

Understanding Surface Scatter Phenomena

A LINEAR SYSTEMS FORMULATION

James E. Harvey

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Fax: +1 360.647.1445

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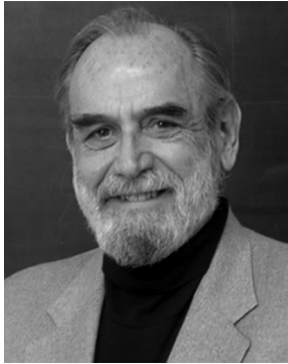
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Roland V. Shack

This book is dedicated to Dr. Roland V. Shack, Professor Emeritus, who was my dissertation adviser at the Optical Sciences Center at the University of Arizona in the early 1970s. In April of 1972, Professor Shack presented a series of four colloquium talks in which he reformulated scalar diffraction theory in terms of the direction cosines of the propagation vectors of the angular spectrum of plane waves described by the Fourier integral transform of the diffracting aperture. The fourth lecture, entitled “Radiometry and Lambert’s Law,” described diffuse reflectance and surface scatter as merely a diffraction phenomenon caused by random phase variations in the optical system pupil function. In 1974, Professor Shack elegantly condensed these four lectures into a single colloquium talk entitled “A Global View of Diffraction.”

I was a graduate student just finishing my course work at the University of Arizona in 1972, and this global view of diffraction, which removed the inherent paraxial limitation in the conventional linear systems formulation of scalar diffraction theory, soon became the basis for my Ph.D. dissertation on surface scatter phenomena. After completing my dissertation entitled “Light-Scattering Characteristics of Optical Surfaces,” I worked in a variety of other areas of applied optics for about a decade. However, things came full circle when I found myself involved in NASA’s X-ray space telescope, the Chandra Observatory. Surface scatter was a dominant image-degradation mechanism for short-wavelength imaging applications. During the previous decade, several commercially available optical analysis codes included in their software various aspects of what they referred to as the Harvey–Shack surface scatter theory, or the Harvey–Shack BRDF model.

After accepting a faculty position at CREOL—the College of Optics and Photonics at the University of Central Florida in 1990, several of my students and I went back to Professor Shack’s “Global View of Diffraction” and developed a linear systems formulation of nonparaxial scalar diffraction theory. This then became the basis for what my students referred to as the generalized Harvey–Shack (GHS) surface scatter theory, which is the primary topic of this book.

Contents

<i>Preface</i>	<i>xi</i>
<i>Acknowledgments</i>	<i>xiii</i>
<i>List of Acronyms</i>	<i>xv</i>
1 Introduction and Overview	1
1.1 A Linear Systems Formulation of Surface Scatter Theory	2
1.2 Motivation for this Book	4
1.3 Organization of the Book	5
References	7
2 Technical Background	9
2.1 Surface Characteristics	10
2.1.1 Mid-spatial-frequency surface irregularities	12
2.1.2 Bandlimited, or relevant, surface roughness	13
2.2 Specular and Diffuse Reflectance (Total Integrated Scatter)	14
2.3 The Bidirectional Reflectance Distribution Function (BRDF)	17
2.4 Vector Analysis and Direction Cosine Space	19
2.4.1 The direction cosines of a vector	20
2.4.2 Direction cosine space and the direction cosine diagram	21
2.4.3 Relationship between direction cosine parameters and spherical coordinates	23
2.4.4 Sign convention for diffraction gratings and surface scatter phenomena	24
2.5 Mathematical Description of Optical Wave Fields	30
2.5.1 The complex amplitude of an electromagnetic field	30
2.5.2 Plane wave fields	31
2.5.3 Spherical wave fields	32
2.5.4 The angular spectrum of plane waves	32
2.5.5 The Poynting vector and irradiance	33
2.6 Radiometric Quantities and their Relationship to Complex Amplitude	35
2.6.1 The solid angle	35
2.6.2 Definitions and terminology	36
2.6.3 The fundamental theorem of radiometry	37
2.6.4 Lambertian sources and Lambert's cosine law	37

2.6.5	Radiometry of imaging systems and the brightness theorem	39
2.6.6	Numerical aperture and focal ratio (F-number)	41
2.6.7	The cosine-fourth illumination fall-off	42
	References	43
3	Historical Background of Surface Scatter Theory	49
3.1	Rayleigh–Rice Surface Scatter Theory	51
3.2	Beckmann–Kirchhoff Surface Scatter Theory	64
3.3	The Original Harvey–Shack Surface Scatter Theory	71
3.4	The Modified Harvey–Shack Surface Scatter Theory	85
	References and Notes	89
4	A Modified Beckmann–Kirchhoff Surface Scatter Model	95
	<i>James E. Harvey, Andrey Krywonos, and Cynthia L. Vernold</i>	
4.1	Nonintuitive Surface Scatter Measurements	95
4.2	Qualitative Explanation of Nonintuitive Surface Scatter Data	97
4.3	Empirical Modification of the Classical Beckmann–Kirchhoff Theory	102
4.4	Experimental Validation: Rough Surfaces at Large Angles	103
4.5	Comparison with the Rayleigh–Rice Theory for Smooth Surfaces	105
	References	108
5	The Generalized Harvey–Shack Surface Scatter Theory	111
	<i>Andrey Krywonos, James E. Harvey, and Narak Choi</i>	
5.1	Evolution of the Linear Systems Formulation of Surface Scatter Theory	113
5.1.1	Inadequate state-of-the-art in surface scatter analysis (1997)	116
5.1.2	Roadmap to successful image degradation analysis (1997)	116
5.1.3	Nonparaxial scalar diffraction theory (1999)	117
5.1.4	Derivation of the GHS surface transfer function (2011)	119
5.2	Numerical Calculations of Scattering Behavior for Rough Surfaces	123
5.2.1	Surfaces characterized by a Gaussian PSD	124
5.2.2	Surfaces characterized by an inverse power law PSD	126
5.2.3	Surfaces characterized by more-general PSDs	131
5.3	Smooth Surface Approximation of the Generalized Harvey–Shack Theory	134
5.4	Comparison of the GHS_{Smooth} and the Rayleigh–Rice Theories	135
5.4.1	Comparison of GHS_{Smooth} and Rayleigh–Rice scattered intensity predictions	137
5.4.2	The inverse scattering problem: predicting PSDs from BRDFs	142
5.4.3	Predicting BRDFs from surface metrology data	147
5.5	Inherent Angular Limitation of the Rayleigh–Rice Surface Scatter Theory	149
5.5.1	Searching for limiting assumptions	150
5.5.2	The GHS_{Smooth} obliquity factor: more general than in RR theory	151

5.5.3	The GHS_{Smooth} obliquity factor: direct result of sinusoidal grating behavior	154
5.5.3.1	Derivation of the classical paraxial efficiency of sinusoidal phase gratings	154
5.5.3.2	Generalizing the classical paraxial expression for diffraction efficiency	161
5.5.3.3	Comparison of predicted diffraction efficiencies with rigorous theory	163
5.6	Predicting BRDFs for Arbitrary Wavelength and Angle of Incidence for a Moderately Rough Surface from Measured BRDF Data at a Single Wavelength and Incident Angle	169
5.7	Summary	171
	References and Notes	173
6	Numerical Validation of the GHS Surface Scatter Theory	179
	<i>Narak Choi and James E. Harvey</i>	
6.1	Surfaces with Gaussian Statistics	179
6.2	Surfaces with an Inverse Power Law PSD	183
6.3	Summary	187
	References	189
7	Empirical Modeling of Rough Surfaces and Subsurface Scatter	191
7.1	The Helmholtz Reciprocity Theorem	192
7.2	Example 1: Rough Ground Glass with Oblique Incident Angles	195
7.3	Example 2: Modeling Subsurface Scatter—Unknown Material #1	202
7.4	Example 3: Modeling Subsurface Scatter—Unknown Material #2	205
7.5	Concluding Remarks	210
	References and Notes	210
8	Integrating Optical Fabrication and Metrology into the Optical Design Process	213
	<i>James E. Harvey and Narak Choi</i>	
8.1	Surface Scatter in the Presence of Aberrations	213
8.1.1	The geometrical PSF for multi-element imaging systems	214
8.1.2	Image degradation due to the surface scatter PSF	216
8.1.3	Derivation of the PSF due to scattering in the presence of aberrations	217
8.1.4	Numerical validation for the case of a two-mirror EUV telescope	218
8.1.5	Summary and conclusions	223
8.2	A Systems Engineering Analysis of Image Quality	223
8.3	Deriving Optical Fabrication Tolerances to Meet Image Quality Requirements	227
	References and Notes	229
	<i>Index</i>	233

Preface

The material in this book was first developed as the seventh and final chapter in a manuscript entitled *Diffraction for Engineers: Including Surface Scatter Phenomena*. However, that chapter on a rather specialized application of diffraction theory grew to over 200 pages. The topic of surface scatter phenomena is probably of limited interest to many people looking for a book on diffraction, and the small community of optical engineers specializing in surface scatter and stray light may rather have access to that material without having to purchase a 400-page book on diffraction. It was thus decided to strip off that final chapter and offer it as a separate book entitled *Understanding Surface Scatter Phenomena: A Linear Systems Formulation*.

Scattering effects from microtopographic surface roughness are merely nonparaxial diffraction phenomena resulting from random phase variations in the reflected or transmitted wavefront. The Rayleigh–Rice, Beckmann–Kirchhoff, or Harvey–Shack surface scatter theories are commonly used to predict surface scatter effects. Smooth-surface approximations and/or moderate-angle limitations have severely reduced the range of applicability of each of the above theoretical treatments.

The true nature of most physical phenomena, including the propagation of light, becomes evident when simple elegant theories and mathematical models conform to experimental observations. Often the simple nature of some natural phenomenon is obscured by applying a complex theory to model an inappropriate physical quantity in some cumbersome coordinate system or parameter space. By integrating sound radiometric principles with scalar diffraction theory, it has been shown that diffracted radiance (not irradiance or intensity) is the natural quantity that exhibits shift invariance with respect to incident angle if formulated in terms of the direction cosines of the incident and diffracted angles. Thus, simple Fourier techniques can be used to predict a variety of wide-angle diffraction phenomena. These include redistributing radiant energy from evanescent diffraction orders into propagating ones, and calculating diffraction grating efficiencies with accuracy usually thought to require rigorous electromagnetic theory.

Since a random rough surface can be modeled as a superposition of sinusoidal reflection gratings of different frequencies, amplitudes,

orientations, and phases, the resulting scattered light distribution is merely the superposition of a myriad of diffraction grating orders. The above linear systems formulation of nonparaxial scalar diffraction theory was thus applied to surface scatter phenomena and resulted first in an empirically modified Beckmann–Kirchhoff surface scatter model, then a generalized Harvey–Shack (GHS) surface scatter theory characterized by a two-parameter family of surface transfer functions. This GHS surface scatter theory produces accurate results for rougher surfaces than the Rayleigh–Rice theory and for larger incident and scattered angles than either the classical Beckmann–Kirchhoff or Rayleigh–Rice theories. The GHS theory also agrees with Rayleigh–Rice predictions within their domain of applicability for smooth surfaces and moderately large scattering angles (up to 50 or 60 deg). These new developments simplify the analysis and understanding of nonintuitive scattering behavior from rough surfaces for large incident and scattering angles.

The transfer function characterization of scattering surfaces can be readily incorporated into the linear systems formulation of image formation, thus allowing a systems engineering analysis of image quality as degraded by diffraction effects, geometrical aberrations, surface scatter effects, and a variety of other miscellaneous error sources. This allows us to derive the optical fabrication tolerances necessary to satisfy a specific image quality requirement, which further enables the integration of optical fabrication and metrology into the optical design process.

The fact that scattered radiance (not irradiance or intensity) is shift-invariant with respect to changes in incident angle *only when expressed in terms of the direction cosines of the propagation vectors* makes a strong case for always displaying scatter measurements as a bidirectional scatter distribution function (BSDF) (i.e., radiance), not angle-resolved scatter (i.e., intensity) as a function of $\beta - \beta_0$. Even BSDF measurements from unknown materials exhibiting subsurface scatter frequently produce simple, elegant behavior that allows empirical parametric modeling when plotted in this format.

Before becoming an associate professor at CREOL—The College of Optics and Photonics at the University of Central Florida, I spent over fifteen years in industry working on real-life optical engineering problems in major DoD and NASA programs. Many of those problems were adequately modeled by the simple and direct application of the linear systems theory and Fourier techniques I learned in Jack Gaskill’s Fourier Optics course (and Joe Goodman’s textbook entitled *Introduction to Fourier Optics*) at the University of Arizona. However, a frequent frustration concerned the fact that many of those real-life problems did not satisfy the paraxial assumption in the conventional linear systems formulation of scalar diffraction theory.

My goal in writing this book is to present the above recent developments and understanding made possible by a linear systems formulation of surface

scatter phenomena to my students as well as to practicing optical engineers. Integrating the subject of radiometry (a neglected step-child in the field of physics) into mainstream optics was particularly satisfying to me (and I hope to my former mentor, Professor Emeritus William L. Wolfe at the Optical Sciences Center at the University of Arizona from whom I learned the fundamentals of radiometry).

Acknowledgments

I am indebted to numerous people without whom this book would never have been written. In particular, I am grateful for the training I received as a graduate student from Professors Jack D. Gaskill, Roland V. Shack, William L. Wolfe, and others at the Optical Sciences Center at the University of Arizona. I also wish to thank all of my graduate students in the College of Optics and Photonics at the University of Central Florida. In particular, Cindi Vernold, whose dissertation research encompassed the topics of diffracted radiance and surface scatter phenomena, and Andrey Krywonos and Narak Choi, who continued that work and made it all come together. Andrey also contributed in various other ways with his modeling efforts (creating appropriate figures) and endless technical discussions.

I have also benefited much from a myriad of technical discussions over the years with Bob Breault, John Stover, Sven Schröder, and Rich Pfisterer.

Bob Breault and I went to graduate school together, and he is responsible for considerable name recognition for me in the surface scatter community by making extensive use of the shift-invariant nature of measured BRDF data from my 1976 Ph.D. dissertation when plotted in the $\beta - \beta_0$ format discussed in Section 3.3 of this book. Bob referred to the Harvey–Shack surface scatter theory or the Harvey–Shack BRDF model and included graphs of this data as justification for his two-parameter and three-parameter “Harvey functions” in hundreds of ASAP software tutorials for thousands of optical engineers over a thirty-year period. This name recognition has been both a curse and a blessing for me.

John Stover has been a friend and colleague for almost 40 years, and I have become intimately acquainted with all three editions of his popular book entitled *Optical Scattering: Measurement and Analysis*. I have made extensive use of his BRDF measurements over the years, both to better understand surface scatter behavior from various surfaces and materials, and to experimentally validate different surface scatter theories and models. I have nothing but admiration for the breadth and depth of his understanding, experience, and expertise in the area of surface scatter measurements spanning several different industries. It is my sincere hope that this book might become a useful complement to John’s scatter measurement book for those scientists and engineers finding themselves—in John’s words—“thrust (sometimes

kicking and screaming) into the position of becoming the company scatter expert as new applications are recognized.”

Sven Schröder was the first person to actually cite the generalized Harvey–Shack surface scatter theory. This citation appeared in his Ph.D. dissertation entitled “Light Scattering of Optical Components at 193 nm and 13.5 nm,” from the Friedrich-Schiller-University, Jena, Germany in 2008. As an employee of the Fraunhofer Institute for Applied Optics and Precision Engineering in Jena, he subsequently spent a year as a visiting scientist with my research group in the Optical Design and Image Analysis Laboratory at CREOL—the College of Optics and Photonics at the University of Central Florida. This was a mutually beneficial collaboration on a research project entitled Universal Light Scattering Technology for the Characterization of Precision Optical and Functional Surfaces. I hope that Sven benefited as much as I did from our extensive interactions during that year-long collaboration.

It has been my good fortune to work with Rich Pfisterer, noted lens designer, developer of the FRED optical analysis software package, entrepreneur, and founding president of Photon Engineering, LLC. Rich is a master at the practical application of radiometry and radiometric principles to the design of optical systems, and is also the author and presenter of a phenomenally popular Stray Light Short Course. When I retired from CREOL at the University of Central Florida and returned to Tucson in 2012, I was fortunate to have the opportunity to work with Rich at Photon Engineering, LLC. Thus, I still benefit from stimulating discussions about surface scatter and occasionally get to contribute an additional chart or two to his Stray Light Short Course or FRED tutorials, which are taught several times a year both state side and internationally.

Finally, I am grateful for the patience and support of my wife, Marva, who has tolerated my occupation and pre-occupation with optics for the past fifty years.

James E. Harvey
June 2019

Chapter 1

Introduction and Overview

Scattered light is a blessing for all of us as it provides the means by which we observe the world around us, but it is also often a curse because unwanted scattered light (or stray light, as it is often called) can seriously degrade the performance of precision optical instruments. There is surface scatter caused by the residual roughness of a highly reflecting mirror, subsurface scatter from many objects or materials such as paints or coatings, particulate scatter caused by contamination of otherwise very smooth and clean optical surfaces, and even bulk scatter from random refractive index fluctuations in the transmissive optical glass used to produce lenses and other optical components.

This book deals primarily with surface scatter phenomena that continue to be an important issue in diverse areas of science and engineering in the 21st century. In many applications it is not only the amount of scattered light, but also the direction of the scattered radiation that is important. This is particularly true for the following applications:

- The design and analysis of stray light rejection systems required by imaging systems used to view a relatively faint target in the vicinity of a much brighter object;
- The fabrication of supersmooth surfaces for high-resolution x-ray and extreme-ultraviolet (EUV) imaging systems;
- Determining whether diamond-turned metal mirrors need to be postpolished to satisfy image quality requirements; and
- Inverse scattering applications where scattered light signatures are used to remotely infer target characteristics.

There are both geometric microfacet models of surface scatter and physical optics or diffractive models. These seemingly disparate approaches are compared in detail in Ref. 1. We deal almost exclusively with physical optics models in this book.

Surface scatter of electromagnetic radiation is due primarily to the surface irregularities inducing a phase variation on the transmitted or reflected

wavefront. The propagation of these perturbed wavefronts then results in scattered light behavior that is strongly affected by

- the propagating wavelength,
- the statistical characteristics of the surface,
- the angle of incidence, and
- the refractive index of the media both before and after the interface or surface encountered.

Surface scatter is a physical optics phenomenon and can be described or modeled with either scalar wave theory or the more rigorous electromagnetic (vector) theory.

The following optical theories are listed in order of increasing mathematical rigor and completeness:

- geometrical optics,
- scalar wave theory, and
- electromagnetic theory.

My personal philosophy is that the effective (most productive) optical systems engineer will always use the simplest theory adequate for the job at hand. The difficulty lies in knowing when a given theory is not adequate, and a more rigorous theory is necessary. The ability to have this insight is the mark of a really good optical engineer.

1.1 A Linear Systems Formulation of Surface Scatter Theory

Scattering effects from microtopographic surface roughness are merely nonparaxial diffraction phenomena resulting from random phase variations in the reflected or transmitted wavefront. As such, they are ideally suited to model with linear systems theory as has been done for conventional diffraction phenomena by Goodman and Gaskill.^{2,3} A systems approach to modeling physical phenomena often makes use of mathematical operators that produce the system output when applied to the system input, as illustrated in Fig. 1.1(a). The condition for linearity is given by³

$$L[a_1f_1(x, y) + a_2f_2(x, y)] = a_1L[f_1(x, y)] + a_2L[f_2(x, y)]. \quad (1.1)$$

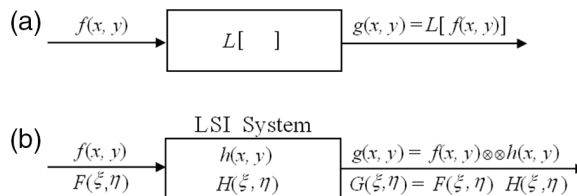


Figure 1.1 (a) General system characterized by a mathematical operator L and (b) a LSI system characterized by a system transfer function.

If, in addition, the system is shift-invariant (i.e., when the input is shifted, the output is merely shifted without a change in functional form), we then have³

$$L[f(x - x_0, y - y_0)] = g(x - x_0, y - y_0). \quad (1.2)$$

If both conditions hold, we have the linear, shift-invariant (LSI) system illustrated schematically in Fig. 1.1(b). The output of a LSI system is given by convolving the input with the system impulse response; alternatively, upon applying the convolution theorem of Fourier transform theory (or frequency analysis), the output spectrum of the system $G(\xi, \eta)$ is given by the product of the input spectrum $F(\xi, \eta)$ and the system transfer function.³

The symbolic notation $\otimes \otimes$ in Fig. 1.1(b) represents the two-dimensional (2D) convolution integral:³

$$g(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\alpha, \beta) h(x - \alpha, y - \beta) d\alpha d\beta, \quad (1.3)$$

where α and β are dummy variables of integration. Also, in Fig. 1.1(b),

$$F(\xi, \eta) = \mathcal{F}\{f(x, y)\} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\alpha, \beta) \exp[-j2\pi(\alpha\xi + \beta\eta)] d\alpha d\beta, \quad (1.4)$$

where \mathcal{F} is the symbolic notation for the Fourier transform operation defined by the integral in Eq. (1.4), and ξ and η are the (reciprocal) spatial frequency variables corresponding to the x and y directions, respectively.³ Likewise, $H(\xi, \eta) = \mathcal{F}\{h(x, y)\}$, and $G(\xi, \eta) = \mathcal{F}\{g(x, y)\}$.

LSI systems can thus be completely characterized by the system transfer function, which is defined as the ratio of the output spectrum to the input spectrum:

$$\text{Transfer Function} = \frac{H(\xi, \eta)}{G(\xi, \eta)}. \quad (1.5)$$

The linear systems formulation of surface scatter phenomena was first developed by Harvey and Shack in 1976 as described in Section 3.3 of this text; however, that treatment was limited to moderate incident and scattered angles. A somewhat less restrictive version of this linear systems formulation of surface scatter theory valid for larger incident angles (but still restricted to moderate scattered angles) is described in Section 3.4. This modified Harvey–Shack (MHS) surface scatter theory is no longer shift-invariant as it requires a different surface transfer function for each incident angle; however, the linear

systems formulation still provides insight and understanding for optical and electrical engineers with a background in linear systems theory.

Rayleigh–Rice (RR),^{4–6} Beckmann–Kirchhoff (BK),⁷ or the original Harvey–Shack (OHS)^{8,9} surface scatter theories are commonly used to predict surface scatter effects. Smooth surface and/or moderate angle limitations have severely limited the range of applicability of each of the above theoretical treatments. A recent linear systems formulation of nonparaxial scalar diffraction theory^{10,11} applied to surface scatter phenomena resulted first in an empirically modified BK surface scatter model,¹² then a generalized Harvey–Shack (GHS)¹³ theory that produces accurate results for rougher surfaces than the RR theory and for larger incident and scattered angles than the BK, the OHS, and even the RR theories. This GHS theory is also no longer shift-invariant, as it is characterized by a two-parameter family of surface transfer functions; i.e., a different transfer function is required for *each incident and each scattered angle*. These new developments enable the analysis and understanding of nonintuitive scattering behavior from rough surfaces illuminated at arbitrary incident angles.

1.2 Motivation for this Book

Most linear systems treatments of diffraction phenomena are limited to Fraunhofer and Fresnel diffraction. Both of these formulations include an implicit paraxial (small angle) limitation. This paraxial limitation severely limits the conditions under which diffraction behavior is adequately described. In this text, a linear systems approach to modeling *nonparaxial* scalar diffraction theory^{10,11} is applied to the development of a linear systems formulation of wide-angle surface scatter phenomena that is not limited to optically smooth surfaces. This treatment not only provides much more insight than the conventional treatment, but is accurate for a much larger range of parameters than usually thought possible.

Wide-angle scalar diffraction phenomena are shift-invariant with respect to changes in incident angle *only when diffracted radiance is expressed in terms of the direction cosines of the propagation vectors*. Likewise, it is the scattered *radiance* (not intensity or irradiance) that is shift-invariant in direction cosine space for optically smooth surfaces. It is this realization that greatly extends the range of parameters over which simple Fourier techniques can be used to make accurate calculations concerning wide-angle surface scatter behavior.

Why should we be surprised that diffracted *radiance* (not *intensity* or *irradiance*) is the fundamental quantity that is shift-invariant with respect to incident angle when properly formulated in direction cosine space? After all, we have the *brightness theorem* in geometrical optics that states that *radiance* is invariant with axial position throughout a lossless imaging system! That this new insight took so long to surface may be due to the fact that the merging of

communications theory with optics (1950s) and the development of Fourier optics (1960s) was accomplished primarily by electrical engineers, and there is no electrical engineering quantity that corresponds to the radiometric quantity called *radiance*.

These new developments will be applied to wide-angle applications such as diffraction from gratings and scattering (due to residual optical fabrication errors) from optical surfaces.

The intent of the author of this text is to help the reader develop the technical approach and insight required for solving practical optical engineering problems involving scattered light, and image degradation due to scattered light behavior. Fourier transform techniques and linear systems theory provide the foundation upon which to perform such detailed optical systems analyses.

1.3 Organization of the Book

In Chapter 2 the surface characteristics that relate to surface scatter behavior are reviewed. We then define and discuss specular and diffuse reflectance and total integrated scatter (TIS). The bidirectional reflectance distribution function (BRDF) is then discussed, as are the associated quantities referred to as the bidirectional transmittance distribution function (BTDF) and the bidirectional scatter distribution function (BSDF). The definition and use of the direction cosines of a vector as widely used in optics and optical design computer programs are introduced. We then proceed with a fairly detailed discussion of the invaluable direction cosine diagram and the concept of direction cosine space. Finally, we discuss the definitions of some basic radiometric quantities and concepts, and their relationship to the complex amplitude of an electromagnetic wave or disturbance.

Chapter 3 provides a historical background of surface scatter phenomena. We start with a review of the RR surface scatter theory and proceed to a discussion of the classical BK surface scatter theory. We then discuss the original Harvey–Shack surface scatter theory, which was limited to moderate incident and scattered angles, and finally the modified Harvey–Shack (MHS) surface scatter theory, which allowed for extremely large incident angles but was still restricted to moderate scattering angles.

An important step in the evolution of a linear systems formulation of a generalized surface scatter theory that remains valid for rough surfaces at arbitrary incident and scatter angles was the development of an empirically modified BK surface scattering model.¹² In Chapter 4 some nonintuitive surface scatter measurements are first presented and discussed. A qualitative explanation of this nonintuitive data is then presented. This leads to an empirical modification of the classical BK theory. Some experimental scatter measurements from rough surfaces at large incident angles are then used to experimentally validate the empirically modified BK model. Finally, the

modified BK surface scatter model is shown to agree with RR predictions of smooth surface scatter behavior.

Chapter 5 discusses the generalized Harvey–Shack (GHS) surface scatter theory that utilizes a two-parameter family of surface transfer functions to characterize surface scatter behavior for moderately rough surfaces at large incident and scattered angles.¹³ This two-parameter family of surface transfer functions includes a different transfer function for *each* incident and *each* scattered angle. As such, predicting the scattered light behavior can be rather computationally intensive. However, if the surface roughness is isotropic, the surface transfer function will be rotationally symmetric, and the 2D Fourier transform reduces to a Hankel transform. Since the Hankel transform operation is one dimensional (1D), this can help to reduce the computation time significantly. Numerical calculations of scatter behavior from rough surfaces characterized with a Gaussian surface power spectral density (PSD) function, inverse power law surface PSDs, and more general surface PSDs are discussed.

The smooth surface approximation to the scalar-based GHS surface scatter theory is then compared to the final result of the classical RR surface scatter theory (a rigorous vector perturbation formulation). We apply deductive reasoning to justify empirically vectorizing the scalar-based $\text{GHS}_{\text{Smooth}}$ theory by simply substituting the polarization-dependent reflectance Q from the RR expression for the scalar reflectance R . Furthermore, because of a little-known or long-forgotten limiting assumption that the surface autocovariance (ACV) length is greater than a wavelength, the RR obliquity factor was found to contain a quadratic approximation to the series expansion for the cosine function, which makes its obliquity factor less general (not valid for scattering angles $> \sim 60$ deg) than that of the $\text{GHS}_{\text{Smooth}}$ theory.¹⁴ It is this inaccurate obliquity factor that causes the annoying “hooks” at the high spatial frequency end of surface PSDs predicted when the RR theory is used to solve the inverse scattering problem of predicting surface characteristics from measured BRDF data. The equally disturbing complementary effect of this limiting obliquity factor of the RR expression causes BRDFs predicted from surface metrology data to dive to zero at ± 90 deg regardless of the nature of the surface PSD.

In addition, the GHS theory has a renormalization factor that compensates for large incident and/or scattering angles that cause a significant portion of the scattered radiance to fall outside of the unit circle in direction cosine space, i.e., when evanescent waves are formed.^{13,14} Likewise, a correction factor in the GHS theory compensates the *relevant* rms surface roughness when it is less than the total intrinsic root-mean-square (rms) roughness (this is a situation that often occurs for real optical surfaces characterized by inverse power law surface PSDs).¹⁴

In Chapter 6, the GHS surface scatter theory is numerically compared to the classical small perturbation method (RR), the Kirchhoff approximation method (BK), and the rigorous method of moments (MoM) for 1D ideally

conducting surfaces whose surface PSD function is Gaussian or exhibits inverse power law (fractal) behavior. Despite its simple analytic form, our numerical comparison shows that the new GHS theory is valid (with reasonable accuracy) over a broader range of surface parameter space than either of the two classical surface scatter theories.¹⁵

Over the years we have developed an adequate theory and understanding of surface scatter from smooth optical surfaces (RR), moderately rough surfaces with moderate incident and scattered angles (BK), and even for moderately rough surfaces with arbitrary incident and scattered angles, where a linear systems formulation requiring a two-parameter family of surface transfer functions is required to characterize the surface scatter process (GHS). However, there is always some new material or surface manufacturing process that provides nonintuitive scatter behavior. The linear systems formulation of surface scatter is potentially useful even for these situations. In Chapter 7 we present empirical models of several classes of rough surfaces or materials (subsurface scatter) that allow us to accurately model the scattering behavior at any wavelength or incident angle from limited measured scatter data. In particular, scattered radiance appears to continue being the natural quantity that exhibits simple, elegant behavior only in direction cosine space.¹⁶

The validation of a generalized linear systems formulation of surface scatter theory and an analysis of image degradation due to surface scatter in the presence of aberrations¹⁷ have provided credence to the development of a systems engineering analysis of image quality as degraded not only by diffraction effects and geometrical aberrations, but by scattering effects due to residual optical fabrication errors as well. This GHS surface scatter theory provides insight and understanding by characterizing surface scatter behavior with a surface transfer function closely related to the optical transfer function (OTF) of classical image formation theory. Incorporating the inherently bandlimited relevant surface roughness into the surface scatter theory provides mathematical rigor to surface scatter analysis, and implementing a fast Fourier transform algorithm with logarithmically spaced data points facilitates the practical calculation of scatter behavior from surfaces with a large dynamic range of relevant spatial frequencies. Chapter 8 discusses how these advances combined with the continuing increase in computer speed leave the optical design community in a position to routinely derive the optical fabrication tolerances necessary to satisfy specific image quality requirements during the design phase of a project, i.e., to integrate optical metrology and fabrication into the optical design process.¹⁸

Detailed references are provided at the end of each chapter.

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