the fraction of the total reflected radiant power contained in the specular and scattered components of the angle spread function, respectively.

Lambert's Cosine Law states that the irradiance decreases with the angle of incidence as $\cos \theta$. From Equation 2.26 and Lambert's Cosine Law, it is evident that the angle spread function is a scattered *radiance* function since $\gamma = \cos \theta_s$. Because radiant intensity is related to the radiance from a uniformly radiant surface by [21]

$$I = \int_{surface} L \cos \theta dA_{surface} = L \cos \theta A_{surface}, \quad (2.35)$$

Equation 2.26, becomes

$$ASF = \frac{L \cos \theta A_{surface}}{P \cos \theta} = \frac{L A_{surface}}{P}. \quad (2.36)$$

Finally, the bidirectional reflectance distribution function (*BRDF*) is defined as the ratio of scattered radiance to incident irradiance and is a function of incident (θ_i, ϕ_i) and scattering (θ_s, ϕ_s) angles. Knowing the incident irradiance on the surface, Equation 2.36 can be expressed as

$$ASF = \frac{L_{scattered}}{E_{incident}}, \quad (2.37)$$

where $E_{incident} = P/A_{surface}$ is the irradiance incident on the surface and L is the radiance scattered from the surface. Thus, the scattered $ASF(\alpha, \beta)$ is converted to *BRDF* by:

$$BRDF \Big|_{\theta_i, \phi_i} = R \cdot ASF(\alpha, \beta), \quad (2.38)$$

where R is the scalar reflectance of the scattering surface, and $BRDF \Big|_{\theta_i, \phi_i}$ is the scattered *BRDF* for one incident angle. Therefore, the total *BRDF* is made up of a superposition of many two-dimensional angle spread functions, one for each angle of incidence [2].

Modified Harvey-Shack Formulation

The above is essentially a derivation of the Original Harvey-Shack formulation (OHS). Its three main limitations are:

1. It is a scalar theory and does not count for polarization effects.
2. It is limited to small incident *and* scattering angles.
3. It does not account for the redistribution of energy from evanescent to propagating waves.

The last two limitations are addressed in the formulation of the Modified Harvey-Shack (MHS) model and the first limitation is addressed in the GHS formulation for smooth surfaces.

Recall that, in the OHS model, the random phase variations induced upon reflection from the surface were assumed to be given by

$$\phi(\hat{x}, \hat{y}; 0) = (2\pi/\lambda)OPD = 4\pi\hat{h}(\hat{x}, \hat{y}; 0). \quad (2.39)$$

This, however, is only true for an incident wavefront at normal incidence. Thus, this assumption severely limits the theory to very small incident and scattering angles. For an incident ray at an arbitrary angle of incidence, θ_i , the optical path difference of a ray specularly reflected ($\theta_0 = \theta_i$) from the surface is given by

$$OPD = (\cos \theta_i + \cos \theta_0) \hat{h}(\hat{x}, \hat{y}; 0) = 2 \cos \theta_i \hat{h}(\hat{x}, \hat{y}; 0) \quad (2.40)$$

and is depicted in Figure 2.6.

Figure 2.6: Illustration of the OPD for a Specularly Reflected Ray from [2]

This new OPD was used to produce the MHS surface transfer function given by

$$H_s(\hat{x}, \hat{y}) = \exp \left\{ - (4\pi \cos \theta_i \hat{\sigma}_s)^2 \left[1 - \frac{C_s(\hat{x}, \hat{y})}{\sigma_s^2} \right] \right\}, \quad (2.41)$$

The MHS transfer function is therefore different for each incident angle. A wavefront incident on a scattering surface at an angle θ_i is essentially a linear phase shift across the pupil. If the plane of incidence is the x-z plane, this will cause a shift of the scattering function in direction cosine space of $\alpha - \alpha_0$, where $\alpha_0 = \sin \theta_0$. The *ASF* is then given by the Fourier transform of the MHS transfer function multiplied by a linear phase shift:

$$ASF(\alpha, \beta) = \mathcal{F}\{H_{eff}(\hat{x}, \hat{y}, 0) \exp(-i2\pi\alpha_0\hat{x})\} = A\delta(\alpha - \alpha_0, \beta) + S(\alpha - \alpha_0, \beta), \quad (2.42)$$

where

$$S(\alpha - \alpha_0, \beta) = B \mathcal{F}\{G(\hat{x}, \hat{y}) \exp(-i2\pi\alpha_0\hat{x})\}. \quad (2.43)$$

As stated previously, $ASF(\alpha, \beta)$ contains components with (α, β) that are outside the unit circle in direction cosine space. These components thus produce evanescent waves which do not produce propagated energy. Thus, to ensure conservation of energy, the por-

tion of the total energy within these waves must be redistributed to the waves that actually propagate. Thus, a renormalization constant, K , is introduced as

$$K = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} ASF(\alpha, \beta) d\alpha d\beta}{\int_{\alpha=-1}^{\alpha=1} \int_{\beta=-\sqrt{1-\alpha^2}}^{\beta=\sqrt{1-\alpha^2}} ASF(\alpha, \beta) d\alpha d\beta}. \quad (2.44)$$

However, because the numerator of Equation 2.44 is defined as unity, K is calculated as

$$K = \frac{1}{\int_{\alpha=-1}^{\alpha=1} \int_{\beta=-\sqrt{1-\alpha^2}}^{\beta=\sqrt{1-\alpha^2}} ASF(\alpha, \beta) d\alpha d\beta}. \quad (2.45)$$

The scattered intensity is thus given by

$$I(\alpha, \beta) = P_i ASF(\alpha, \beta) \cos \theta_s, \quad (2.46)$$

where

$$ASF(\alpha, \beta) = K \mathcal{F}\{H_s(\hat{x}, \hat{y}) \exp(-i2\pi\alpha_0\hat{x})\}. \quad (2.47)$$

Generalized Harvey-Shack Formulation

Though an improvement over the OHS, the MHS still had shortcomings. Most notably, the MHS cannot be expected to work well for wide scattering angles, especially at large incident angles. Thus, the generalized Harvey-Shack (GHS) method was formulated to work for arbitrary incident and scattering angles.

Figure 2.7 illustrates the same optical path difference concept as before but now applied for arbitrary incident *and* scattering angle. This OPD can be written as

$$OPD = (\cos \theta_i + \cos \theta_s) \hat{h}(\hat{x}, \hat{y}; 0). \quad (2.48)$$

This new OPD was used to produce the GHS surface transfer function given by

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp \left\{ - [2\pi \hat{\sigma}_s (\gamma_i + \gamma_s)]^2 \left[1 - \frac{C_s(\hat{x}, \hat{y})}{\sigma_s^2} \right] \right\}, \quad (2.49)$$

where $\gamma_i = \cos \theta_i$ and $\gamma_s = \cos \theta_s$. The GHS transfer function is now different for each incident angle and each scattering angle. The angle spread function for light scattered in

Figure 2.7: Illustration of the OPD for a Ray Reflected at an Arbitrary Angle from [2]
the (α_s, β_s) direction is now

$$ASF(\alpha, \beta) = \mathcal{F} \left\{ H_s(\hat{x}, \hat{y}, \gamma_i, \gamma_s) \exp(-i2\pi\alpha_0\hat{x}) \right\} \Big|_{\alpha=\alpha_s, \beta=\beta_s}, \quad (2.50)$$

where

$$\gamma_s = \sqrt{1 - \alpha_s^2 - \beta_s^2}. \quad (2.51)$$

The surface transfer function may again be written in the form

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = A + B G(\hat{x}, \hat{y}; \gamma_i, \gamma_s), \quad (2.52)$$

where

$$A = \exp \left[- (2\pi(\gamma_i + \gamma_s)\hat{\sigma}_s)^2 \right], \quad (2.53)$$

$$B = 1 - \exp \left[- (2\pi(\gamma_i + \gamma_s)\hat{\sigma}_s)^2 \right], \quad (2.54)$$

and

$$G(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \frac{\exp \left\{ [2\pi(\gamma_i + \gamma_s)]^2 \hat{C}(\hat{x}, \hat{y}) \right\} - 1}{\exp [2\pi(\gamma_i + \gamma_s)\hat{\sigma}_s]^2 - 1}. \quad (2.55)$$

The ASF is then written as

$$ASF(\alpha, \beta) = [A\delta(\alpha - \alpha_0, \beta) + S(\alpha - \alpha_0, \beta)] \Big|_{\alpha=\alpha_s, \beta=\beta_s}, \quad (2.56)$$

where

$$S(\alpha - \alpha_0, \beta) = B \mathcal{F} \{ G(\hat{x}, \hat{y}; \gamma_i, \gamma_s) \exp(-i2\pi\alpha_0\hat{x}) \}. \quad (2.57)$$

The renormalization and conversion to intensity is the same as for the MHS model. Now, however, a different surface transfer function must be calculated for every combina-

tion of incident and scattering angles. Thus, a different Fourier transform is required to calculate the ASF for each scattering angle [2].

2.1.2.3 Current Experimental Validation and Implementations of the GHS Surface Scatter Theory

Experimental Validation

The experimental comparisons discussed here only include comparisons with the GHS theory and do not include comparisons from the preceding theories, the OHS and MHS. These are not included in this section as they are assumed to be less valid over the whole domain of applications.

Experimental comparisons with results from the GHS model start with the results in the original development of the GHS model in [2] and [15]. These references compare GHS data with experimental data for a rough surface measured by O'Donnell and Mendez [22]. Reference [2] also includes analysis of a smooth mirror in which the author demonstrates the usage of a smooth-surface approximation of the GHS model that results in a form very similar to the Rayleigh-Rice formulation. The author uses measured $BRDF$ data to back out the surface PSD and compares the forward and backward scattered results that match the Rayleigh-Rice results well. Next, predicted and measured $BRDF$ results are shown for the same mirror for a single wavelength where the GHS model more closely matches the measured data. References [23] and [24] feature some of these same results. Harvey's 2010 work, [25], demonstrates the use of the GHS model for accurate prediction of the bidirectional transmission distribution function (BTDF) for an interface between glass and a thin film silicon solar cell at one wavelength and one incident angle. Reference [6] again shows comparison with data from [22]. Reference [6] also shows comparative results between the GHS model, Rayleigh-Rice, and measurements for the back side of a clean silicon wafer for three wavelengths and incident angles. These are measurements of a "smooth" surface at one wavelength at which the surface is smooth and two at which it is no longer considered smooth. For all cases, the GHS and Rayleigh-Rice models match the measured data well. Note that all of these results feature Harvey as an author and are from

the same research group at the University of Central Florida (UCF).

In 2009, Wang et al. used the smooth-surface approximation of the GHS model and the Rayleigh-Rice model to backout surface PSDs from x-ray ($\lambda = 0.154 \text{ nm}$) reflectance measurements as compared to PSDs generated from surface profile measurements [26]. The results for three samples of varying roughness at fixed incident angles agree well with PSD results via AFM.

In 2011, Schroder used both rigorous computations and experimental data to validate the GHS model [27]. First, the GHS model is compared to Rayleigh-Rice and the Rigorous Coupled Wave Analysis (RCWA) for sinusoidal phase gratings at one wavelength for sinusoids of differing periods and amplitudes. In general, the GHS model agrees well with the RCWA results. Schroder also measured the surface roughness of three steel surfaces, spanning the spectrum of surface roughness, at three different wavelengths. He then used the surface roughness to predict the resultant scatter with the GHS and Rayleigh-Rice models. The Rayleigh-Rice model fit well for the only smooth surface. However, the GHS model fit all measurements rather well. This is likely the best example of experimental validation of the GHS model in the literature currently.

In 2012, Choi examined the domain of validity of the Rayleigh-Rice, Kirchhoff, and GHS models with comparison to a rigorous method of moment code for one-dimensional ideally conducting surfaces [28]. Choi's publication gives many error function plots demonstrating the dependence of the accuracy of these models on surface roughness and incident/scattered angle. Choi's summary was that the GHS method has a much broader domain of validity than the other two methods and that it applies well for smooth and rough surfaces as well as small and large angles of incidence. In 2013, Choi demonstrated similar analysis along with comparative plots of scattered intensity distributions [29]. Again, Harvey is an author of these articles from their research group at UCF.

In 2014, the first of two applications of the GHS model to millimeter wave scattering appeared in [30]. The authors measured and predicted the scatter off of 40-grit gold coated sandpaper at 0.8 THz and 37 degrees incidence. Only one figure is shown comparing the experimental and predicted data. There is a significant lack of detail in the application

of the GHS method, and the predicted results indicate possible error in application. The experimental and predicted results do not match well. Additionally, it is stated that the measured data was shifted by 17 dB.

In 2016, Harvey again demonstrated the comparison of the smooth surface approximation of the GHS model to the Rayleigh-Rice model for a smooth molybdenum mirror at 488 nm [31]. This data is very similar to that shown in [2].

Also in 2016, Lee used the GHS model to verify measurements of a scattered light measurement system [32]. However, it appears that Lee used the smooth surface approximation of the GHS model with reasonable agreement for one wavelength and one incident angle.

In 2017, a thorough experiment was done at NIST of bistatic scattering measurements of Aluminum Oxide grit reference targets from 325 - 500 GHz and 650 GHz [33]. The results are compared to the modified integral equation method and the GHS model. The authors go into significant detail on the background, application, and capabilities of the GHS model. The experimental comparisons are shown for a few different incident angles and wavelengths for all samples. The surfaces inspected were found to be Gaussian distributed through surface topography measurements. In general, the authors state that the overall agreement must be considered disappointing. Specifically, the GHS model predicts little to no scattering in the backward direction at many angles while it is clearly present in the measured data. The authors state that the GHS model may not be valid for rough surfaces, such as theirs, with short correlation lengths relative to the wavelength ($l_c/\lambda < 1$). Along this line of thought, the authors also theorize that the failure of the GHS model may have arisen due to considering surface reflection and not bulk reflection and viewing the surface as a single sharp dielectric interface with a specific PSD. Perhaps, they argue, rough surfaces with short correlation lengths should be regarded as a graded-density layer. This flaw in the GHS model may also be attributable to effects from multiple scattering as the short correlation lengths would likely provide ample opportunity for incident light to reflect several times within the surface roughness. The authors do not state this possible limitation, but it is very likely that the end of the domain of validity of the GHS model is met at surfaces with potential for multiple reflections such as surfaces with volumetric

scattering or short correlation lengths.

Also in 2017, Lee et al. demonstrated the use of the GHS model in the simulation of speckle for laser displays [34]. The authors provide some detail of the application of the GHS model before discussing the application to their research. The GHS model is then used to predict the scatter from a piece of computer paper at a wavelength of 520 nm. The GHS model was used within simulation software that predicts the speckle contrast as a function of detection angle. The authors display simulation results with and without the use of the GHS model and experimental results. The data clearly indicate that the simulations correspond much better to experimental values with the use of the GHS model.

Documented Implementations

Documented implementations of the GHS model are as scarce as experimental comparison. The derivation of the GHS model originated from the work by Krywonos in 2006 in [2] and [15]. The proceedings article published near Krywonos' dissertation features a summarized version of the work presented in the dissertation. This dissertation naturally describes the GHS model in full, including historical background, diffraction theory, the original and modified Harvey-Shack methods, and numerical examples. Of particular interest is Section 5.3.4 of the dissertation in which Krywonos describes the process of numerically calculating the GHS prediction for arbitrarily rough surfaces. Krywonos describes the steps involved and even provides example intermediate calculations to further explain the detailed process. Lastly, Krywonos provides numerous example results for the GHS model compared with some measurements and other scatter theories such as the Rayleigh-Rice model.

Another helpfully documented implementation of the GHS model was published in 2009 by Harvey, Choi, and Krywonos [35]. Here, the authors describe the process of calculating $BRDF$ from surface PSDs for rough surfaces. They describe the process of calculating the 2-D surface PSD and fitting that PSD to a K-correlation form. The authors then describe the $BRDF$ calculation process, providing detail into the computational complexity required. Because of this complexity, the authors describe the implementation and

verification of the FFTLog algorithm that calculates the fast Fourier transform of a periodic sequence of logarithmically spaced data points. This is particularly useful for PSDs that span many orders of magnitude. *BRDF* curves are then plotted for the same surface parameters at varying wavelengths. This reference provides an illustrative process that addresses the computational complexity of the GHS method.

The next implementation was authored by Krywonos, Harvey, and Choi in 2012 and describes the entire history of Harvey-Shack scattering theory as well as providing brief discussions on surface roughness and applications of the GHS model [6]. The article begins with the requisite historical background and motivation for the work before discussing surface characteristics. The discussion provides a general overview as well as a formulation of the *relevant* surface roughness, σ_{rel} . This relevant surface roughness replaces the first appearance of the standard roughness, σ_s , in the GHS surface transfer function in Equation 2.49. σ_{rel} is discussed further in the implementation of the GHS model in Section 3.1.1. The 2012 article then walks through the origins and formulations of the OHS and MHS models as well as the application of these models to predicting *BRDF*. The article then provides the same level of detail, if not more, in explaining the GHS model. This article does not provide additional information into the implementation of the GHS model over [2] except for the inclusion of σ_{rel} . The article is helpful, however, in providing GHS algorithm results that include σ_{rel} that are useful for comparison.

One of the more helpful implementations overall is by Johansen in 2015 [36]. The first sentence of its abstract is, “The paper shows how to implement the generalized Harvey-Shack (GHS) method for isotropic rough surfaces discretized in a polar coordinate system and approximated using Fourier series.” The author also states that one of the main purposes of the paper is “to present a minimalistic, ready-to-use implementation of the GHS method in order to make it accessible for researchers in need of a scattering model for rough surfaces.” To this end, the author provides the implementation in software form in the appendix, written in Python. The article begins with an introduction to notation and the discrete ordinates method (the numerical method employed). The author then discusses rough surfaces with detail regarding relative roughness and Gaussian ACVs. The author

then provides an overview of, and all equations for, the GHS model. This section, and the corresponding lines of code, were invaluable in understanding that the GHS model results are generally used to predict the *diffusely scattered* portion of the reflected light. The only information needed regarding the specularly reflected light is its intensity, as its location is determined by the incident angle.

Before introducing the Python implementation, the author discusses the formulation of the GHS model for the discrete ordinates method. The author explains nearly every line of code and even includes specific details regarding the Python language. The author also includes several example results, including in-plane scattering curves as well as polar intensity plots of scattered intensity.

The final relevant implementation of the GHS model is found in 2017, by Grossman, et al. [33]. This reference provides a rare application of the GHS model to scattering at terahertz frequencies. In it, the authors discuss rough surface scattering in general, including the Rayleigh-Rice, Kirchhoff, and GHS models. Next, an introduction to *BRDF* and radiometric quantities used in surface scattering is provided. The authors also describe the methods of surface roughness characterization, including data and equations, showing the surfaces under inspection have Gaussian ACV functions. An entire scattering theory section is included that discusses the limitations, applications, and usage of the GHS model. The authors then provide a discussion-based overview, interpreting the GHS model's application. Finally, the author presents measurement data and conclusions. The findings are discussed above.

2.2 *BRDF* Measurement Background

The measurement of surface scatter has a long history spanning many fields. This section will provide a theoretical and application-driven background of the measurement of *BRDF* for providing experimental validation of the GHS model, as stated in Section 1.3. This section will include measurement best practices derived from sources such as a standard textbook, [37], and an ASTM standard, [38].

2.2.1 Definition of $BRDF$

The derivation and notation for $BRDF$ is regularly credited to F.E. Nicodemus as he sought to create nomenclature to describe the reflectance of optics that were neither completely diffuse nor completely specular [39]. As mentioned above briefly, $BRDF$ is defined as the ratio of scattered surface radiance, L , to incident surface irradiance, E . The surface irradiance is the light flux incident on the surface per illuminated surface area, represented as power per area or W/m^2 . The scattered surface radiance is the light flux scattered through the solid angle Ω per unit illuminated surface area per unit projected solid angle. This projected solid angle is the solid angle times $\cos \theta_r$ [37]. Surface radiance is thus represented as power per solid angle per area or $W/m^2/sr$.

$BRDF$ is formally derived as a differential quantity, or as a ratio of infinitesimals, as

$$BRDF = \frac{dL}{dE}. \quad (2.58)$$

Thus, the $BRDF$ has instantaneous values that can never be measured directly. Hence, real measurements involve non-zero intervals and can only yield average values over those intervals. Thus, Equation 2.58 becomes

$$BRDF \approx \frac{\Delta L}{\Delta E} \approx \frac{\Delta P_r / \Delta \Omega_r}{P_i \cos \theta_r}, \quad (2.59)$$

where ΔP_r is the reflected power over the solid angle $\Delta \Omega_r$, P_i is the power of the incident light, and θ_r is the reflected elevation angle. This definition and approximation of the $BRDF$ relies upon the assumption of a collimated incident beam of spatially uniform power and that the scatter from the surface is all due to surface roughness, not from volumetric scattering. Furthermore, the illuminated area on the sample should be representative of the entire surface roughness. This also implies that the surface contains uniform roughness characteristics. The approximation to the differential form is very poor when measuring focused specular peaks with large collecting apertures, as the peak will be averaged over an area much larger than its actual width.

The geometry depicting the definition of $BRDF$, as well as the convention for spherical angles, is shown in Figure 2.8. For sufficiently small collecting apertures, the solid angle

Ω is small and Equation 2.59 becomes

$$BRDF \approx \frac{\Delta P_r / \Delta \Omega_r}{P_i \cos \theta_r} \approx \frac{P_r / \Omega_r}{P_i \cos \theta_r}. \quad (2.60)$$

Figure 2.8: Geometry for the Definition of $BRDF$ from [4]

Because the $BRDF$ is defined as the ratio of scattered and incident quantities, it is dependent on the scattered and incident angles (θ_i, ϕ_i) and (θ_r, ϕ_r) respectively. Additionally, the $BRDF$ is dependent upon the wavelength of light and polarization of the incident and detected light. The units of $BRDF$ are inverse steradians (sr^{-1}). $BRDF$ values for very specular mirrors, where $P_r/P_i \approx 1$, approach $1/\Omega$ and can be as high as $10^6 sr^{-1}$ for small solid angles. Conversely, $BRDF$ values for very specular mirrors acquired far away from the specular beam approach noise-limiting values from the surrounding air molecules on the order of $10^{-9} sr^{-1}$. Thus, a very large dynamic range may be required by the measurement instrumentation.

One particular example of a simple $BRDF$ is the case of a Lambertian reflector. A Lambertian reflector, as its name suggests, obeys Lambert's Cosine Law in that the irradiance scattered from the surface, E , decreases with the scattered angle as $\cos \theta$, and the scattered radiance, L , is constant. Since $BRDF$ is defined as scattered radiance over incident irradiance, the $BRDF$ of a Lambertian reflector is constant as both the incident irradiance and scattered radiance are constant. Though no real object acts completely Lambertian, there are a few surfaces that approximate this behavior. A low-cost approximately

Lambertian reflector is white computer paper. In contrast, many optical fabrication companies manufacture surfaces made of fluoropolymers such as polytetrafluoroethylene, commonly known as Teflon. Approximately Lambertian reflectors are often used as standard test targets since their $BRDF$ is well-known.

Lambertian reflectors lie in stark contrast to high-fidelity smooth mirrors. These reflectors feature virtually zero diffuse scatter and only reflect light in the specular direction. The reflected power thus only depends on the input power and the reflectivity of the surface. Specular reflectors may provide useful test targets if the reflectivity of the surface is well-known.

2.2.2 $BRDF$ Measurement Principles

This section discusses the general principles of $BRDF$ measurement as well as measurement best practices. As with the above section, this section is generally derived from two references: [37] and [38].

A $BRDF$ measurement system is generally comprised of five components: light source, sample mount, receiver, computer/electronics package, and the controlling software, as shown in Figure 2.9.

Figure 2.9: Components of a Typical *BRDF* Measurement System from [5]

The light source is often a laser that is chopped, spatially filtered, expanded, and brought to a focus onto the detector. If the light source is not a laser, its bandwidth must be specified. The incident beam should be collimated or slightly converging to avoid discrepancy in the incident angle and to achieve high angular resolution in the scattered specular direction. The polarization of the incident light must be controlled, as the *BRDF* is generally dependent on polarization. If unpolarized results are desired, it is often best to perform two measurements with both linear polarizations, with the average being reported [38]. The light source is sometimes modulated or chopped to provide phase-sensitive lock-in detection of the scattered signal to lessen the effect of scatter from other sources. Lastly, the profile of the illuminated spot should be nearly uniform and should underfill the receiver field of view. In order to improve the quality of the incident beam, spatial filters and focusing optics are used, as shown in Figure 2.9.

The sample holder should provide a secure mount that ensures the sample is kept flat and immovable. Because incident and scattering angles are with respect to the sample surface, positioning can be accomplished by orienting the sample holder, source, or receiver, or some combination. The sample holder should not block any incident light, nor should

it contribute to the scattered light. It is common practice to mount the sample to a combination of rotation stages to provide the necessary articulation. It is also desirable that the sample mount is capable of being positioned both laterally and along the path of the incident beam. The former allows for *BRDF* measurements of different spots on the sample to inspect roughness uniformity. The latter allows for measurements of samples with varying thickness.

The receiver must have a well-defined aperture, as the *BRDF* is directly related to the detecting solid angle, Ω . For most systems where there are no optical elements between the detector and aperture, the solid angle is

$$\Omega \approx \frac{A_{rec}}{r^2} \quad (2.61)$$

where the approximation is due to the fact that solid angle is properly defined as the area on a sphere at a given radius. For small apertures, the approximation holds well.

When using coherent incident light, the aperture must be large enough to reduce the effects of speckle on the measured scatter. This, in practice, only applies for very small apertures at close distances. When performing *BRDF* measurements, there are two common ways of calculating P_i from Equation 2.60. The first method is called “relative” calibration in which a sample with a known *BRDF* is measured. In order to then obtain the *BRDF* of arbitrary samples, Equation 2.60 is rearranged to solve for P_i , with a known *BRDF* at each incident and scattered angle. The second method, and the one employed in this research, is called “absolute” calibration in which the incident irradiance is measured directly by positioning the receiver directly in the path of the incident light with the sample removed. For this method, the detector either must accommodate the power of the direct incident source or neutral density filters with known transmittance are used to attenuate the incident light to a power that will not harm the detector. In either case, the receiver aperture must be large enough to detect all of the incident light.

The receiver field of view should be large enough to ensure that all of the light scattered by a sample into the detector solid angle is captured by the detector. In general, the field of view must be at least as large as the largest projected incident spot. The field of view should

therefore be characterized by moving a small diffuse source laterally in the sample plane and recording the change in received signal [38]. Finally, the receiver detector must be linear over the entire signal range of the measurement and should have uniform sensitivity over its area. The detector should also have a known spectral responsivity curve to account for differing sensitivities with respect to wavelength.

The electronics package of *BRDF* measurement systems vary but may include amplifiers, source monitors, and A/D converters. These electronics may be used and changed out for different sample requirements such as samples with low reflectivity, high specular reflection, or very large samples. The controlling software of a *BRDF* measurement system must be completely integrated with all electronics and motion controllers and ensure that user inputs are easily accessible and documented [37]. Lastly, as with any sensitive measurement, extraneous signals and sources should be mitigated. For *BRDF* measurements, this primarily includes stray light, whether from unwanted sources or scatter off of instruments and other objects. To accomplish this, shrouds and baffles are often used to block highly-reflective objects such as optical posts and sample mounts. The field of view of the receiver may also be decreased to only allow for light scattered off the sample to be detected. An unnecessarily large field of view increases the chance of detecting light scattered off of other sources.

Chapter 3

Methods

This chapter describes the methodologies and processes undertaken in this research to properly address the objectives described in Section 1.3. Specifically, these entailed the development and verification of the GHS algorithm in software and the design and execution of a *BRDF* measurement system.

3.1 Generalized Harvey-Shack Algorithm Development

First, the GHS algorithm was developed in MATLAB[®] to operate with arbitrary inputs of surface roughness, incident angle, and wavelength. The development of this software included validation via the GHS Python code developed by Johansen [36] and results shown in literature for known surfaces.

3.1.1 Characterization of Surface Roughness

The Generalized Harvey-Shack (GHS) method, as discussed in Section 2.1, is based on a linear systems treatment of surface scattering. The GHS method, as well as its “Original” and “Modified” predecessors, defines a surface transfer function that acts as a phase disturbance on the incoming radiation. For the GHS theory, the surface transfer function, H_s , is

defined as

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp\{-[2\pi\hat{\sigma}_{rel}(\gamma_i + \gamma_s)]^2[1 - C_s(\hat{x}.\hat{y})/\sigma_s^2]\}. \quad (3.1)$$

As clearly seen in Equation 3.1, the surface transfer function is dependent on the surface autocovariance (ACV) function, C_s . All surface scatter theories use some numerical description of the surface roughness to formulate the resultant scatter. As discussed in Section 2.1, the Rayleigh-Rice model is similarly directly dependent upon the surface power spectral density (PSD) function.

Consider the one-dimensional surface profile in Figure 3.1. The surface is defined to have a zero mean with surface height, h , varying as a function of position. Two very relevant statistical surface characteristics are the surface height distribution function and the surface ACV function. Very often, the surface heights feature a Gaussian distribution and the root-mean-square (rms) surface roughness, σ_s , is the standard deviation of that distribution. However, the ACV function is not necessarily Gaussian and is material and process dependent. The correlation length, l_c , is defined as the half-width of the ACV function at the $1/e$ height and generally describes the spacing of surface roughness features. The squared rms roughness is the value of the ACV function at the origin and generally describes the height of surface roughness features. The ACV function can be calculated from a two-dimensional surface profile $h(x, y)$ by multiplying the function by the translated version of itself, and then averaging. Note that the autocorrelation and autocovariance functions are identical when the mean of the signal is zero (as it is here). The ACV is essentially the average of a function convolved with itself [37]:

$$C(x', y') = \lim_{L \rightarrow \infty} \frac{1}{L} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} h(x, y)h(x + x', y + y')dxdy. \quad (3.2)$$

Another highly relevant roughness statistic is the surface PSD function. This function describes the spatial frequency content of the surface and, per the Wiener-Khinchin Theorem, is the Fourier transform pair of the ACV function. Thus, the ACV and PSD express the same information in different domains. The PSD expresses surface statistics in the spatial frequency domain while the ACV expresses the same information in the “lag length” space. Due to the central ordinate theorem of Fourier transforms, the peak in one domain is

Figure 3.1: Surface Roughness Parameters [6]

the integral over all space in the other domain. Since the peak of the ACV is the square rms roughness, the volume under the PSD curve is also defined as the square rms roughness. The PSD (or ACV) function is often used as the main input to *BRDF* prediction. The PSD function can be calculated from a two-dimensional surface profile $h(x, y)$ by:

$$PSD(f_x, f_y) = \lim_{L \rightarrow \infty} \frac{1}{L^2} \left| \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} h(x, y) e^{-j2\pi(f_x x + f_y y)} dx dy \right|^2. \quad (3.3)$$

Here, f_x and f_y are the spatial frequencies in the x and y dimensions and L is the length of the surface profile in both dimensions. Note, however, that for finite surface profiles ($L < \infty$), these quantities become band-limited in their calculation. The minimum frequency, f_{min} , is determined by the profile length and the maximum frequency, f_{max} , is determined by the number of points in the profile scan. Furthermore, the “relevant” surface roughness is also dependent on the wavelength and incident angle. For normal incidence, spatial frequencies greater than $1/\lambda$ produce evanescent waves that do not result in scattered radiant power. For an arbitrary incident angle, θ_i , the boundary of the appropriate band-limited portion of the surface PSD is a circle of radius $1/\lambda$ whose center is shifted to a spatial frequency $f_0 = \sin \theta_o / \lambda$, where $\theta_o = -\theta_i$. The corresponding relevant roughness, σ_{rel} , is the square root of the volume under the relevant portion of the surface PSD [6]:

$$\sigma_{rel}(\lambda, \theta_i) = \sqrt{\int_{-1/\lambda + f_0}^{1/\lambda + f_0} \int_{-\sqrt{1/\lambda^2 - (f_x - f_0)^2}}^{\sqrt{1/\lambda^2 - (f_x - f_0)^2}} PSD(f_x, f_y) df_x df_y}. \quad (3.4)$$

This relevant roughness determines the fraction of the total reflected light contained in

the reflected specular beam. For normal incidence, the above equation simplifies to:

$$\sigma_{rel}(\lambda, \theta_i) = \sqrt{2\pi \int_{f_0}^{1/\lambda} PSD(f) f df}. \quad (3.5)$$

Because the main dependency of the GHS algorithm is the surface roughness, described either by the ACV or PSD function, it is imperative that surface roughness is accurately characterized numerically. To accomplish this, sinusoidal and random Gaussian surfaces were generated and their ACV and PSD functions computed and analyzed. First, the ACV and PSD functions were computed via Equations 3.2 and 3.3 respectively. Since the ACV and PSD functions are Fourier pairs, the computed functions may be compared to their transform-derived counterparts. In other words, because the ACV and PSD represent the same information in different domains, there are two ways of generating each function. One may calculate the ACV or PSD directly from the data, or one may calculate one (e.g. the ACV) and then apply a Fourier transform to obtain the other (e.g. the PSD):

$$PSD(f_x, f_y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} ACV(x, y) e^{-j2\pi(f_x x + f_y y)} dx dy. \quad (3.6)$$

3.1.1.1 Sinusoidal Surface

First, a two-dimensional surface consisting of a one-dimensional sinusoid, the surface with the simplest PSD, was constructed and analyzed. This one-dimensional sinusoidal surface was created with a smooth spatial frequency of $f = 0.03/\lambda$, where λ is the wavelength of light. For this case, a wavelength of 632 nm was used. Figure 3.2 shows the resultant surface and a horizontal cut of the surface on which analysis was performed.

First, the ACV of the surface cut in Figure 3.2b was obtained using the one-dimensional equivalent of Equation 3.2 and is shown in Figure 3.3a. In MATLAB[®], this requires looping through each element in the array and each possible lag length. Because of this nested-loop process, the direct calculation of the ACV is relatively inefficient compared to calculation of the PSD through the use of the Fast-Fourier-Transform (FFT). For example, a 512 x 512 surface takes nearly 7 minutes to compute the 2-D ACV, compared to less than half a second for the 2-D PSD of the same surface.

Next, the PSD of the surface cut in Figure 3.2b was obtained using the one-dimensional

Figure 3.2: Surface Plots of 1-D Sinusoidal Surface

equivalent of Equation 3.3. This calculation is fairly simple and results in the one-dimensional PSD in Figure 3.3b. In order to provide verification of the numerical calculation of the ACV and PSD, the Fourier transforms of each were compared to their directly calculated counterparts. The results of this are shown by the dashed lines of Figures 3.3a and 3.3b, displaying excellent agreement between the direct and FFT methods.

Figure 3.3: ACV/PSD of 1-D Sinusoidal Surface - Both Methods

Lastly, the two-dimensional ACV and PSD are calculated for the full two-dimensional surface and are shown in Figure 3.4. Because of the greater efficiency of the PSD calculation, surface roughness will be quantified via the PSD calculation and converted to the ACV when needed.

Figure 3.4: ACV/PSD of 2-D Sinusoidal Surface

3.1.1.2 Gaussian Surface

The next simplest model of a rough surface is an isotropic Gaussian surface. A surface is “isotropic” if its surface roughness statistics are invariant with respect to position. Most surfaces with Gaussian distributions feature Gaussian ACV functions. If the surface is isotropic and has a Gaussian ACV, the ACV is azimuthally symmetric and can be expressed by:

$$ACV_{gauss} = \sigma^2 e^{-l_c^2(x^2+y^2)}. \quad (3.7)$$

Here, σ is the rms roughness and l_c is the correlation length, as discussed previously. Because the Fourier-transform of a Gaussian is a Gaussian, the corresponding PSD of a Gaussian surface is:

$$PSD_{gauss} = \pi \sigma^2 l_c^2 e^{-\frac{f_x^2 + f_y^2}{l_c^2}}. \quad (3.8)$$

Surfaces with Gaussian ACV are common in both rough surface scatter modeling and measurement and are therefore an important class of surfaces. As will be seen in Section 4.1, most literature results for the GHS algorithm are for surfaces with Gaussian ACVs. As shown in Section 4.1, this provides a useful way to validate the correct implementation of the GHS algorithm.

As a second example surface, a Gaussian surface is constructed with a target rms height and correlation length using a Gaussian filter and convolution of Fourier transforms. A map of this surface and a one-dimensional cut through the surface are shown in Figure 3.5.

Figure 3.5: Surface Plots of Gaussian Surface

The resultant ACV and PSD functions of the one-dimensional cut are shown in Figure 3.6, showing high agreement between both methods of direct calculation and calculation through FFT. It is evident from these plots that the surface does not exhibit strictly Gaussian surface statistics. The ACV in Figure 3.6a follows a Gaussian shape until about 12 wavelengths in lag length. The corresponding PSD in Figure 3.6b lacks a clear Gaussian form due to the spatial frequency contribution of the data in the ACV past 12 wavelengths. The two-dimensional ACV and PSD functions of the constructed 2-D Gaussian surface are shown in Figure 3.7. The Gaussian nature of the ACV function of this surface is well-pronounced in Figure 3.7a.

Figure 3.6: ACV/PSD of 1-D Gaussian Surface - Both Methods

Figure 3.7: ACV/PSD of 2-D Gaussian Surface

3.1.2 Algorithm Implementation

Once surface roughness is numerically characterized, the ACV (or PSD) function, wavelength, and incident angle are declared as inputs to the GHS algorithm. This section discusses some of the details in the implementation of the GHS algorithm in MATLAB®.

3.1.2.1 GHS Method Overview

The general process of the GHS model from Section 2.1.2.2 is repeated here to describe the purpose of sections of the software algorithm. As discussed previously, the GHS is built on the development of the surface transfer function approach to surface scatter theory. This surface transfer function, repeated here in Equation 3.9, is dependent on the incident and scattering angle and a new transfer function must therefore be generated for each combination of incident and scattering angle:

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp\{-[2\pi\hat{\sigma}_{rel}(\gamma_i + \gamma_s)]^2[1 - C_s(\hat{x}, \hat{y})/\sigma_s^2]\}. \quad (3.9)$$

The angle spread function, ASF , is then the Fourier transform of the surface transfer function, H_s , shifted to the location of the specular reflection, $\alpha_0 = \sin(-\theta_i)$:

$$ASF\{\alpha_s, \beta_s\} = \mathcal{F}\{H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) \exp(-i2\pi\alpha_0\hat{x})\}|_{\alpha=\alpha_s, \beta=\beta_s}. \quad (3.10)$$

This ASF then describes the light scattered in the (α_s, β_s) direction. This two-dimensional Fourier transform must be calculated for every (α_s, β_s) direction, unless the analytical form

is known and can be solved for a priori. The direction cosines α_s and β_s are related to γ_s by:

$$\gamma_s = \sqrt{1 - \alpha_s^2 - \beta_s^2} \quad (3.11)$$

Krywonos and Harvey commonly break the surface transfer function into two components: a constant term, A , and a frequency and angle dependent term, G :

$$H_s(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = A + B G(\hat{x}, \hat{y}; \gamma_i, \gamma_s). \quad (3.12)$$

Where

$$A = \exp \{ -[2\pi(\gamma_i + \gamma_s)\hat{\sigma}_{rel}]^2 \}, \quad (3.13)$$

$$B = 1 - \exp \{ -[2\pi(\gamma_i + \gamma_s)\hat{\sigma}_{rel}]^2 \}, \quad (3.14)$$

and

$$G(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \frac{\exp \{ [2\pi(\gamma_i + \gamma_s)]^2 \hat{C}(\hat{x}, \hat{y}) \} - 1}{\exp \{ [2\pi(\gamma_i + \gamma_s)\hat{\sigma}_{rel}]^2 \} - 1}. \quad (3.15)$$

This separation of the surface transfer function is done so that the resultant ASF is made up of a specular term, a Dirac delta function, and a scattered term, S :

$$ASF(\alpha_s, \beta_s) = \mathcal{F}\{A + BG(\hat{x}, \hat{y}; \gamma_i, \gamma_s)\} = [A\delta(\alpha - \alpha_0, \beta) + S(\alpha - \alpha_0, \beta)]_{\alpha=\alpha_s, \beta=\beta_s}, \quad (3.16)$$

where

$$S(\alpha - \alpha_0, \beta) = B \mathcal{F}\{G(\hat{x}, \hat{y}; \gamma_i, \gamma_s) \exp(-i2\pi\alpha_0\hat{x})\}. \quad (3.17)$$

Therefore, Equation 3.13 corresponds to the portion of the total incident light that is reflected into the specular direction when $\gamma_s = \gamma_i$. When this is the case,

$$A = \exp \{ -[4\pi\gamma_i\hat{\sigma}_{rel}]^2 \}. \quad (3.18)$$

Likewise, Equation 3.14 corresponds to the portion of the total incident light that is diffusely scattered and is given by:

$$B = 1 - A = 1 - \exp \{ -[4\pi\gamma_i\hat{\sigma}_{rel}]^2 \}. \quad (3.19)$$

It is important to note that, in practice, the only piece of Equation 3.16 that is often shown in results is the *scattered* distribution of the reflected light. Most literature results omit the specular peak predicted by Equation 3.16 since its location, $-\theta_i$, and its amplitude, A , are known. The inclusion of the specular peak in plotted results would dominate and

obfuscate the diffusely scattered portion.

Lastly, the ASF must be renormalized to unit volume within the unit circle in direction cosine space to ensure conservation of energy.

3.1.2.2 Software Structure and Numerical Calculations

This section describes the steps and structure in the development of software to implement the GHS method. This section includes some of the details and nuances of programming such a code in order to provide the field with an example to allow for easier implementation by others in the future. This section also includes intermediate results from an isotropic Gaussian surface that depict the functionality and purpose of the software.

1. Inputs and Settings

First, the user must define several inputs. These inputs include a surface height map along with the sampling points in both dimensions. Currently, the software enforces that the sampling of the surface is at least as fine as $\lambda/5$. This is so that the ACV function is well-sampled near the origin. Inputs also include the wavelength and incident angle. The ASF must be calculated for all scattered angles in the hemisphere so that the ASF can be properly normalized. The user may, however, input the number of points to sample in the hemisphere when calculating the ASF . The user must also supply the reflectance of the surface, R , as well as a directory in which to save results.

2. Setup Spatial and Spatial Frequency Domains

The software then proceeds to setup the spatial (x, y) and spatial frequency (f_x, f_y) domains. The spatial domain is input from the user. The spatial frequency domain is determined by the spatial domain and the sampling criteria. If the x and y domains are setup such that a “bar” ($\bar{}$) denotes the extent of the variable, i.e. $\bar{x} = x(end) - x(1)$, and Δx denotes the difference between adjacent entries in x , then

$$x = -\bar{x}/2 : \Delta x : \bar{x}/2, \quad y = -\bar{y}/2 : \Delta y : \bar{y}/2, \quad (3.20)$$

and

$$f_x = -\bar{f}_x/2 : \Delta f_x : \bar{f}_x/2, \quad f_y = -\bar{f}_y/2 : \Delta f_y : \bar{f}_y/2. \quad (3.21)$$

The Nyquist-Shannon sampling criteria states that a signal must be sampled at a rate that is twice the highest frequency of interest. Here, however, transforming into the frequency domain means that the frequency domain is being sampled. Thus, the Nyquist sampling criteria for this case states that the frequency domain must be sampled at a rate that is twice the extent of the spatial domain. Mathematically, this is equivalent to

$$\Delta f_x < \frac{1}{2\bar{x}}. \quad (3.22)$$

Because $\Delta f_x = \bar{f}_x/N$, where N is the number of samples when transforming into the spatial frequency domain, the Nyquist criteria is written as

$$\Delta f_x = \frac{\bar{f}_x}{N} < \frac{1}{2\bar{x}}. \quad (3.23)$$

Finally, since $\bar{f}_x = 1/\Delta x$,

$$\frac{1}{N\Delta x} < \frac{1}{2\bar{x}} \implies N > 2\frac{\bar{x}}{\Delta x}. \quad (3.24)$$

Because the FFT function in MATLAB[®] operates most efficiently when N is a power of 2, the function `nextpow2` is used to ensure N meets the sampling criteria as a power of 2. If N is exactly $2\frac{\bar{x}}{\Delta x}$, then the frequency domain is critically-sampled. Best practices, however, dictate that the data is at least slightly oversampled. Oversampling, though it produces a small amount of extra computation, ensures that the proper information is obtained during the transform.

An additional sampling constraint is placed on the spatial frequency domain to ensure sufficient sampling in the spatial frequency domain of interest. As discussed in Section 2.1 and in [2], the calculation of the *ASF* is most conveniently done in direction cosine space. These direction cosines are related to the spherical angles by

$$\alpha = \sin \theta \cos \phi, \quad \beta = \sin \theta \sin \phi, \quad \gamma = \cos \theta. \quad (3.25)$$

The spatial frequencies are related to these angles by the conical diffraction grating

equations:

$$f_x = \frac{\sin \theta_s \cos \phi_s - \sin \theta_i}{\lambda}, \quad f_y = \frac{\sin \theta_s \sin \phi_s}{\lambda}. \quad (3.26)$$

Substituting in the direction cosines yields

$$f_x = \frac{\alpha_s - \alpha_0}{\lambda}, \quad f_y = \frac{\beta_s}{\lambda}. \quad (3.27)$$

Because the ASF in Equation 3.16 features a frequency shift, the α_0 in Equation 3.27 is dropped, yielding an equation for the direction cosines in terms of the spatial frequencies, f_x and f_y

$$\alpha_s = \lambda f_x, \quad \beta_s = \lambda f_y. \quad (3.28)$$

As discussed in Section 2.1, only spatial frequencies beneath $\frac{1}{\lambda}$ produce propagating waves. Therefore, it is important to ensure that the region from $-\frac{1}{\lambda}$ to $\frac{1}{\lambda}$ (the unit circle in direction cosine space) is well-sampled. The software, after finding the number of points to satisfy Nyquist-Shannon sampling via Equation 3.24, if necessary, increases the sampling to at least $N \geq 50\lambda\bar{f}$ for both f_x and f_y . This guarantees that α and β include 100 points between -1 and 1. This importance is increased because the ASF will need to be interpolated at requested scattered angles, (θ_s, ϕ_s) , since the ASF is calculated in direction cosine space.

3. Calculate Surface PSD/ACV

Once the spatial frequencies, f_x and f_y , are calculated, Equation 3.3 is performed, yielding the PSD of the surface. This is calculated in MATLAB® via `fft2`. As an example of a software calculation, the specific MATLAB® command issued is:

$$\text{PSD} = \text{abs}(\text{fftshift}(\text{fft2}(S, \text{NFFT}_y, \text{NFFT}_x)))^2 * \\ dx * dy / \text{length}(x) / \text{length}(y)$$

Here, S is the two-dimensional surface array, $\text{length}(x)$ and $\text{length}(y)$ are the number of elements in x and y respectively, and NFFT_x and NFFT_y are the number of samples in the x and y dimensions. Note that the MATLAB® `fft` function requires scaling the outputs by the Δ of the input array (e.g. $dx * dy$). This PSD is then used to calculate the surface's ACV, as discussed above in Section 3.1.1. Lastly, the PSD

is used to calculate the relevant, band-limited, surface roughness, σ_{rel} , via Equation 3.4.

4. Loop Over All Scattered Angles

Once the above calculations are performed, the loop over all scattered angles commences. The ASF is preallocated to the size specified by the user. The scattered direction cosines are also predefined and are linearly spaced from -1 to 1 with the number of samples determined by the ASF . The software then features two nested for loops over all combinations of α_s and β_s .

- (a) **Define Direction Cosines** At each iteration, (j, k) , the direction cosines are selected from the precomputed arrays and are now defined as $\alpha_{s,j}$ and $\beta_{s,k}$. $\gamma_{s,jk}$ is defined as

$$\gamma_{s,jk} = \sqrt{1 - \alpha_{s,j}^2 - \beta_{s,k}^2} \quad (3.29)$$

The ASF is then calculated for any combination of $\alpha_{s,j}$ and $\beta_{s,k}$ that remain in the unit circle. For combinations of $\alpha_{s,j}$ and $\beta_{s,k}$ that fall outside the unit circle, the ASF is set to zero.

- (b) **Calculate Surface Transfer Function (A , B , and G)**

Next, the surface transfer function is calculated in terms of A , B , and $G(\hat{x}, \hat{y}; \gamma_i, \gamma_s)$. These are calculated using Equations 3.13 - 3.15. A surface transfer function for an isotropic Gaussian surface with $\sigma = 0.5\lambda$, $l_c = 5\lambda$, $\alpha_s = 0.88$, and $\beta_s = 0$ is shown in Figure 3.8.

- (c) **Obtain Intermediate ASF via 2-D FFT of G**

Next, for each scattered angle, a new *intermediate* ASF must be calculated. This necessitates that a two-dimensional Fourier transform is performed for each combination of (α_s, β_s) . Then, *one* point from this intermediate ASF corresponding to (α_s, β_s) is retained in the final ASF [2].

As discussed in Section 3.1.2.1, the ASF is only calculated for the *scattered* portion of the reflected light, i.e. $G(\hat{x}, \hat{y}; \gamma_i, \gamma_s)$. Thus, the intermediate ASF is calculated by taking the Fourier transform of G . Note that in MATLAB[®],

Figure 3.8: Surface Transfer Function of Gaussian Surface
 requesting a FFT with N larger than the number of samples in the input array “zero-pads” the input data to produce finer sampling in the output array. Simply “zero-padding” the transfer function produces a *rect* function in the transfer function, resulting in an unwanted *sinc* function in the *ASF*. To prevent this, the surface transfer function must be padded with its minimum, or steady-state, value. The transfer function of Figure 3.8 thus becomes padded as the one shown in Figure 3.9.

With a padded surface transfer function, the intermediate *ASF* is obtained through a frequency-shifted two-dimensional Fourier transform, as in Equation 3.17. However, when the surface, and thus the surface transfer function, is isotropic, the two-dimensional Fourier transform of a radially symmetric function is equivalent to a Hankel transform of order zero [3]. Let $f(r)$ be a radially-dependent function. Its Fourier transform is then:

$$g(f_x, f_y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(r) e^{-j2\pi(f_x x + f_y y)} dx dy. \quad (3.30)$$

If we substitute x and y for the usual spherical coordinates r , θ , and ϕ and let

Figure 3.9: Properly Padded Surface Transfer Function of Gaussian Surface

$q = \sqrt{f_x^2 + f_y^2}$, then

$$g(q) = \int_0^\infty \int_0^{2\pi} f(r) e^{-j2\pi r q (\cos \phi \cos \theta + \sin \phi \sin \theta)} r dr d\theta, \quad (3.31)$$

which is reduced to

$$g(q) = \int_0^\infty f(r) \left[\int_0^{2\pi} f e^{-j2\pi r q \cos \theta} d\theta \right] r dr, \quad (3.32)$$

and finally,

$$g(q) = 2\pi \int_0^\infty f(r) J_0(2\pi r q) r dr, \quad (3.33)$$

where J_0 is the zeroth order Bessel function of the first kind. Therefore, the two-dimensional FFT is substituted for a one-dimensional Hankel transform. The code for the discrete Hankel transform is from [40]. The time to generate the *ASF* for an isotropic surface is then *greatly* reduced. An intermediate *ASF* corresponding to the surface transfer function of Figure 3.9 is shown in Figure 3.10.

5. Renormalize Final *ASF*

Once the final *ASF* is known for every scattered angle, the *ASF* must be renormalized to unit volume within the unit circle in direction cosine space. Thus, $ASF(\alpha_s, \beta_s)$

Figure 3.10: Intermediate ASF of Gaussian Surface must be scaled by a constant, K , which is computed as:

$$K = \frac{1}{\int_{\alpha=-1}^{\alpha=1} \int_{\beta=-\sqrt{1-\alpha^2}}^{\beta=\sqrt{1-\alpha^2}} ASF(\alpha, \beta) d\alpha d\beta}. \quad (3.34)$$

However, since this is only the scattered portion of the ASF , K is then multiplied by B as given by 3.19. The final ASF is then multiplied by the coefficient BK . The final ASF for the same Gaussian surface is shown in Figure 3.11. Lastly, the $BRDF$ for one incident angle is simply calculated as the scalar reflectance of the surface, R , multiplied by the ASF :

$$BRDF(\theta_s, \phi_s) \Big|_{\theta_i, \phi_i} = R \cdot ASF(\alpha_s, \beta_s). \quad (3.35)$$

The conversion from $BRDF$ to intensity, I , is calculated by multiplying by the cosine of the scattered angle:

$$I(\theta_s, \phi_s) \Big|_{\theta_i, \phi_i} = R \cdot ASF(\alpha_s, \beta_s) \cos \theta_s. \quad (3.36)$$

Figure 3.11: Final Renormalized ASF of Gaussian Surface

6. Plot and Save

Once all calculations are completed, plots are constructed of the final *ASF*, the scattered intensity of the *BRDF* in the plane of incidence, and the scattered radiance in the plane of incidence. Then all settings, inputs and outputs, and plots are saved to the hard disk.

(a) ASF of Gaussian Surface in Plane of Incidence (b) *BRDF* of Gaussian Surface in Plane of Incidence

Figure 3.12: In-Plane *ASF* and *BRDF* of Gaussian Surface

3.2 *BRDF* Measurement System Development

This section includes the discussion of the design, construction, testing, and validation of a *BRDF* measurement system. This section is broken down into parts that discuss the requirements of each system component, the chosen implementation for each component, and how each component satisfies its requirements.

3.2.1 Measurement Design

In general, a *BRDF* measurement system must independently manipulate the incident and scattered angles in both azimuth and elevation. The design of this system should allow for measurement of the entire hemisphere for both incident scattered angles, save for a few special cases. This requires positioning that accommodates four angular degrees of freedom for θ_i , ϕ_i , θ_r , and ϕ_r . This is often accomplished, and is done in this research, through mounting the sample holder to a three-axis stage and rotating the source or receiver on an arc about the center of the sample.

This is also the measurement design used by NIST's Robotic Optical Scatter Instrument (ROSI) and ROSI's predecessors, STARR and STARR II [8], [41], [42], [43], [7]. The configuration of the measurement system in this research is highly adapted from the design of NIST's measurement system and is shown in Figure 3.13. ROSI utilizes a six-axis robotic arm for rotation and translation of the sample, and a receiver mounted to an arm on a rotary stage that moves the receiver about the center of the sample [7]. The system also includes a stationary light source which illuminates the center of the sample.

Figure 3.13: *BRDF* Measurement System Setup

3.2.1.1 Coordinate System

In the configuration described above, the four angles θ_i , ϕ_i , θ_r , and ϕ_r are manipulated by three angles associated with the robotic arm and one angle associated with the receiver rotation stage. These two motorized units make up what is henceforth referred to as the goniometer. The four spherical angles are shown in Figure 3.14. In order to control these angles via the goniometer, the angles α , β , γ , and δ are defined as described in [8] and depicted in Figure 3.15.

Figure 3.14: Definition of Spherical Angles from [7]

Figure 3.15: Definition of Goniometer Angles from [8]

The following derivations closely follow [8]. Let $\hat{x}, \hat{y}, \hat{z}$ be the coordinate system fixed to the sample and $\hat{x}', \hat{y}', \hat{z}'$ be the coordinate system fixed to the laboratory. When $\alpha = \beta = \gamma = 0$, the two coordinate systems are identical. Applying a rotation of angle γ about $\hat{z}'$, followed by a rotation of angle β about $\hat{x}'$, and lastly followed by a rotation of angle α about $\hat{y}'$, the conversion from goniometer angles to sample frame angles is expressed by:

$$\theta_i = \arccos(\cos \alpha \cos \beta), \quad (3.37a)$$

$$\theta_r = \arccos(\cos \beta \sin \alpha \sin \delta + \cos \alpha \cos \beta \cos \delta), \quad (3.37b)$$

$$\phi_i = \text{atan2}(-\cos \gamma \sin \alpha - \cos \alpha \sin \beta \sin \gamma, \cos \alpha \cos \gamma \cos \beta - \sin \alpha \sin \gamma), \quad (3.37c)$$

$$\begin{aligned} \phi_r = \text{atan2}[-\cos \delta (\cos \gamma \sin \alpha - \cos \alpha \sin \beta \sin \gamma) + \\ \sin \delta (\cos \alpha \cos \gamma - \sin \alpha \sin \beta \sin \gamma), \\ \sin \delta (\cos \gamma \sin \alpha \sin \beta + \cos \alpha \sin \gamma) + \\ \cos \delta (\cos \alpha \cos \gamma \sin \beta - \sin \alpha \sin \gamma)], \end{aligned} \quad (3.37d)$$

where $\text{atan2}(x, y)$ is the 2 argument arctangent that takes into account which quadrant

the point (x, y) lies in:

$$\text{atan2}(x, y) = \begin{cases} \tan^{-1}\left(\frac{y}{x}\right), & \text{if } x > 0 \\ \tan^{-1}\left(\frac{y}{x}\right) + \pi, & \text{if } x < 0 \\ \frac{\pi}{2}, & \text{if } x = 0 \text{ and } y > 0 \\ -\frac{\pi}{2}, & \text{if } x = 0 \text{ and } y < 0. \end{cases} \quad (3.38)$$

The conversion from sample frame angles to goniometer angles is expressed in [43] by:

$$\delta = \text{sgn}(\sin(\phi_r - \phi_i)) \arccos(\sin \theta_i \sin \theta_r \cos(\phi_i - \phi_r) + \cos \theta_i \cos \theta_r), \quad (3.39a)$$

$$\alpha = \arctan\left(\frac{\cos \theta_r - \cos \delta \cos \theta_i}{\sin \delta \cos \theta_i}\right), \quad (3.39b)$$

$$\beta = \arccos\left(\frac{\cos \theta_i}{\cos \alpha}\right), \quad (3.39c)$$

$$\gamma = \begin{cases} \text{atan2}(-\tan \alpha, \sin \beta) - \phi_i, & \text{if } \theta_i \neq 0 \\ \text{atan2}(\tan(\delta - \alpha), \sin \beta) - \phi_r, & \text{if } \theta_i = 0, \end{cases} \quad (3.39d)$$

where

$$\text{sgn}(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ -1, & \text{if } x < 0. \end{cases} \quad (3.40)$$

These equations thus define the goniometer angles, α , β , γ , and δ , required for a given θ_i , ϕ_i , θ_r , and ϕ_r .

3.2.1.2 Motion Control

As discussed, the goniometer angles, α , β , γ , and δ , are controlled via the six-axis robotic positioner and a rotary stage. For this research, the robotic positioner used was a Yaskawa Motoman HP20F, with repeatability of 60 μm and a maximum payload of 20 kg. This robotic positioner was programmed via LabVIEW to perform the appropriate translations and spherical rotations to accomplish all positioning needed by it in the measurement system. This was accomplished utilizing the Yaskawa Motoman Robotics Library by Digimetrix [44]. The rotation stage responsible for positioning the receiver was a Daedal 20501 stage with a Compumotor S57-51-M0 motor capable of 5.0 arcmin accuracy and 0.3 arcmin repeatability.

The illumination source and rotation stage for this measurement system are on an optical table next to the robot. The illumination source, a Helium-Neon (HeNe) laser, is positioned at a height of 15.75 in. and lateral location of (39.5 in., 12.5 in.) with respect to the corner of the optical table, as shown in Figure 3.17. The rotation stage is fixed to the table such that the axis of rotation is about the point (39.5 in., 12.5 in.) with respect to the same corner of the optical table, as shown in Figure 3.17. This configuration ensures that the illumination source and the axis of the rotary stage are orthogonal to one another and define the plane of the sample when $\alpha = \beta = \gamma = 0$.

Figure 3.16: Diagram of Measurement Layout

Figure 3.17: Locations of Components in Measurement Layout

The robotic positioner used to articulate the sample is commonly used for pick-and-place applications in factories. As such, the robot's usage had to be adapted for use in complex articulation. This was accomplished through the use of programming a "tool" attached to the end of the robot. After attaching a "tool" to the end of the robot, the user can calibrate to a particular point on the tool. The robot is now able to perform all normal functions, including rotations about the Cartesian axes, with that point as the point of rotation. This became the basis of goniometric rotation about a point on the sample face. With this calibrated tool, the robot is also able to learn user-defined coordinate frames. In order to align the sample with the illumination source and the rotation stage, the robot is taught a coordinate frame defined by the optical table. Once the sample is calibrated as a tool, the robot is able to position the face of the sample at a point in space above the optical table directly over the axis of the rotation stage while aligned with the incident light source.

3.2.2 The Illumination Source

As discussed in Section 2.2, the system must also include an illumination source with known spectral content, polarization, and beam size. The incident light should also be collimated or slightly converging in order to limit the variance in incident angle. The illumination source employed in this research is a Helium-Neon (HeNe) laser, operating at 632.8 nm. This particular HeNe is of an unknown manufacturer or model number. As such, the exact beam diameter or polarization is not known. However, the beam is clearly smaller than the detector aperture of 9.5 mm diameter. It is conservatively estimated that the beam size is about 3mm, which is more than sufficiently small for this measurement system. Were the polarization known, it would not impact the results since the GHS model does not include polarization effects.

3.2.3 The Receiver

The requirements of a receiver for the accurate measurement of $BRDF$ include dynamic range, aperture size, field of view, and spectral responsivity. Because $BRDF$ is defined for each given wavelength, the responsivity of the receiver must be known for the

wavelength(s) tested. This is generally accomplished through calibration by the manufacturer.

Recall that, from Section 2.2, $BRDF$ is equivalent to:

$$BRDF = \frac{P_r}{P_i \Omega \cos \theta_r} \quad (3.41)$$

where P_i is incident power, P_r is the reflected power, θ_r is the reflected elevation angle, and Ω is the solid angle of the receiver [38]. Because the calculation of $BRDF$ is highly dependent on the receiver solid angle, Ω , it is imperative that the receiver have a well-defined aperture.

Additionally, $BRDF$ values may range from 10^6 sr^{-1} for highly specular mirrors and small apertures to 10^{-9} sr^{-1} for a noise-limited system measuring the surrounding air molecules [37]. As such, the receiver used must produce a linear response over quite a large dynamic range. The dynamic range of the system is then a product of the aperture size, reflected elevation angles, incident power, and minimum detectable power.

The final consideration for a receiver is the field of view. In order to properly measure the scatter off of a sample, the field of view of the receiver must always be larger than the projected illumination spot on the sample. Since this field of view is generally constant throughout the measurement, the field of view is set to be larger than the largest projected spot size on the sample. This occurs at the largest incident elevation angle since the projected area, A_p , becomes an ellipse at nonzero incident elevation with area

$$A_p = \frac{A_0}{\cos \theta_i}, \quad (3.42)$$

where A_0 is the spot size of the illumination at $\theta_i = 0^\circ$. If absolute calibration is desired, as it is in this research, all of the incident irradiance and scattered radiance must be measured by the receiver. The field of view, and the solid angle Ω will be defined by the size of the receiver optic nearest the sample and the distance from that optic to the sample.

The receiver utilized in this research employs a silicon photodiode detector, the Thorlabs S120VC. The specifications of this detector are shown in Table 3.1. The detector features spectral calibration performed by the manufacturer and wavelength selection to ensure proper spectral responsivity. The console used in operating the detector is the Thor-

labs PM100D. The control console also employs a zeroing function to help alleviate the effect of electronic noise within the detector. The detector also features a power dynamic range of six orders of magnitude. Additionally, though the detector’s reported minimum optical power working range is 50 nW, the PM100D console reports power in the range of hundreds of pW. As will be shown in measurement results below, it is likely that the 50 nW recorded in Table 3.1 is a conservative estimate, as the detector reports optical power down to hundreds of pW with no illumination. Below 50 nW, the detector still reports apparently linear values in actual *BRDF* measurements.

Detector Type	Silicon Photodiode (UV extended)
Wavelength Range	200 - 1100 nm
Optical Power Working Range	50 nW - 50 mW
Max Average Power Density	20 W/cm ²
Linearity	±0.5%
Resolution	1 nW
Measurement Uncertainty	±3% for 440 - 980 nm
Input Aperture	∅9.5 mm

Table 3.1: Thorlabs S120VC Detector Specifications from [9]

The field of view (FOV) of the receiver is set by the aperture and its distance from the sample. Since the diameter of the incident beam is less than 3 mm, the maximum FOV was conservatively set at 3 inches. The aperture in the receiver is a Newport UPA1-.5 mirror mount adapter with an 11.1 mm diameter aperture mounted to the detector through three 1 inch lens tubes to limit the FOV. This aperture was set at 9 27/32 inches from the sample face.

The FOV calculations follow the illustration in Figure 3.18. The goal of these calculations is to set the FOV at 3 inches and find the ray with the most extreme angle that is still able to arrive at the detector. This then allows for the determination of the distance between the sample and the aperture. This “extreme” angle is defined as α in the figure below.

Figure 3.18: Calculation of Field of View - Receiver Geometry

The diagram on the right of Figure 3.18 begins the calculations through the determination of θ by

$$\tan \theta = L / (d + (a - d)/2). \quad (3.43)$$

α is then related to θ by

$$\alpha = 180^\circ - 2\theta. \quad (3.44)$$

l and h are then

$$l = \frac{FOV}{2 \tan \alpha/2}, \quad h = \frac{d}{2 \tan \alpha/2}. \quad (3.45)$$

Which gives

$$D = l - (L - h). \quad (3.46)$$

The distance from the aperture to the detector, L , is set at 3 in. of lens tube plus the distance from the end of the threads to the detector within the powermeter, which is about 3.3 mm. The size of the detector, d , is set at 9.5 mm and the size of the aperture, a , is set at 11.1 mm. For a FOV of 3 in., the corresponding D is 9.89 in.

Once the receiver assembly was set at the above distance, a FOV characterization measurement was performed as discussed in Section 2.2. In this measurement, a small flashlight with a high divergence angle was used to resemble a small diffuse source. This source was mounted to the robotic positioner and moved so that the beam emanated from the sample plane. This was done to simulate scatter from the surface (or other objects) from a particular location in the sample plane to determine whether the receiver could detect scatter from that location. The robot then positioned the source in both lateral dimensions across the sample plane while the powermeter detected the “scattered” light.

Figure 3.19 shows the results of this measurement. The lateral positioning was performed from -3 in. to 3 in. every 0.25 in. in both dimensions. The results indicate that little to no light outside of the 3 in. calculated FOV is able to be detected. The red circle in Figure 3.19 corresponds to the intended FOV of 3 in. diameter. In fact, 97.79% of the total power is contained within the central 3 in. of the FOV. Thus, the FOV of the receiver is confirmed to be nearly exactly 3 in.

Figure 3.19: Characterization of Field of View

3.2.4 Measurement Control Software

The entire software suite controlling the measurement system is programmed in LabVIEW utilizing the Yaskawa Motoman Robotics Library mentioned above [44] and various other instrument drivers. Each measurement starts with recording measurement parameters such as sample name, incident and scattering angles, receiver distance, file paths, notes, and the many required instrument settings. These settings are saved to disk upon starting the measurement. The user may also select whether only in-plane measurements are required. Though the entire system was designed and built to perform in- and out-of-plane measurements, only in-plane measurements were performed and presented here due to time and scope constraints. The relevant research questions are still sufficiently answered with in-plane measurements.

Once the user starts the LabVIEW program, the robot moves up and out of the way while the receiver arm rotates to $\delta = 180^\circ$ to acquire an incident power measurement. This is performed before each measurement, and the corresponding *BRDF* calculations are all done with respect to each measurement's incident irradiance measurement.

After the incident power measurement, the software loops through all combinations

of $(\phi_i, \phi_r, \theta_i, \theta_r)$, in that order. In the future, a more mechanically efficient order may be implemented that loops through combinations of $(\alpha, \beta, \delta, \gamma)$. For each incident angle where $\phi_i \neq \phi_r$ (forward scatter), θ_r is more finely sampled in the specular region. For the $\pm 10^\circ$ surrounding the expected specular peak, the sampling criteria is automatically doubled. This is to help capture the rapidly-varying behavior of the specular region and to successfully capture the location of the specular peak.

First, the robot rotates the sample face about $\hat{z}'$ in the User Frame. Next, the robot rotates the sample about $\hat{z}$ (sample surface normal). When out-of-plane measurements are desired, the robot then rotates about β . This movement presents a challenge as the sample's lateral plane is not easily defined. As discussed above, the axis about which β rotates is calculated by rotating $\hat{x}'$ about the angle α . To accomplish this in the robot's coordinate systems, extrinsic Euler angles are used to rotate about an arbitrary axis in Cartesian space by rotating about each of the stationary (extrinsic) axes $\hat{x}', \hat{y}', \hat{z}'$, in that order. Finally, the receiver arm rotary stage is rotated an angle δ . To conserve time, any of the movements above are only executed for nonzero movements. Before each iteration, the new positions of the robot and rotary stage are checked to avoid collision. If collision will happen within the next iteration, the movement order is swapped so that the rotary stage moves out of the way of the robot.

The software, after waiting for each movement to complete, triggers the powermeter. The powermeter takes and averages 300 measurements, and the corresponding reflected power is stored in an array. Once all movements are completed, the reflected power and incident and scattering angles are written to disk. If there is already data stored in the assigned folder, new files are created instead of overwriting the existing data and settings. Finally, the receiver and robot positioners are returned to their starting positions.

3.2.5 Capabilities and Limitations

As discussed above, the design of this system should allow for measurement of the entire hemisphere for both incident scattered angles, save for a few special cases. These special cases include incident and scattering elevation angles near 90° , where, for incident

angles near 90° , the projected area of the incident light approaches infinity and, for scattered angles near 90° , the surface becomes infinitesimally small from the receiver's point of view. Most *BRDF* measurement systems therefore limit the incident and scattered elevation angles to a hard limit near 75° or 80° . The chosen limit in the system developed here is 80° . These special cases also include backscatter, where the incident and scattered angles are the same and the receiver blocks the source or vice versa. Most *BRDF* measurement systems either interpolate these very small areas or do not report measured values, while others employ optics such as beamsplitters. For this system, backscattered *BRDF* will be obscured by the receiver. As such, it will be measured and reported as virtually 0 in all cases.

The dynamic range of any *BRDF* measurement system is essentially limited by the dynamic range of the detector, the power of the incident illumination, and the solid angle. For the system developed here, the incident power, P_i , is nearly constant at 1 mW. Furthermore, the solid angle, Ω , is chosen to be constant with a 0.374 in. (9.5 mm) aperture at 12 27/32 in. from the sample face. This translates to a fixed solid angle of 0.000666 sr. Because the minimum optical working range of the detector is 50 nW from Table 3.1, the minimum and maximum *BRDF* can be calculated as a function of angle, as shown in Figure 3.20. The maximum *BRDF* values range from 8647 sr^{-1} to 1501 sr^{-1} for scattered angles of $\pm 80^\circ$ and 0° respectively. Conversely, the minimum *BRDF* values range from 0.4323 sr^{-1} to 0.07507 sr^{-1} for scattered angles of $\pm 80^\circ$ and 0° respectively. Though the minimum optical working range of the sensor is 50 nW, the detector console will report values as low as 100 pW. These values will be below the reported working range of the detector and will be below the minimum *BRDF* shown here. These values should therefore be treated with caution.

Figure 3.20: *BRDF* Measurement System Dynamic Range

3.3 Surface Roughness Measurement

In order to properly test the validity of the GHS model, the surface roughness of the measured surfaces must be characterized. To accomplish this, atomic force microscopy (AFM) measurements were performed for several samples. First, these samples are introduced. Second, the usage of the AFM is discussed. Below in Section 4.3, the roughness of these surfaces is characterized via PSD and ACV functions.

3.3.1 Sample Surfaces

Because the GHS model claims validity over all domains of surface roughness and incident and scattering angles, surfaces with varying roughness and scattering profiles were desired. For example, from Equation 2.53, it becomes apparent that the amount of light reflected in the specular direction is directly dependent upon the rms surface roughness, σ_s . Likewise, it is well established that surfaces with low correlation lengths, and thus low separation between peaks, feature a wider scattering profile [2]. Because models for smooth surfaces have been well-verified in the past, surfaces with roughness much less than one wavelength ($\sigma \ll \lambda$) and surfaces with correlation lengths much higher than the

wavelength ($l_c \gg \lambda$) are not highly desired for this research.

Therefore, it was intended that sample surfaces be made of the same material with varying rms roughness and varying correlation length. The science of designing surfaces based on particular surface roughness, however, is complicated and is beyond the scope of this research. For example, the surfaces in [22] were fabricated via spin-coating glass plates with three layers of high-resolution photoresist. Next, the plates were exposed to laser speckle produced by an argon-ion laser a large number of times. Next, the plates were processed in photoresist developer so as to produce a linear relation between exposure and surface height. Finally, the plates were coated with a layer of gold or aluminum, using vacuum-coating methods. The resulting surfaces featured excellent Gaussian ACV functions and varying rms roughness.

Such surfaces or processes were not available during this research. However in order to best achieve a change in surface roughness, sandpaper with differing grits were used on aluminum and high-density polyethylene (HDPE). These surfaces were chosen due to their high reflectivity (aluminum) or malleability (HDPE). It is imperative that the surfaces feature negligible transmitted light because the surfaces are backed by a black-anodized aluminum plate. Any transmitted light will reflect off of this plate, transmit through the material a second time through a different point on the sample, and appear as reflected light at an angle uncaused by surface reflections. Initially, ABS plastic was used instead of HDPE due to being easily sanded. The ABS samples, however, were slightly transparent and featured undesirable measured $BRDF$ values.

First, a random orbital sander was used to uniformly and randomly sand the HDPE samples with 50, 120, 220, and 320 grit sandpaper. All but the 320 grit HDPE proved too rough for AFM measurements and did not vary in their distribution of light scatter. Next, the aluminum samples were wet-sanded by hand with 400, 600, 1200, and 2000 grit sandpaper. The wet-sanding was done in small circular motions, intended to provide negligible directional bias. Lastly, an electrically-polished aluminum sample was obtained to provide a very smooth sample.

Sample surfaces consisted of:

1. 6061 Aluminum:
 - (a) Wet-Sanded with 400-grit
 - (b) Wet-Sanded with 600-grit
 - (c) Wet-Sanded with 1200-grit
 - (d) Wet-Sanded with 2000-grit
2. HDPE Plastic:
 - (a) Sanded with 320-grit
3. Electrically Polished 304 Stainless Steel

Figure 3.21: All Aluminum and HDPE Samples

Figure 3.22: 400 Grit and 600 Grit Sanded Aluminum Samples

Figure 3.23: 1200 Grit and 2000 Grit Sanded Aluminum Samples

Figure 3.24: Electrically Polished Aluminum Sample and 320 Grit Sanded HDPE Sample

3.3.2 Atomic Force Microscopy Measurements

Surface roughness measurements were performed using a Bruker Dimension Icon AFM at Ohio State University's Nanosystems Lab, shown in Figure 3.25. For all measurements, $40\ \mu\text{m} \times 40\ \mu\text{m}$ scan sizes were used with 256×256 points, providing 156 nm resolution. At 632.8 nm, this resolution corresponds to 0.247λ and supplies a spatial frequency bandwidth from -3.2×10^6 to $3.2 \times 10^6\ 1/\text{m}$. In terms of direction cosines, this spans from -2.025 to 2.025 and is double the range needed for the GHS calculations. The AFM was used in "Tapping Mode" in which the cantilever is oscillated at its resonant frequency. Any perturbation to its native travel caused by the tip contacting the surface is then detected by a laser and sophisticated photodiodes. The lateral positioning noise is at most 0.15 nm, while the height sensor noise is 50 pm. The "TESP" etched silicon tip radius was approximately 10 nm in radius, with a front angle of 25° and a back angle of 15° .

Due to time constraints, three or four AFM measurements were conducted for each sample at locations near the center and approximately 10 mm from the center towards the top, bottom, and left of the sample face. Images of the surface obtained from a microscopic imager on the AFM are shown below in addition to examples of the surface maps produced by the AFM.

Figure 3.25: Bruker Dimension Icon Atomic Force Microscope

Figure 3.26: Microscope Images of 400 Grit and 2000 Grit Sanded Aluminum

Figure 3.27: Microscope Images of 320 Grit Sanded HDPE and Polished Aluminum

Figure 3.28: AFM Image and Surface Plot of 400 Grit Sanded Aluminum

Figure 3.29: AFM Image and Surface Plot of 2000 Grit Sanded Aluminum

Figure 3.30: AFM Image and Surface Plot of 320 Grit Sanded HDPE

Figure 3.31: AFM Image and Surface Plot of Electrically Polished Aluminum

One of the first things noticed when examining the above images are the large features seen in the sanded aluminum samples. These large “gashes” are seen in much of the wet-sanded data and may be due to particulates stuck between the surface and sandpaper, resulting in an effectively lower grit size and nonuniformity. Conversely, there also seems to be a very clear and desirable “micro-roughness” pattern in the sanded aluminum images.

Secondly, the roughness of the sanded HDPE sample is much larger than any of the aluminum samples, even the 400 grit aluminum, and appears quite uniform. This is likely due to the fact that a power random orbital sander was used for this sample, generating a statistically large number of passes. The aluminum samples, sanded by hand, likely did not feature enough passes to create consistent uniformity in both surface height and feature direction.

Lastly, the electrically polished aluminum sample is very smooth and features a one-dimensional grain pattern that is even clearly detectable by the naked eye. Even this pattern, though, is only on the order of tens of nanometers and will appear very smooth optically.

Chapter 4

Results

This chapter describes all results following the implementation of the efforts described in Chapter 3. First, the validation of both the GHS model implementation and the *BRDF* measurement system are discussed. Next, the characterization of the surfaces analyzed through AFM is described. Once the needed roughness characteristics are obtained, the GHS model is used to predict the *BRDF* from the sample surfaces. *BRDF* measurements of the individual sample surfaces are discussed along with the corresponding uncertainty analysis. Finally, the comparison of predicted and measured *BRDF* results is analyzed.

4.1 Generalized Harvey-Shack Algorithm Verification

First, the verification of the implementation of the GHS algorithm was accomplished through comparison with GHS results published in literature for surfaces with Gaussian ACV.

Comparative results are gathered from two main sources: Krywonos' 2006 Dissertation, [2], and 2011 article, [6], and the Python program from Johansen in [36]. Results from [2] and [6] will be compared side by side with results from the GHS implementation in this research. The plots from [2] and [6] are screenshots from electronic versions of the references since the raw data was not available. Results from [36] are calculated numeri-

cally using the referenced author’s included Python code (“Python-GHS”) and are overlaid with results from this research (“MATLAB-GHS”).

All results are for surfaces with Gaussian ACV functions of known form. As such, the surfaces themselves are not constructed. Rather, Equations 3.7 and 3.8 are used to completely describe the surface. Plots from [2] also include results from the Rayleigh-Rice smooth surface approximation (RR) and the Modified Harvey-Shack (MHS) model in addition to the GHS results. Results from [6] are for a particular surface with specified roughness parameters since data for this surface was available for two incident angles. These results include experimental data for two specific incident angles: 20° and 70° . For all incident angles, the results from [6] include data from the Original, Modified, and Generalized Harvey-Shack method.

Literature Results: $\sigma/\lambda = 0.02, l_c/\lambda = 5$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.1: Literature Comparison for $\sigma/\lambda = 0.02, l_c/\lambda = 5, \theta_i = 0^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.2: Literature Comparison for $\sigma/\lambda = 0.02$, $l_c/\lambda = 5$, $\theta_i = 20^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.3: Literature Comparison for $\sigma/\lambda = 0.02$, $l_c/\lambda = 5$, $\theta_i = 50^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.4: Literature Comparison for $\sigma/\lambda = 0.02, l_c/\lambda = 5, \theta_i = 70^\circ$

Literature Results: $\sigma/\lambda = 0.02, l_c/\lambda = 0.5$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.5: Literature Comparison for $\sigma/\lambda = 0.02, l_c/\lambda = 0.5, \theta_i = 0^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.6: Literature Comparison for $\sigma/\lambda = 0.02$, $l_c/\lambda = 0.5$, $\theta_i = 20^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.7: Literature Comparison for $\sigma/\lambda = 0.02$, $l_c/\lambda = 0.5$, $\theta_i = 50^\circ$

(a) Literature Results from [2]

(b) Current Implementation and Python Implementation from [36]

Figure 4.8: Literature Comparison for $\sigma/\lambda = 0.02, l_c/\lambda = 0.5, \theta_i = 70^\circ$

Literature Results: $\lambda = 10.6\mu m, \sigma = 2.27\mu m, l_c = 20.9\mu m$

(a) Literature Results from [6]

(b) Current Implementation and Python Implementation from [36]

Figure 4.9: Literature Comparison for $\lambda = 10.6\mu m, \sigma = 2.27\mu m, l_c = 20.9\mu m, \theta_i = 20^\circ$

(a) Literature Results from [6]

(b) Current Implementation and Python Implementation from [36]

Figure 4.10: Literature Comparison for $\lambda = 10.6\mu m$, $\sigma = 2.27\mu m$, $l_c = 20.9\mu m$, $\theta_i = 40^\circ$

(a) Literature Results from [6]

(b) Current Implementation and Python Implementation from [36]

Figure 4.11: Literature Comparison for $\lambda = 10.6\mu m$, $\sigma = 2.27\mu m$, $l_c = 20.9\mu m$, $\theta_i = 60^\circ$

Figure 4.12: Literature Comparison for $\lambda = 10.6\mu m$, $\sigma = 2.27\mu m$, $l_c = 20.9\mu m$, $\theta_i = 70^\circ$

As clearly seen in the data above, excellent agreement exists in all cases between the Python results from [36] and the results from this research. Comparisons between the 2006 results from [2] match moderately well with the results of this research. The shapes and locations of the main peak show excellent agreement in all cases. Discrepancies between results are only apparent in the scale of the data. For most cases, the difference is small. There exists, however, one particularly mismatched case for $\sigma/\lambda = 0.02$, $l_c/\lambda = 0.5$, $\theta_i = 70^\circ$, shown in Figure 4.8, where the results from [2] are nearly double the results of this research and the Python code.

Lastly, comparisons between results from [6] match very well with the results of this research. The 2011 results in [6] are from the same authors (Krywonos, Harvey, et al.) as the 2006 results in [2], but 5 years later. Upon further investigation, it appears that the main difference between these two references are the inclusion and usage of the bandlimited “relevant” surface roughness, σ_{rel} . The surface transfer function in [2] is formulated as:

$$H_s^{2006}(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp\{-[2\pi\hat{\sigma}_s(\gamma_i + \gamma_s)]^2[1 - C_s(\hat{x}, \hat{y})/\sigma_s^2]\}, \quad (4.1)$$

while the surface transfer function in [6] is formulated as:

$$H_s^{2011}(\hat{x}, \hat{y}; \gamma_i, \gamma_s) = \exp\{-[2\pi\hat{\sigma}_{rel}(\gamma_i + \gamma_s)]^2[1 - C_s(\hat{x}, \hat{y})/\sigma_s^2]\}. \quad (4.2)$$

This difference does not have a large impact when σ_s and σ_{rel} are nearly identical, as in Figure 4.2 where σ_s and σ_{rel} are the same up to three decimal places. The effect is com-

pounded in cases such as Figure 4.8 where $\sigma_{rel}/\sigma_s = 0.676$ and there is poor agreement between [2] and the results of this research. This effect is likely responsible for discrepancies in the magnitudes mentioned above. Note that the Python code from [36] includes σ_{rel} .

This “relevant” surface roughness is discussed fully in Section 3.1.1. The difference between σ_s and σ_{rel} stems from the fact that only the portion of the PSD with spatial frequencies less than $1/\lambda$ contribute to propagating waves. Thus, any difference between σ_s and σ_{rel} arises from the presence of high spatial frequency terms, often encountered with surfaces with short correlation lengths. This notion corresponds well with the disagreement in Figure 4.8, where the short correlation length produces large differences in σ_s and σ_{rel} . Conversely, σ_s and σ_{rel} are nearly identical for surfaces with highly specular reflection, commonly seen in smooth surfaces with negligible high frequency content.

These results indicate successful implementation of the GHS model in MATLAB®. The strong agreement with the Python code developed in [36] and with the 2011 results of [6] for varying surface roughness and incident angles show that the algorithm, when supplied proper inputs, generates the outcome predicted by the GHS model.

4.2 *BRDF* Measurement of Diffuse Reflectance Standard

In order to verify the performance of the *BRDF* measurement system, a calibrated reflectance standard was obtained and measured. The results of this standard are discussed before results from actual surface samples. This is done to provide a measure of validation to results of unknown surfaces.

The specific standard used was a diffuse reflectance standard known as Spectralon. The standard, fabricated by Labsphere, is used very widely in industry and is regarded as an excellent example of an approximate Lambertian reflector. The specific Spectralon standard used was a 12 in. x 12 in. 99% reflective target and is shown mounted in Figure 4.13. The target is calibrated to have a hemispherically-integrated reflectance of 0.9921 when illuminated from 8° elevation.

Labsphere also supplied a technical report in which the $BRDF$ of a typical 99% reflective Spectralon target was measured for an incident angle of 30° elevation and 90° azimuth. $BRDF$ curves are reported for all reflected elevation angles and for reflected azimuth angles of -90° , -45° , 0° , 45° , and 90° and are shown in Figure 4.14. Unfortunately, only a digital image of Labsphere's results are available. Without the actual numerical data from Labsphere, only graphical comparison may be performed. Comparisons are then made between Labsphere's light blue curve representing an in-plane ($\phi = -90^\circ$) measurement. The dip shown for the in-plane data ($\phi = -90^\circ$) in Figure 4.14 is caused by the inability to measure backscatter since the receiver blocks the incident light source. This dip is also present in the data from the measurement system developed here for the same reason. The flat black curve labeled " $0.99/\pi$ " corresponds to the $BRDF$ of an ideal Lambertian reflector with 99% reflectance.

Figure 4.13: $BRDF$ Measurement of Spectralon

Figure 4.14: *BRDF* Curves of Typical Spectralon, Measured by Labsphere

BRDF measurements were then performed for the acquired Spectralon target. Measurements were executed for 30° incident elevation for both “sides” of the target (i.e. incident azimuth angles of 0° and 180°). These results are shown in Figure 4.15. These measurements were also performed at both surface orientations by rotating the target 90° about its normal. These results are shown in Figure 4.16. Each measurement was performed 5 times in succession to gain insight into the repeatability of the measurements.

Both sets of data clearly indicate generally good agreement between Labsphere’s measurements and the measurements presented here. The measured results also closely resemble the *BRDF* of a Lambertian reflector, given by the horizontal black line in all plots. Each figure, like the results by Labsphere, features slight asymmetry between the forward and backward scattered *BRDF*. This is to be expected as virtually all real surfaces exhibit some specular reflection. Furthermore, the data seems to be in agreement regardless of the “side” of the target and regardless of orientation. The lack of dependency on the “side” of the target indicates that the laboratory setup is somewhat uniform with respect to noise and stray light, since the two incident azimuth angles are performed by rotating the sample

about the laboratory z axis clockwise or counterclockwise.

Figure 4.15: Spectralon $BRDF$ Results for $\phi_i = 0^\circ$ and $\phi_i = 180^\circ$

Figure 4.16: Spectralon $BRDF$ Results for Both Polarizations

Although the above agreement between the measured results and results from Lab-sphere is quite good, there is still likely error due to background noise and stray light. This is compounded by the fact that the Spectralon target is 99% reflective and will diffusely scatter any incident light. In order to quantify the amount of “extra” light detected during the Spectralon measurement, the difference in the $BRDF$ for the measured results are subtracted by the $BRDF$ of an ideal Lambertian reflector. This difference is then converted to reflected power. Then, a background measurement of the Spectralon was performed in which the incident light source was turned off, but the rest of the measurement remained the same. This provides a quantitative analysis of the stray light in the laboratory that

contributes to measured $BRDF$ values. The “additional” P_r of the measured Spectralon compared to a Lambertian reflector is shown in Figure 4.17. The measured $BRDF$ and P_r from a “dark” measurement, in which the illuminator was turned off, are shown in Figure 4.18. Note that the Dark $BRDF$ is calculated assuming the incident power is 1 mW.

Figure 4.17: Extra P_r of Spectralon When Compared with Ideal Lambertian Reflector

Figure 4.18: Dark Measurement of Spectralon

Figure 4.18b shows that any stray sources of light in the laboratory and background noise are on the order of tens of pW, far below the conservative minimum power threshold of the detector. This data clearly indicates that any stray sources of light in the laboratory are negligible and do not appreciably affect measured $BRDF$ results. This data is not sufficient to quantify the stray light from the source that is scattered off of other objects during the measurement. The agreement shown between Labsphere’s results and the measured

results here indicate reasonably low levels of stray light scatter.

4.3 Roughness Characterization Results for Sample Surfaces

Next, the characterization of surface roughness for the sample surfaces is discussed for use as an input to the GHS model. After obtaining AFM surface data, the data was imported to the associated analysis software. Here, the surfaces were “flattened” by removing 1st order tilt that may have arisen due to the surfaces not featuring flatness on the order of nanometers. Then, the surfaces were exported to text files to be analyzed in MATLAB®.

In MATLAB®, the surfaces were characterized according to the discussion in Section 3.1.1. When converting real sampled surface profiles into PSDs, it is well-known that individually-sampled “local” profiles often contain much noise and vary greatly from the true “global” PSD of the surface. This is the resultant from a localized area not containing statistically significant information on the surface as a whole. Thus, an ensemble average of the PSDs of many different profiles acquired across the surface must be calculated. Generally, this process would require an exorbitant amount of time, as upwards of 20 profiles at different locations would need to be acquired. There is, however, another way to provide an ensemble averaged PSD without acquiring such large datasets that involves breaking a few sampled profiles into smaller subprofiles. Then, the PSD is calculated from each subprofile, and the estimated PSDs are averaged together. This method is generally valid when the correlation length of the relevant surface’s features is much shorter than the total profile length. This method is credited to Elson and Bennett from [45], in which they state that the length of the subprofiles must be many times the correlation length. The example analysis shown in [45] features subprofile lengths roughly 10-20 times the correlation length.

The surface maps obtained from the AFM are analyzed by first breaking the individual maps into “blocks” whose PSDs are calculated and averaged together. First, the data is imported into MATLAB®. Because correlation lengths (calculations entailed below) are on the order of 2 -3 μm , the 40 μm x 40 μm surface maps are only able to be broken up into 20 μm x 20 μm blocks, generating 4 blocks per surface.

Each block's PSD is then calculated and averaged together with blocks from measurements at different points on the surface. Since each surface was measured 3 or 4 times, there are 12 or 16 blocks for each surface. An example of this process is shown for the 2000 grit sanded aluminum in Figure 4.19. The corresponding two-dimensional PSD for 2000 grit sanded aluminum is shown in Figure 4.20.

Figure 4.19: Raw and Averaged PSDs of 2000 Grit Sanded Aluminum

Figure 4.20: Averaged PSD of 2000 Grit Sanded Aluminum

Next, the ACV of the averaged PSD is calculated as the two-dimensional Fourier transform of the PSD. The ACV for the 2000 grit sanded aluminum is shown in Figure 4.21. This process is performed for each of the sample surfaces. The resulting PSD and ACV for each surface is shown below.

Figure 4.21: ACV of 2000 Grit Sanded Aluminum

Figure 4.22: Averaged PSD and ACV of 400 Grit Sanded Aluminum

Figure 4.23: Averaged PSD and ACV of 600 Grit Sanded Aluminum

Figure 4.24: Averaged PSD and ACV of 1200 Grit Sanded Aluminum

Figure 4.25: Averaged PSD and ACV of 320 Grit Sanded HDPE

Figure 4.26: Averaged PSD and ACV of Polished Aluminum

The above data indicate many differences between the surfaces. For example, the drop off present in the ACV of the 400 grit aluminum (Figure 4.22) is much faster than the other

sanded aluminum samples. This is generally indicative of a lack of lower spatial frequency (higher lag length) content. This corresponds with the 400 grit PSD in Figure 4.22 as the first peaks are further away from the origin than the other sanded aluminum samples.

Another feature that varies between samples is the angle of the distribution in the ACV functions. Since the ACV is the covariance/correlation between the surface and itself, the ACV would be circular in shape and Gaussian in distribution if the surface were actually random. If the two dimensions were uncorrelated but had differing variances, then the ACV would be a Gaussian with two different variances and eigenvectors parallel to the main axes. However, when the eigenvectors are not parallel to the main axis, as they are not here, then the two dimensions are correlated and the eigenvectors are tied to the variances and covariances of the two dimensions. All of the surfaces, besides the polished aluminum, feature eigenvectors at an angle with respect to the main axes [46].

The polished aluminum sample clearly contains a dominant spatial frequency component related to the grains running parallel to one another in the material. Along these grains, there is essentially no roughness and the ACV function never reaches zero. Perpendicular to these grains, the ACV rapidly decays and provides a correlation length directly related to the spacing of the grains.

Finally, the sanded HDPE sample features the most Gaussian ACV function, shown by the slower decay from its peak near the origin. Additionally, the overall spacing of features is evidently larger as shown by the extent of the nonzero portion of the ACV extending to $\pm 5 \mu m$. Furthermore, the high peak value of the ACV of the HDPE indicates the higher rms roughness expected from the HDPE sample.

For this research, the sample surfaces are assumed to be isotropic. In reality, of course, they are not perfectly isotropic, as seen by the angled eigenvectors in the above ACVs. To accommodate for this, *BRDF* measurements were taken with the sample's orientation at 0° and 90° and were averaged together. Thus, the plane of incidence rotates between the two lateral surface dimensions.

As stated previously, the fabrication of surfaces to desired roughness characteristics is quite complicated and is beyond the scope of this research. Thus, the surfaces shown here

feature nonuniformity and non-standard roughness characteristics. Like the fabrication of engineered surfaces, the endeavor of detailed characterization of surface roughness is beyond the scope of this research. This is the reason the surfaces were intended to have uniform roughness and standard characteristics during fabrication. Though this is not the case in a strict sense, the surfaces still feature random and very Gaussian distributions. The distribution of the surface height for each surface, for all blocks, is shown below.

Figure 4.27: Surface Height Distribution of 400 and 600 Grit Sanded Aluminum

Figure 4.28: Surface Height Distribution of 1200 and 2000 Grit Sanded Aluminum

Figure 4.29: Surface Height Distribution of 320 Grit HDPE and Polished Aluminum

Because the surface height distribution is generally Gaussian in shape, the ACVs shown above each resemble Gaussians (in each dimension), the specific surface dimensions are not well-defined, and to simplify computations, each surface will be regarded as having a Gaussian ACV with one rms roughness, σ_s , and one correlation length, l_c . Clearly from the ACVs shown above, the surfaces generally do not have the same decay in the x and y dimensions and will therefore have different correlation lengths in each dimension. The discrepancy in these two correlation lengths will be the most important contributor to the analyzed uncertainty in the GHS simulations of these surfaces. To quantify this effect, GHS simulations will be performed for three correlation lengths, l_c^x , l_c^y , and their mean, l_c , for each surface to bound the uncertainty in correlation length. Because the method of averaging PSDs to remove noise from individual profiles does not consider each profile as a sampling of the same value, there is not a clear method of further quantifying the uncertainty in the surface roughness. Ideally, these surfaces would be governed by σ_s and l_c , each with an uncertainty bound encompassing the spread of possible actual values. Instead, the surfaces, and thus the GHS simulations, here will have uncertainty associated with l_c but not σ_s .

The rms roughness, σ_s , of any surface is easily calculated as

$$\sigma_s = \frac{1}{M N} \sum_{i=0}^M \sum_{j=0}^N h_{ij}, \quad (4.3)$$

where h_{ij} is the surface height at the (i^{th}, j^{th}) element. In order to calculate the correlation

lengths of the ACVs of the surfaces, the horizontal and vertical cuts of the ACV were analyzed by finding the lag length at which the ACV had fallen to $1/e$ times its maximum. The resulting surface roughness parameters are shown in Table 4.1.

Sample	σ_s	l_c^x	l_c^y	l_c	σ_s/λ	l_c/λ
400G Al	0.204 μm	2.52 μm	2.20 μm	2.36 μm	0.323	3.73
600G Al	0.200 μm	3.31 μm	2.20 μm	2.76 μm	0.316	4.36
1200G Al	0.200 μm	1.89 μm	2.36 μm	2.13 μm	0.315	3.36
2000G Al	0.200 μm	2.36 μm	2.05 μm	2.20 μm	0.315	3.48
320G HDPE	1.31 μm	4.25 μm	3.31 μm	3.78 μm	2.06	5.97
Polished Al	0.0251 μm	10.7 μm	0.787 μm	5.75 μm	0.0397	9.08

Table 4.1: Surface Roughness Parameters for Sample Surfaces

Table 4.1 clearly indicates a lack of appreciable or predictable change in roughness for the sanded aluminum surfaces. Section 3.3.2 discusses the possible causes. Because the sanded aluminum surfaces do not vary much, only two of the four surfaces will be simulated and measured. The two chosen were the 600 grit and 2000 grit samples due to the unexpectedly long correlation length of the 600 grit sample and the fact that the 2000 grit sample should be the smoothest of the sanded aluminum samples. Additionally, the 320 grit sanded HDPE and the polished aluminum are both simulated and measured.

4.4 *BRDF* Results for Sample Surfaces

As mentioned above, the four samples to be measured were the 600 and 2000 grit sanded aluminum, the 320 grit HDPE, and the polished aluminum. Plane of incidence *BRDF* measurements were conducted for these four samples. For each surface besides the polished aluminum, measurements were performed at five different locations on the surface. Note that all locations are relative to each other and are not registered to absolute positions on the surface. These locations were at the center of the surface and the four “corners” 10 mm laterally and vertically on the sample as depicted in Figure 4.30. The

inversion of the coordinate system is due to the method of changing the measurement location. This was done by changing the robot's "tool center position" to $X = 10$ mm and $Y = -10$ mm for "p10m10". The robot then positioned this spot on the sample at the location of the incident beam and center of rotation.

Figure 4.30: Measurement Locations on Sample

Measurements were also conducted with the sample at a normal position and with the sample rotated 90° counter-clockwise. This was done in order to average the surface roughness of the two lateral dimensions since, as discussed previously, the samples are treated as isotropic. Therefore, measurements are done in both orientations are averaged together. Measurements were performed for $\phi_i = 0^\circ$ and $\phi_i = 180^\circ$ at each incident angle. Because the surface is assumed to be isotropic, measurements for both values of ϕ_i are compared with each other.

For each sample (besides polished aluminum), the five locations and two values of ϕ_i provide ten total *BRDF* measurements per sample. The spread of these measurements is discussed below in quantifying measurement uncertainty. The polished aluminum sample was only measured in three locations: center, top, and bottom, where top and bottom are separated from center by 10 mm vertically. Only three locations were needed as the polished aluminum is a very uniform and carefully made surface. Furthermore, its *BRDF* consists only of a specular beam with very low diffuse scattering.

$BRDF$ measurements were done for incident elevation angles of 30° , 45° , and 60° . These angles were chosen to provide a general sampling of near-normal, moderate, and wide incident angles. Scattered angles were spaced every 5° from -80° to 80° . The $\pm 10^\circ$ surrounding the specular region was sampled twice as fine at 2.5° . All measurements were performed in the same configuration with all possible sources of light blocked or turned off. Each sample was measured in one session lasting two hours.

Figure 4.31: $BRDF$ Measurements of 600 Grit Sanded Aluminum - $\theta_i = 30^\circ$

Figure 4.32: $BRDF$ Measurements of 600 Grit Sanded Aluminum - $\theta_i = 45^\circ$

Figure 4.33: *BRDF* Measurements of 600 Grit Sanded Aluminum - $\theta_i = 60^\circ$

Figure 4.34: *BRDF* Measurements of 2000 Grit Sanded Aluminum - $\theta_i = 30^\circ$

Figure 4.35: *BRDF* Measurements of 2000 Grit Sanded Aluminum - $\theta_i = 45^\circ$

Figure 4.36: *BRDF* Measurements of 2000 Grit Sanded Aluminum - $\theta_i = 60^\circ$

Figure 4.37: *BRDF* Measurements of 230 Grit Sanded HDPE - $\theta_i = 30^\circ$

Figure 4.38: *BRDF* Measurements of 320 Grit Sanded HDPE - $\theta_i = 45^\circ$

Figure 4.39: *BRDF* Measurements of 320 Grit Sanded HDPE - $\theta_i = 60^\circ$

Figure 4.40: *BRDF* Measurements of Polished Aluminum - $\theta_i = 30^\circ$

Figure 4.41: *BRDF* Measurements of Polished Aluminum - $\theta_i = 45^\circ$

Figure 4.42: *BRDF* Measurements of Polished Aluminum - $\theta_i = 60^\circ$

Overall, the above data indicate generally consistent values with respect to sample position. The largest variance is seen in the HDPE sample, where small variations in the detected power are more impactful on the low *BRDF* values. As expected, the 600 and 2000 grit sanded aluminum samples are quite specular and are very similar in shape with the 2000 grit sample having slightly wider scatter. To show an overall comparison between the 600 and 2000 grit aluminum results, the *BRDF* of each sample is averaged over all locations and values of ϕ_i . The resultant averaged *BRDF* results for each incident angle are shown in Figure 4.43. These plots show that, for all incident angles, the 600 grit aluminum had more specular scatter than the 2000 grit aluminum. This finding agrees with the longer correlation length found in the 600 grit sample.

Also shown in the above data is the highly specular scatter produced by the polished aluminum sample. Because the *BRDF* features such rapidly varying features, the results for the polished aluminum sample are displayed on a log scale. As expected, the *BRDF* decays rapidly from a high value in the one data point in the specular direction. There is a stark difference in the *BRDF* between the two orientations of the sample. Because “LR” indicates that the grain pattern is in the incident plane, there is negligible effective roughness. However for the “UD” case, the grain pattern is orthogonal to the plane of incidence. Therefore, the surface has a nearly fixed-frequency roughness in this dimension. This is very evident in the PSD of the polished aluminum as seen in Figure 4.26. Because the surface roughness is obviously different between the two orientations, the results from

the polished aluminum sample will not be averaged between its two dimensions. Instead, they will be treated independently.

In stark contrast, the HDPE sample has quite low $BRDF$ values across all scattered angles. Another point of interest in the HDPE data is the apparent slight upward trend when nearing the backscattered direction. Though the data exactly at backscatter is not available due to the receiver obfuscating the illumination, one could easily see a trend to achieve a local maxima at the backscatter angle. This phenomena is often referred to as the “opposition effect” where a surge in reflected intensity is observed when the directions of illumination and reflectance are parallel [47]. There are multiple theories explaining this phenomena, but all generally theorize that it arises with scattering from features that are large compared to the wavelength. This idea is consistent with the presence of an opposition effect seen in the HDPE results, where the surface roughness is certainly larger than the wavelength.

Figure 4.43: Averaged $BRDF$ Measurements of Sanded Aluminum

4.4.1 Uncertainty in $BRDF$ Measurement System

For the measurements presented here, there are essentially two categories of uncertainty. The first category is the uncertainty in the measurement process itself and is associated with the precision of the measurement devices used. Since $BRDF$ is defined as

$$BRDF = \frac{P_r}{P_i \Omega \cos \theta_r}, \quad (4.4)$$

then the total uncertainty equation is [48]

$$\frac{\Delta BRDF}{BRDF} = \left[\left(\frac{\Delta P_r}{P_r} \right)^2 + \left(\frac{\Delta P_i}{P_i} \right)^2 + \left(\frac{\Delta \Omega}{\Omega} \right)^2 + \left(\frac{\Delta \theta_r \sin \theta_r}{\cos \theta_r} \right)^2 \right]^{1/2}. \quad (4.5)$$

Each of the above contributors to the total measurement uncertainty are discussed below. Much of the measurement uncertainty presented here is based on [48].

4.4.1.1 Uncertainty in P_r

First, the uncertainty associated with the measurement of reflected power, P_r , has four main sources:

1. Receiver polarization misalignment
2. Receiver aperture misalignment
3. System noise
4. Detector nonlinearity

The first source, polarization misalignment, is neglected here because the polarization is unspecified and fixed. Because the detector has no polarization preference, there is no effective uncertainty associated with polarization misalignment.

The second source, receiver aperture misalignment, is uncertainty produced by misalignment of the receiver aperture out of the incident plane. To quantify this, the reflected power, P_r , is assumed to be linear on a log-log scale for a small region. This assumption, as stated in [48], often holds for many samples. When this assumption is true, the reflected power may be given as

$$P_r = Ae^{m \ln \theta}, \quad (4.6)$$

where A is a constant, m is the slope of the log-log curve, and θ is the angle from specular ($\theta = \theta_s - \theta_i$). If the scatter is assumed isotropic, the uncertainty can be written as

$$\frac{\Delta P_r}{P_r} = \frac{m}{\theta}(\theta' - \theta), \quad (4.7)$$

where θ' is the actual angle at which the reflected light is measured due to the aperture

alignment. θ' is given by

$$\theta' = \cos^{-1} \left[\frac{R \cos \theta}{(\Delta y^2 + R^2)^{1/2}} \right], \quad (4.8)$$

where R is the distance from the sample to the receiver aperture and Δy is the linear aperture misalignment. For this system, R is set at 12 27/32 in. while Δy is estimated to be 0.5 mm. This value for Δy originates from the alignment of the source and receiver. This process is done by moving the receiver to $\delta = 0^\circ$, then slightly moving the illuminator so the beam is centered on the back of the receiver, moving the receiver back to $\delta = 180^\circ$, and again adjusting the illuminator so the beam is centered on the detector. This process is repeated until adjusting the illuminator is no longer necessary. It is thus estimated that the alignment process could feature misalignment up to 0.5 mm in any direction. The parameter m is obtained by fitting a line to the $BRDF$ in log-log space plotted with the maximum as the first point. The $BRDF$ is trimmed so only half is fitted to a line. In general, the assumption holds well.

The third and fourth sources of uncertainty in the measurement of P_r are system noise and detector nonlinearity. For the detector used here, an uncertainty value is actually supplied and is given in Table 3.1 as $\pm 3\%$. This value will replace the system noise and nonlinearity, as this value encompasses the entire detector system.

4.4.1.2 Uncertainty in Incident Power

The uncertainty in measuring the incident power depends on the uncertainty with respect to the detector as well as uncertainty resulting from aperture clipping and the temporal stability of the incident source. The first source, aperture clipping, results from the receiver aperture having a smaller diameter than the incident beam. For the system developed here, the incident beam is at most 3 mm in diameter while the detector aperture is 9.5 mm. Thus, this uncertainty source is negligible.

The second source, the temporal instability of the source, has a much greater impact. As stated above, the HeNe laser used is of unknown make or model. As such, much of its characteristics were not known ahead of time. One of these unknown characteristics

is power stability. Because many measurements were desired, large amounts of time in excess of 30 minutes were not available to allow the laser to warm up fully. As such, the power variation over time is very apparent in many measurements. In order to characterize the power stability, power measurements were initially acquired for 40 minutes. The resulting stability is shown in Figure 4.44a. Another measurement was performed just after the 40 minute measurement in which the stability was observed for two hours. This data is shown in Figure 4.44b. As is clearly seen, the same instability is still observed but with longer periods. Therefore, it should be assumed that all measurements may feature a temporal change in the power of the laser between 1.05 mW and 1.085 mW, resulting in an uncertainty of $\pm 1.66\%$.

(a) Laser Power Stability Over 40 Minutes

(b) Laser Power Stability Over 2 Hours *Following* 40 Minute Test

Figure 4.44: HeNe Laser Power Stability

4.4.1.3 Uncertainty in Solid Angle

The third source of uncertainty in measuring $BRDF$ is the solid angle of the receiver. Assuming a small circular aperture, the solid angle is given by

$$\Omega = \frac{\pi r^2}{R^2}, \quad (4.9)$$

where r and R are the same as above. The uncertainty in solid angle is then simply given by

$$\frac{\Delta\Omega}{\Omega} = \left[\left(\frac{2\Delta r}{r} \right)^2 + \left(\frac{2\Delta R}{R} \right)^2 \right]^{1/2}, \quad (4.10)$$

where a Δ indicates the uncertainty in the quantity. For this system, Δr is conservatively estimated to be 0.1 mm since this is the aperture of the power meter supplied by the manufacturer. The uncertainty in measuring R is much higher and is estimated to be 1/16 in. or 1.6 mm. The uncertainty in solid angle is therefore fixed at $\Delta\Omega = 1.54 \times 10^{-5}$ sr for the fixed solid angle of 0.000666 sr.

4.4.1.4 Uncertainty in Reflected Angle

The final contributor to $BRDF$ uncertainty is the uncertainty in reflected angle. Though the accuracy and repeatability of the rotary stage is very high, the uncertainty resulting from aligning the sample, illuminator, and rotary stage is conservatively estimated to be $\pm 0.5^\circ$.

The total uncertainty in the measurement system itself is then combined from the above components using Equation 4.5. This uncertainty will depend on specific $BRDF$ values and scattered and incident angles. Two examples of the measurement system uncertainty are shown in Figure 4.45 as “ $\Delta Meas$ ” where error bars are used to represent the uncertainty for each scattered angle.

Figure 4.45: Measurement System Uncertainty for 600 Grit Sanded Al and 320 Grit Sanded HDPE

4.4.2 Uncertainty in Sample $BRDF$

As mentioned above, there are essentially two categories of uncertainty for the results presented here. The first category was the uncertainty in the measurement process itself and is associated with the precision of the measurement devices used. This uncertainty is most

like systematic uncertainty that results from an imperfect measurement system. The second category, discussed here, is the uncertainty resulting from the variance of the $BRDF$ with respect to position on the surface. This uncertainty is more related to random uncertainty as it will depend on the random distribution of the surface itself. The repeatability of the measurement system is also discussed here.

As discussed above, there are ten measurements performed for each sample surface. These are made up of the five locations on the surface and the two values of ϕ_i . Since these measurements are meant to represent the possible variations of the $BRDF$ for a given sample, they are treated as samplings of a random variable. Unfortunately, ten measurements does not constitute a sufficiently large sample set. Therefore, without convergence, the standard deviation of these measurements is used as the basis for uncertainty bounds. Two examples of the uncertainty in the sample are shown in Figure 4.46 as “ $\Delta Samp$ ”. As clearly seen in these plots, the uncertainty with respect to the sample is at least on the order of the uncertainty produced by the measurement system.

Figure 4.46: Sample Uncertainty for 600 Grit Sanded Al and 320 Grit Sanded HDPE

In addition to the ten measurements for each sample, the 2000 grit sanded aluminum was measured five successive times, without removing the sample or realigning, to observe the actual repeatability of the measurement system for one specific measurement. Some of the results are shown in Figure 4.47. Clearly, the data indicate that the general repeatability of the system falls well within the uncertainty bounds of the measurement system discussed above.

Lastly, measurements were conducted to investigate the benefit and resolution obtained by a sampling criteria of 2.5° instead of 5° . The same 2000 grit sanded aluminum sample was measured at a sampling interval of 2.5° except for the 1.25° sampling in the specular region. This data is also shown below in Figure 4.48. The results clearly indicate that doubling the measurement time was not justified by the negligible gain in resolution produced by 2.5° sampling.

Figure 4.47: Measurement System Repeatability Test

Figure 4.48: Comparison of 2.5° and 5° Sampling

4.4.3 Total Uncertainty

The total net uncertainty of each measurement is then combined in a root-sum-squares process as

$$\Delta Total = \sqrt{\Delta Meas^2 + \Delta Samp^2}, \quad (4.11)$$

where $\Delta Meas$ is the uncertainty associated with the measurement system and $\Delta Samp$ is the uncertainty in the $BRDF$ of each sample. Note that the uncertainty associated with the measurement system itself is included in the uncertainty with respect to each sample since the measurements yielding $\Delta Samp$ were performed with the measurement system associated with $\Delta Meas$. Thus, $\Delta Total$ provides a conservative estimation of the total uncertainty in resultant $BRDF$ values. These results are overlaid with the ten measurements for that sample and incident angle. Overall, the total uncertainty is generally low for the sanded aluminum samples. The uncertainty increases nearing the specular peak due to the spread in the measurements across the sample shown above and the increased impact of aperture misalignment near the specular region. The same may be said of the uncertainty in the polished aluminum samples. Here, the uncertainty is very low for all but the specular peak, save for an increase in uncertainty for large scattered angles.

The largest relative spread is seen in the HDPE measurements where the $BRDF$ values are generally low. The increase in uncertainty at large scatter angles is caused by the larger impact of the uncertainty in scattered angle due to the $\cos \theta_r$ term in the denominator of Equation 4.5.

Figure 4.49: *BRDF* and Total Uncertainty of 600 Grit Sanded Aluminum

Figure 4.50: *BRDF* and Total Uncertainty of 2000 Grit Sanded Aluminum

Figure 4.51: *BRDF* and Total Uncertainty of Polished Aluminum - UD

Figure 4.52: *BRDF* and Total Uncertainty of Polished Aluminum - LR

Figure 4.53: *BRDF* and Total Uncertainty of 320 Grit Sanded HDPE

4.4.4 Reciprocity Tests

With the quantification of uncertainty, the measured $BRDF$ results were checked for consistency through a simple reciprocity test. To satisfy reciprocity, interchanging the incident and scattering angles should result in the same measured $BRDF$ value. This test is performed by comparing the results with $\theta_i = 30^\circ$, $\theta_r = 45^\circ$ and $\theta_i = 45^\circ$, $\theta_r = 30^\circ$. The same analysis is performed for all combinations of $\theta_i = 30^\circ$, 45° , 60° . Reciprocity tests for HDPE and aluminum are shown in Figures 4.54 - 4.58. The black circles indicate values that should agree. Within uncertainty bounds, the data shows high reciprocal agreement.

Figure 4.54: Reciprocity Tests for HDPE

Figure 4.55: Reciprocity Tests for HDPE and Aluminum

(a) Reciprocity -600 Grit Al for $\theta = 30^\circ, 60^\circ$

(b) Reciprocity - 600 Grit Al for $\theta = 45^\circ, 60^\circ$

Figure 4.56: Reciprocity Tests for Aluminum

(a) Reciprocity - 2000 Grit Al for $\theta = 30^\circ, 45^\circ$

(b) Reciprocity - 2000 Grit Al for $\theta = 30^\circ, 60^\circ$

Figure 4.57: Reciprocity Tests for Aluminum

(a) Reciprocity Test for 2000 Grit Al for $\theta = 45^\circ, 60^\circ$

(b) Reciprocity Test for Polished Al - LR for $\theta = 30^\circ, 45^\circ$

Figure 4.58: Reciprocity Tests for Sanded and Polished Aluminum

(a) Reciprocity Test for Polished Al - UD for $\theta = 30^\circ, 60^\circ$ (b) Reciprocity Test for Polished Al - UD for $\theta = 45^\circ, 60^\circ$

Figure 4.59: Reciprocity Tests for Sanded and Polished Aluminum

4.5 GHS Results for Sample Surfaces

Once the surface roughness of the sample surfaces were characterized, GHS simulations were performed with the roughness parameters listed in Table 4.1, assuming Gaussian ACV. As stated previously, GHS simulations were performed for the correlation lengths in each lateral dimension and the mean correlation length. The GHS simulations were executed as discussed in Section 3.1.2 utilizing Gaussian ACV functions similar to the calculations in Section 4.1.

Note that all results shown in this section feature the *diffusely* scattered portion of the $BRDF$. In other words, the specular peak is not shown or calculated in this data. This is due to the fact that the specular peak is theoretically a Dirac delta function with infinitesimally small width. This, of course, is not the case in actual measured $BRDF$. In measurements, the reflected power contained in the specular peak is averaged over the collecting aperture. Thus, the peak of the specular lobe will depend on the specific measurement scenario. The implementation of this is discussed more in the comparison of predicted and measured $BRDF$ in Section 4.6.

Finally, each plot features text that indicates the scalar reflectance value used in the GHS simulations, R , and the calculated fraction of diffusely scattered light, B . As discussed

above, the parameters A and B are calculated when expressing the GHS transfer function in terms of a specular term and a diffuse term. The coefficients corresponding to each are A and B respectively and define the fraction of light scattered specularly and diffusely. The inclusion of the B parameter is to provide information about how much light is contained in the specular lobe since the specular lobe is not featured in these simulated results. The order of the B values correspond to the order of the plot's legend.

4.5.1 Sanded Aluminum

For the sanded aluminum samples, GHS simulations were performed for incident angles of $\theta_i = 30^\circ, 45^\circ$, and 60° . Simulations were also, as discussed above, performed for the correlation lengths in each of the x and y dimensions as well as their mean. The resultant data is shown below in Figures 4.60 and 4.61. The only other input to the GHS model not yet discussed is the scalar reflectance of the surface under consideration. This scalar reflectance refers to the Fresnel reflectance of a very smooth surface of the same material as the rough surface. Because bare aluminum is a very common optical surface, its reflectance is known well and is widely reported as approximately 90% [49]. Thus, this 90% reflectance value is used for the sanded and polished aluminum samples.

The data below is generally difficult to assess without comparison to measured data. In general, though, the dependence on correlation length is appropriate. For shorter correlation lengths, the spacing of surface features is closer and the surface appears rougher. Thus for shorter correlation lengths, the scattering profile is wider. This trend is observed in both sets of simulated results for sanded aluminum. Additionally, the B values for each case indicate very low or even negligible fractions of specular scatter.

What will become apparent when overlaid with measurement data is that the decay from the specular peak is very gradual and Gaussian. This is clearly not the case in the measured data, where the $BRDF$ falls off more rapidly. The cause of this discrepancy lies in the assumption of Gaussian ACV/PSD for the aluminum samples. As will be discussed further in Section 4.6, their PSDs have better resemblance to a modified Lorentzian.

Figure 4.60: GHS Simulation of 600 Grit Aluminum

Figure 4.61: GHS Simulation of 2000 Grit Aluminum

4.5.2 Sanded HDPE

For the sanded HDPE sample, GHS simulations were performed for incident angles of $\theta_i = 30^\circ, 45^\circ$, and 60° . Simulations were also, as discussed above, performed for the correlation lengths in each of the x and y dimensions as well as their mean. The resultant data is shown below in Figures 4.64, 4.65, and 4.66.

Unlike the aluminum samples, the reflectance value for this particular HDPE sample is not readily known. Because of this, the scalar reflectance had to be measured using the actual material in possession. As discussed for the aluminum samples, the scalar, or Fresnel, reflectance is defined by reflectance off of a smooth surface. Unfortunately, even the unsanded side of the HDPE sample was too rough for this measurement. When this is the case, directional hemispherical reflectance (DHR) measurements are required. DHR measurements consist of illuminating at one particular incident angle, collecting all reflected angles in the hemisphere, and integrating over that hemisphere. The DHR is essentially the integral of the out-of-plane $BRDF$ over all reflected angles for one incident angle and is equal to the scalar reflectance. Though the $BRDF$ measurement system developed here is capable of measuring out-of-plane $BRDF$ and thus DHR, this measurement scenario was not yet tested and confirmed. Furthermore, a DHR measurement would likely take up to 30-40 times as long as one in-plane measurement.

With measuring DHR proving infeasible, another method of measuring the reflectance of the sample was needed. The employed method used reciprocity to avoid the measurement of DHR. Thus, instead of measuring all reflected angles for one incident angle, one reflected angle was measured for “all” incident angles. Instead of DHR, this measurement is defined as HDR. This method generally still requires an out-of-plane $BRDF$ measurement. However, the simple approach of acquiring an optical image with a camera in ambient lighting serves as a good approximation for an HDR measurement.

The process of using an image of the HDPE surface in ambient lighting required the use of calibrated standards, since the camera used was not radiometrically calibrated. Therefore, a target with calibrated reflectance values, known as a “gray card” in photography, was

used as a reference standard for the extraction of the reflectance of the HDPE. This gray card, shown in Figure 4.62 alongside the unsanded HDPE sample, features several patches with known reflectance values. The two patches employed here are the two middle grays in Figure 4.62. These two grays correspond to reflectance values of 12% and 18%. Using the grayscale image of Figure 4.62, the grayscale pixel values of the two middle grays and the HDPE sample were assessed. The distribution of pixel values for each surface is shown on the left in Figure 4.63. The two known gray surfaces were then used to produce a linear mapping from grayscale value to reflectance, as seen on the right in Figure 4.63. This process assumes that the camera is operating in the linear regime of its dynamic range. From previous usage, this 8-bit camera is known to have a linear dynamic range that spans well beyond the values seen here. Using the linear reflectance mapping in Figure 4.63, the reflectance of the HDPE surface was found to be 12.3%. Note that this reflectance value is averaged over the entire visible spectrum as a grayscale image was used without filtering out all but the wavelength of interest, 632.8 nm. However because the actual HDPE surface is gray in appearance and seems to lack spectral dependence, it is safe to assume that the reflectance is relatively constant over the visible spectrum. This reflectance value is then used in the GHS simulations below for the HDPE sample.

Figure 4.62: Gray Card Image for Determination of HDPE Reflectance

Figure 4.63: Distribution and Reflectance Values of Gray Card and Smooth HDPE

Figure 4.64: GHS Simulation of 320 Grit Sanded HDPE - $\theta_i = 30^\circ$

Figure 4.65: GHS Simulation of 320 Grit Sanded HDPE - $\theta_i = 45^\circ$

Figure 4.66: GHS Simulation of 320 Grit Sanded HDPE - $\theta_i = 60^\circ$

The simulated results shown above contain trends similar to those found and discussed for the sanded aluminum samples. As correlation length decreases, the scattering profile increases in width and decreases in magnitude. This HDPE sample produces an interesting result in that there is no discernible peak in the specular direction. This feature is likely caused by the large roughness relative to the wavelength ($\sigma_s = 2.06\lambda$). The large roughness is also the likely cause of the parameter B held constant at 1. This value indicates there is essentially no specular component of the $BRDF$ for this surface.

Another interesting feature of the HDPE results is the convergence of all three curves at a single $BRDF$ value. This convergence is seen in all three incident angles and occurs at nearly the same $BRDF$ value, 0.04 sr^{-1} but at differing scattered angles. When examining the sanded aluminum results closely, the same convergence is seen by all three curves. For the sanded aluminum results, this convergence is seen on both sides of the specular peak. The $BRDF$ value at the convergence is asymmetric, as the scatter profile generally widens with increasing scattered angle.

Lastly, the scales of the HDPE results correspond well with the low reflectance value ($R = 12.3\%$) and the fact that the scatter is distributed over the entire forward scattering region. In other words, to preserve conservation of energy the volume under the $BRDF$ curve must remain constant. Thus, for highly specular surfaces, the majority of the volume is concentrated within the specular lobe, resulting in a high $BRDF$ value for the specular

peak. The opposite is true for diffuse surfaces. For surfaces where the scatter is spread over the hemisphere, the $BRDF$ values are correspondingly lower as the total power is spread over a larger volume. Thus, the $BRDF$ values for HDPE are quite low due to its low reflectance and widely diffuse scatter. Overall, the simulated results are fitting with expectations.

4.5.3 Polished Aluminum

As discussed in Section 4.4, the polished aluminum sample features widely different surface roughness between its two lateral dimensions. In the “UD” orientation, the grains in the sample are oriented vertically and the plane of incidence is orthogonal to the grains. This produces a much lower correlation length of $l_c = 0.24\lambda$. Conversely, the “LR” orientation corresponds to a grain pattern parallel to the plane of incidence. For this orientation, there is negligible roughness and the correlation length is very high ($l_c = 16.9\lambda$). Therefore, it is inappropriate to consider these two orientations and roughness profiles together. As such, the reported $BRDF$ values, both measured and simulated, are reported separately for the two dimensions. In contrast to the other samples, the mean correlation length is not simulated.

Shown below in Figures 4.67, 4.68, and, 4.69 are the GHS simulated diffuse $BRDF$ results for each of the two orientations separately. The “UD” orientation is on the left, while the “LR” orientation is on the right. Because even the diffuse portion of the “LR” orientation features such a sharp specular peak, its $BRDF$ values are plotted on a log scale. All $BRDF$ values outside of the specular peak are virtually zero (10^{-6}). Interestingly, because the diffuse portion still contains a high specular peak, the diffuse portion of the scattered light, B , is well above zero at $B = 0.17, 0.12, 0.06$ for each of the three incident angles.

In stark contrast, the “UD” orientation features widely distributed diffuse scatter. Despite this wide scatter due to the short correlation length, the overall magnitude of the diffuse scatter is very low due to the low overall roughness of the surface ($\sigma_s = 0.0397\lambda$). Thus, the diffuse portion of the scattered light is very low at $B = 0.07, 0.042, 0.019$ for

the three incident angles.

Figure 4.67: GHS Simulation of Polished Aluminum - $\theta_i = 30^\circ$

Figure 4.68: GHS Simulation of Polished Aluminum - $\theta_i = 45^\circ$

Figure 4.69: GHS Simulation of Polished Aluminum - $\theta_i = 60^\circ$

4.6 Comparison of Predicted and Measured Results

Once all simulations, measurements, and uncertainty analyses were completed, the predicted and measured $BRDF$ results are compared. For each sample and incident angle, the measured $BRDF$, including error bars, is overlaid with the simulated GHS results for the three correlation lengths simulated. The only difference between the simulated results in this section and Sections 4.4 and 4.5 is the inclusion of the specular peak in these GHS results.

As discussed previously, the specular peak predicted by the GHS is described by its obvious location, $-\theta_i$, and the calculated portion of the reflected light contained in the specular peak, A . In the GHS model, the specular peak is formulated as a finite Dirac delta function whose volume in direction cosine space is the parameter A . Thus, the height of the specular peak is determined by the sampling of the scattered angle in direction cosine space. For simulated results, the sampling is much finer and thus leads to a higher and narrower specular peak. For comparison to measurements, however, the sampling of the simulated results must be adjusted to match the sampling of the measurement results and the specular peak is averaged over a finite receiver aperture. Therefore, the simulated $BRDF$ is interpolated at the scattered angles used during measurement for each incident angle. Then, the peak of the specular curve is found by using the parameter A and the angular size of the receiver aperture in direction cosine space. This is essentially calculated by setting the volume of the specular lobe to A and solving for the specular peak since the total volume under the ASF curve is 1 ($A + B = 1$). The specular peak, SP , is then given by

$$SP = \frac{A}{d\alpha^2}, \quad (4.12)$$

where $d\alpha$ is the angular size of the receiver in direction cosine space. $\alpha = \sin \theta$ for in-plane measurements. This calculated specular peak value is then added to the diffusely scattered value at the specular location. As shown in the nonzero specular ($B < 1$) aluminum results below, this addition often produces discontinuities in the otherwise smoothly varying curves. The reason for this, discussed below, is likely caused by the assumption of Gaus-

sian ACV for the aluminum samples. In reality, their PSDs are more accurately described by an ABC modified Lorentzian model. PSDs of this model generate more rapidly varying $BRDF$ curves, similar to those measured for the aluminum samples.

4.6.1 Sanded Aluminum

The comparisons between predicted and measured $BRDF$ for the 600 and 2000 grit sanded aluminum samples are shown below in Figures 4.70 and 4.71. Clearly, there is a general lack of agreement in both shape and amplitude. The shape predicted by the GHS model shows very diffuse scatter with a wide, slowly varying profile. The measured data displays a moderately high specular scatter with faster decay in the diffuse regions.

For both samples, the results for 60° incident angle show a large discontinuity in the GHS simulated curves. This is due to the addition of the specular peak in an otherwise very Gaussian curve.

Figure 4.70: Comparison of Predicted and Measured *BRDF* - 600 Grit Aluminum

Figure 4.71: Comparison of Predicted and Measured *BRDF* - 2000 Grit Aluminum

Overall, the agreement for these samples is poor. One likely cause of this is the assumption of Gaussian ACV briefly mentioned above. As discussed fully in Section 4.3, all surfaces were treated as having Gaussian ACVs. This was motivated by the highly Gaussian distribution curves and for simplicity in GHS simulation. In reality, these surfaces do not resemble Gaussian ACVs or PSDs. In fact, the PSD of most smooth surfaces feature an inverse power law falloff [2]. One of the models that is often used to describe and fit these PSDs is the “K-correlation” or “ABC” model. For this model, the ACV is given by a modified Bessel function, “K”, and the one-dimensional PSD is given by

$$PSD_{ABC} = \frac{A}{\left[1 + (Bf_x)^2\right]^{(C+1)/2}}, \quad (4.13)$$

where f_x is the spatial frequency and A , B , and C are the fitting parameters in the ABC model. When examined on a log-log scale, the ABC model consists of a flat line at low frequencies and a sloped line at higher frequencies. In general, A describes the amplitude, B describes the “break point” separating the low and high spatial frequency regions, and C describes the slope of the higher spatial frequency region.

To show the correspondence of the sanded aluminum PSDs to an ABC model, the one sided PSD was calculated for x and y separately. This one-sided PSD was then smoothed with a 5 point window. Then, the parameters A , B , and C were tuned to fit the model to the PSD curve. The results for the 2000 grit aluminum sample are shown in Figure 4.72. These plots clearly indicate that the sanded aluminum samples highly resemble ABC model PSDs.

Figure 4.72: PSD of 2000 Grit Sanded Aluminum Compared to an ABC Fit

The $BRDF$ corresponding to surfaces with ABC model PSDs are very similar to those measured for the sanded aluminum samples. Two examples in literature calculated from ABC model PSDs using the GHS model are shown in Figure 4.73. Below them, in Figure 4.74, is the measured $BRDF$ of the 2000 grit sanded aluminum plotted on a log scale. The general shape of the $BRDF$ curves in Figure 4.73 is a much better match to the shape of the measured results than the GHS results from Gaussian ACVs. It is apparent from these plots that the sanded aluminum surfaces are better approximated with ABC model PSDs and that more accurate simulated $BRDF$ results could be obtained using this model of surface roughness.

Figure 4.73: $BRDF$ Curves for ABC Model PSDs from [6] and [2]

Figure 4.74: Measured $BRDF$ of 2000 Grit Sanded Aluminum on Log Scale

4.6.2 Sanded HDPE

The comparison between predicted and measured $BRDF$ for the 320 grit sanded HDPE sample is shown below in Figures 4.75, 4.76, and 4.77. These results indicate good agreement overall between measured and simulated curves. This agreement worsens, however, for angles in the backscatter region. In all cases, the GHS simulated results feature little to no scatter in the region surrounding the incident angle. The disagreement worsens as the simulated results reach their minimum at grazing scattered angles on the backscatter side.

This disagreement may be caused by the limitation of the GHS model to single-scatter reflections. In other words, the GHS model does not account for multiple reflections within the surface roughness. Multiple reflections are more likely with rough surfaces and for surfaces with shorter correlation lengths. This notion was discussed above in Section 3.1.2. This discussion also includes the findings by NIST in [33] where the GHS model did not match measured results for rough surfaces with very short correlation lengths. Though the correlation lengths of the HDPE sample are not nearly as small as those in [33], the roughness of the surface suggests that multiple reflections may be present. Additionally, O'Donnell and Mendez measured and discussed increased backscatter with shorter correlation lengths [22].

This disagreement occurs as a result of increased measured $BRDF$ in the backscatter region. As discussed in Section 4.4, this phenomena is known as the “opposition effect” and has been studied widely in radar and remote sensing literature. Generally, the opposition effect (local maximum at the monostatic angle) is more pronounced in surfaces with increased roughness and *longer* correlation lengths [50]. This observation suggests that this particular HDPE sample would exhibit high backscatter levels due to its roughness and large correlation length. Regardless of the mechanism by which backscatter is increased, the GHS model would likely not account for this effect due to its negligence of multiple reflections.

Despite the disagreement in the backscatter region likely due to the limitations of the GHS model, the predicted and measured $BRDF$ results agree very well for all incident angles. The worst agreement is seen for $\theta_i = 60^\circ$, though the uncertainty bounds from simulations and measurements still slightly overlap.

Figure 4.75: Comparison of Predicted and Measured $BRDF$ - 320 Grit HDPE - $\theta_i = 30^\circ$

Figure 4.76: Comparison of Predicted and Measured $BRDF$ - 320 Grit HDPE - $\theta_i = 45^\circ$

Figure 4.77: Comparison of Predicted and Measured $BRDF$ - 320 Grit HDPE - $\theta_i = 60^\circ$

4.6.3 Polished Aluminum

The last sample to be examined is the polished aluminum sample. Comparisons between predicted and measured $BRDF$ are shown in Figures 4.78 and 4.79 for the “UD” and “LR” orientations respectively for all incident angles. As seen with the sanded aluminum samples above, the general shape of the diffuse scatter disagrees greatly. The levels of diffuse scatter predicted by the GHS model for the “LR” orientation are difficult to confirm as they are near 10^{-6} sr^{-1} and are certainly below the noise floor of the $BRDF$ measurement system. For the “UD” orientation, however, the measured levels are near 10^{-1} sr^{-1} and are one order of magnitude higher than the measured levels of the “LR” ori-

entation (10^{-3} sr^{-1}). These diffuse $BRDF$ values near 10^{-3} sr^{-1} measured for the “LR” orientation likely represent the system’s noise floor. This suggests that the measured values for the “UD” orientation are not at the noise floor and that the corresponding predicted GHS values could be detected by the measurement system. This confirms that the disagreement for the “UD” orientation are not caused by sensitivity issues. Instead, the predicted GHS results are definitely in disagreement in amplitude and shape.

Interestingly, the value of the specular peak is in general agreement for all cases within uncertainty bounds. This suggests that the characterization of the total rms roughness, σ_s , was valid since σ_s influences the specular fraction of reflected light, A .

Figure 4.78: Comparison of Predicted and Measured *BRDF* - Polished Aluminum - UD

Figure 4.79: Comparison of Predicted and Measured *BRDF* - Polished Aluminum - LR

As discussed above for the comparison of the sanded aluminum samples, it is very likely that the assumption of Gaussian ACV was inappropriate for this surface, especially given its low roughness. Like the sanded aluminum samples, the PSD for each dimension of the polished aluminum was compared to an ABC model fit. These fits are shown in Figure 4.80. The high degree of agreement between the ABC model and the measured PSD for both directions indicate that the PSD of the polished aluminum should be characterized by an ABC model. This argument is reinforced by the similarity in the shape of the $BRDF$ of the ABC model in Figure 4.73 and the measured $BRDF$ for the polished aluminum.

Figure 4.80: PSD of Polished Aluminum Compared to an ABC Fit

Chapter 5

Discussion

5.1 Primary Findings

Before discussing the primary findings, the specific objectives of this research are reiterated here. From Section 1.3, these objectives are:

1. To implement the GHS theory for arbitrary inputs and provide a documented implementation to the field.
2. To design, build, and execute a surface scatter measurement system.
3. To provide a comparison between the GHS theory and experimental results, using real surfaces with characterized roughness.

The first objective, developing and documenting an implementation of the GHS theory, has been met through the detailed discussion in Section 3.1 and the validation of the implementation in Section 4.1. The primary finding or product for this objective are the details provided in implementing the GHS model for comparison with measured data. The literature includes description of the mathematics governing the theory but does not generally include some of the necessary details involved in the implementation. Some of these details withheld in literature, but included here, involve the separation of the transfer function into diffuse and scattered portions, the definition and sampling of spatial and spatial frequency

domains, the steps to calculate the intermediate and final ASF , and the calculation of the specular component for measurement comparison. Much of these details are not easily found or are absent from the current literature. This research thus provides a transparent documentation of the implementation of the GHS theory.

The second objective, designing, building, and executing a surface scatter measurement system, has been met through the discussion of the chosen system design and components in Section 3.2, the validation of the system in Section 4.2, and the uncertainty analysis in Section 4.4. The primary finding or product for this objective is the measurement system itself, the validation in producing correct results, and the documentation of the development of the system.

The third, and most significant, objective was to provide a comparison between the GHS theory and experimental results for real rough surfaces. This was accomplished through the culmination of the efforts in the first two objectives and the characterization of surface roughness. The primary finding for this objective was that the GHS model produced results that generally agreed with measurements for one of the four tested samples. It is likely that the disagreement found for the other three samples is resultant from an oversimplification in roughness characterization. As analyzed in Section 4.6, the three aluminum samples were likely not appropriately characterized by simple Gaussian ACV functions. The fourth sample, the sanded HDPE, was described by a very Gaussian ACV function. It is therefore no surprise that the highest agreement between measured and predicted $BRDF$ was found for the HDPE sample.

For the forward scatter region in the HDPE results, the agreement between prediction and measurement is quite high. The limitation of the GHS model to single scatter interactions is likely the cause of worsening agreement in the backscatter region. Disagreement in the backscatter region for the GHS model has been documented in literature previously and is a current limitation of the model. Therefore, with correct inputs of surface roughness, the GHS model seems to produce correct results in the forward scatter region.

5.2 Caveats and Consequences

5.2.1 Caveats

The caveats to some of the findings in this research are discussed in the sections above and are summarized here.

Once caveat corresponding to the implementation of the GHS model is that it was not fully validated for arbitrary inputs of surface ACV functions. Though it is expected to produce correct results because of the analysis shown here, only Gaussian ACVs with known form were used here for simplicity.

Another caveat related to the $BRDF$ measurement system is the lack of control over polarization. In general, the $BRDF$ of a surface will depend on the incident and detected polarization. The lack of specification or control of polarization in this research does not greatly impact the primary findings as the GHS model is polarization independent. The results of the measurement system would, technically, be altered by more control over polarization.

The final main caveat discussed at length already is the assumption that the sample surfaces had isotropic Gaussian ACVs. This assumption proved to undermine the comparison for the aluminum samples as their PSDs are shown to more closely resemble ABC models.

5.2.2 Consequences

The main consequence drawn from the comparison of $BRDF$ results between predictions from the GHS model and measurements is the domain of validity of the GHS model. If the comparisons for the sanded HDPE sample are representative, the GHS model provides excellent prediction of $BRDF$ in the forward scatter region for a very rough surface with low reflectance at wide incident and scattering angles. In the context of the literature review in Chapter 2, there are few, if any, other surface scatter models that may claim validity in a case such as the one presented here. Though other experimental validation exists in literature, this research provides an independent addition to that validation.

5.3 Future Work

The areas of possible future work are essentially ways to improve upon the caveats stated above. Primary among these, the already measured aluminum sample should be characterized via an ABC model fit. This would allow for more accurate simulation of these surfaces without additional AFM measurements. Additional aluminum surfaces could be fabricated more carefully with random orbital wet sanders to ideally create surfaces with statistics similar to the HDPE sample but with lower roughness. Furthermore, if necessary, the actual ACVs of the aluminum samples could be input to the GHS model to provide a direct link to simulated results and actual surface roughness.

In terms of future work with respect to measurement, out of plane measurements could be conducted and compared to results predicted by the GHS model. Measurements could also be performed for varying wavelengths. Since varying the wavelength would alter the apparent roughness of the surface, multiple wavelengths would provide a way to analyze the wavelength scalability of the GHS model. Additionally, polarization-controlled measurements would lead to more accurate or, at least, more accurately described measured results.

The last source of future work involves the disagreement with the GHS model in the backscattered region when compared with measured results. Because the underlying foundation of the GHS model is scalar diffraction theory, incorporating multiple reflections may prove impossible. Instead, it may prove more fruitful to use or develop a different theory for the prediction of rough surface scatter in the backscatter region. Then, the two theories may be used simultaneously in a complementary way similar to the Uniform Theory of Diffraction in electromagnetic scattering applications.

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