University of Central Florida

CREOL: College of Optics and Photonics

Deriving Optical Fabrication Tolerances to Satisfy Specific Optical Performance Requirements: Beyond the Smooth-surface Limit

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Introductory Comment # 1

Surface scatter phenomena continues 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:

1.) **The design and analysis of stray light rejection required by optical systems used to view a relatively faint target in the vicinity of a much brighter object.**

2.) **The fabrication of "super-smooth" surfaces for high resolution X-ray and extreme ultraviolet (EUV) imaging systems.**

3.) **Determining whether diamond-turned metal mirrors need to be post-polished to satisfy image quality requirements.**

4.) **Inverse scattering applications where scattered light "signatures" are used to remotely infer target characteristics.**

5.) **The engineering of "enhanced roughness" to increase the efficiency of thin-film photo-voltaic solar cell applications.**

Introductory Comment # 2

Surface scatter of electromagnetic radiation is not caused directly by surface roughness, but rather by the effect of the *phase variation* induced upon the transmitted or reflected wavefront as it propagates; i.e., surface scatter is a *diffraction phenomena* caused directly by the *propagation process*. As such, surface scatter is strongly affected by:

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

Introductory Comment # 3

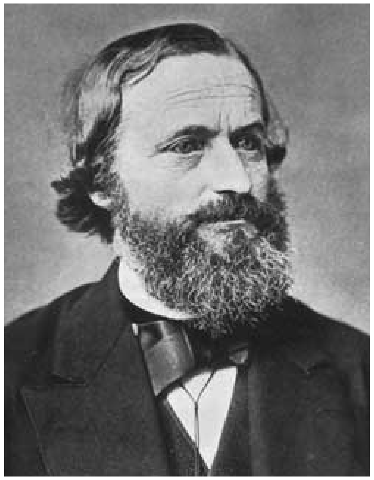
The generalized Harvey-Shack (GHS) surface scatter theory is a linear systems formulation of scattering from *arbitrarily rough surfaces with arbitrary incident and scattering angles*. As such, the scattering surface, and the resulting BRDF is completely characterized by a two-parameter family of surface transfer functions.

It is a scalar theory based almost solely upon the two optical principles:

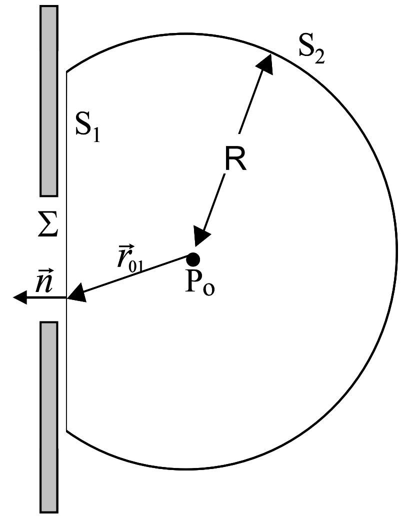
- **The Kirchhoff Assumption**
- **The Rayleigh Hypothesis**

However, it has been quasi-vectorized by substituting the polarization reflectance, Q, from the Rayleigh-Rice vector perturbation theory for the scalar reflectance R.

The Kirchhoff Assumption



Gustav Kirchhoff added some mathematical rigor to the early ideas of Huygens and Fresnel by showing that the amplitudes and phases ascribed to the secondary wavelets are indeed logical consequences of the wave nature of light. He did this by choosing an appropriate Green's function which satisfied the wave equation.



Kirchhoff formulation of diffraction by a plane screen.

However, his formulation was based upon two ***assumptions about boundary values*** of optical disturbances that were inconstant with each other.

Kirchhoff Boundary Conditions

1. Across the open portion of surface S_1 (Σ) the field distribution U and its derivative dU/dn are exactly the same as they would be in the absence of the screen.

2. Over the portion of S_1 that lies in the geometrical shadow of the screen, the field distribution U and its derivative dU/dn are identically zero.

It has been said that—"The sole virtue of Kirchhoff's theory of diffraction lies in its correct predictions and not in its false assumptions". (Andrews 1947)

The Rayleigh Hypothesis

Rayleigh Was Right: Electromagnetic Fields and Corrugated Interfaces *

The Rayleigh hypothesis concerns the diffraction of light by a periodically corrugated interface between two homogeneous media. It simply states that the electromagnetic field in the corrugation is composed of waves outgoing from the interface. There has been a long-standing debate in the optics community as to whether this hypothesis is true or simply an approximation for shallow corrugations.

The dominant opinion is that it is an approximation whose validity limit has been quantified at $h/d < 0.1426$. As a result, *its potential for electromagnetic theory and modeling has been overlooked for a half century*.

Against common sense and pretended mathematical proofs, the author has tested the Rayleigh hypothesis numerically, and found that it is *exactly true* up to a corrugation depth of *at least 15 times the claimed validity limit*!

* Alexandre V. Tishchenko, OPN Optics & Photonics News, Vol. **21** No. 7/8, 51-54 (July/August 2010).

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- Statement of the EUV Imaging Problem (Summary of Results).
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- BRDFs from Real Metrology Data from Moderately Rough Surfaces. (that violate the smooth surface approximation).
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  - Dealing with the "Scattered-Scattered" Light.
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- **Rayleigh (1896, 1907)**
  Investigated scattering of acoustic waves.
  Developed vector perturbation theory for gratings.
- **Fano (1941)**
  Expanded on the Rayleigh approach to explain anomalous grating behavior.
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- **Harvey and Shack (1976)**
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Recent Approximate Approaches

This is still a very active area of research (over 200 references since 1980).

In 2004, Elfouhailey and Guerin* wrote a critical review including over thirty (30) different approximate approaches of predicting surface scatter behavior. These were divided into three categories:

- Small Perturbation Methods
- Kirchhoff Approaches
- Unified Methods

They concluded that

"*there does not seem to be a universal method that is to be preferred systematically. All methods present a compromise between versatility, simplicity, numerical efficiency, accuracy and robustness, with a different weighting in these various fields…There is still room for improvement in the development of approximate scattering methods.*"

* T. M. Elfouhaily and C. A. Guerin, "A Critical Survey of approximate Scattering Wave Theories from Random Rough Surfaces", Waves in Random Media **14**, R1-R40 (2004).

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Other Major Contributor's

- J. M. Elson (1970s): Vector Surface Scatter Theory.
- Bennett & Mattson: Surface Characterization.
- John C. Stover: Scatter Measurements and Analysis.
- Bob Breault: Founder of Breault Research Org., Inc. and co-developer of ASAP optical engineering software.
- Angela Duparré and Sven Schröder: Surface Characterization & Scatter Measurements
- Rich Pfisterer: President of Photon Engineering and co-developer of FRED optical engineering software.

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Statement of the Problem

For many applications, surface scatter effects from residual optical fabrication errors frequently limit the performance of imaging systems rather than geometrical aberrations or diffraction effects!

- **Optical fabrication tolerances necessary to satisfy specific image quality requirements must be derived:**
  - **o Calculate the BRDF from assumed metrology data.**
  - **o Calculate the image degradation caused by that BRDF.**

ZEMAX
ASAP
FRED

- **Optical surfaces aren't always "smooth“ relative to the operational wavelength; hence, surface scatter theories using smooth surface approximations or perturbation techniques (Rayleigh-Rice) are *not* valid.**

- **A new generalized surface scatter theory valid for moderately rough surfaces and non-paraxial incident and scattering angles has been developed.**

- **The large dynamic range in the relevant spatial frequencies of optically polished surfaces poses severe computational problems in implementing any new generalized scatter theory.**

Objective/Technical Approach/Results

Objective:

- Advance the Linear Systems Formulation of Surface Scatter Theory.
  - o Valid for both smooth and rough surfaces.
  - o Valid for both small and large incident and scattered angles.

Technical Approach:

- Surface Scatter is Merely a Diffraction Phenomenon.
  - o Random surfaces can be described as a superposition of sinusoidal phase gratings.
  - o First develop a non-paraxial scalar diffraction model that accurately predicts the diffraction efficiency of sinusoidal phase gratings.

Results:

- We have Developed a Linear Systems Formulation of Non-paraxial Scalar Diffraction Theory (Diffracted Radiance, Direction Cosine space).
- Empirically Modified Beckmann-Kirchhoff Scatter Model (non-paraxial).
- Derived a New Generalized Harvey-Shack (GHS) Surface Scatter Theory.
  - o Valid for smooth and rough surfaces.
  - o Valid for both small and large incident and scattered angles.
  - o Smooth surface approx. leads to an improved inverse scattering solution.

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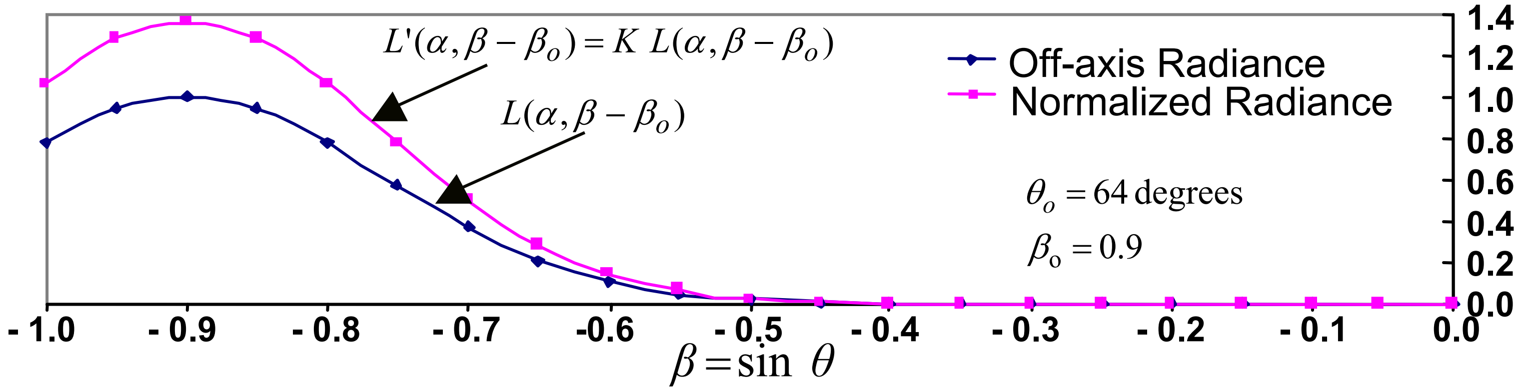
Diffracted Radiance: The Fundamental Quantity Predicted by Scalar Theory *

By formulating scalar diffraction theory in terms of the direction cosines of the propagation vectors of the angular spectrum of plane waves represented by the kernal of the Fourier transform integral, and incorporating sound radiometric principles, we obtained the following expression for diffracted radiance.

$$L'(\alpha,\beta-\beta_o) = K\,\gamma_o \frac{\lambda^2}{A_s}\left|\mathcal{F}\left\{ U_o(\hat{x},\hat{y};0)\,\exp(i2\pi\beta_o\hat{y})\right\}\right|^2 \quad \text{for} \quad \alpha^2+\beta^2 \le 1$$
$$L'(\alpha,\beta-\beta_o) = 0 \quad \text{for} \quad \alpha^2+\beta^2 > 1 \qquad \textbf{(1)}$$

For large incident and diffraction angles, a portion of the diffracted radiance distribution function will fall outside of the unit circle in direction space.



Parseval's theorem from Fourier transform theory then requires that a re-normalization constant be applied.

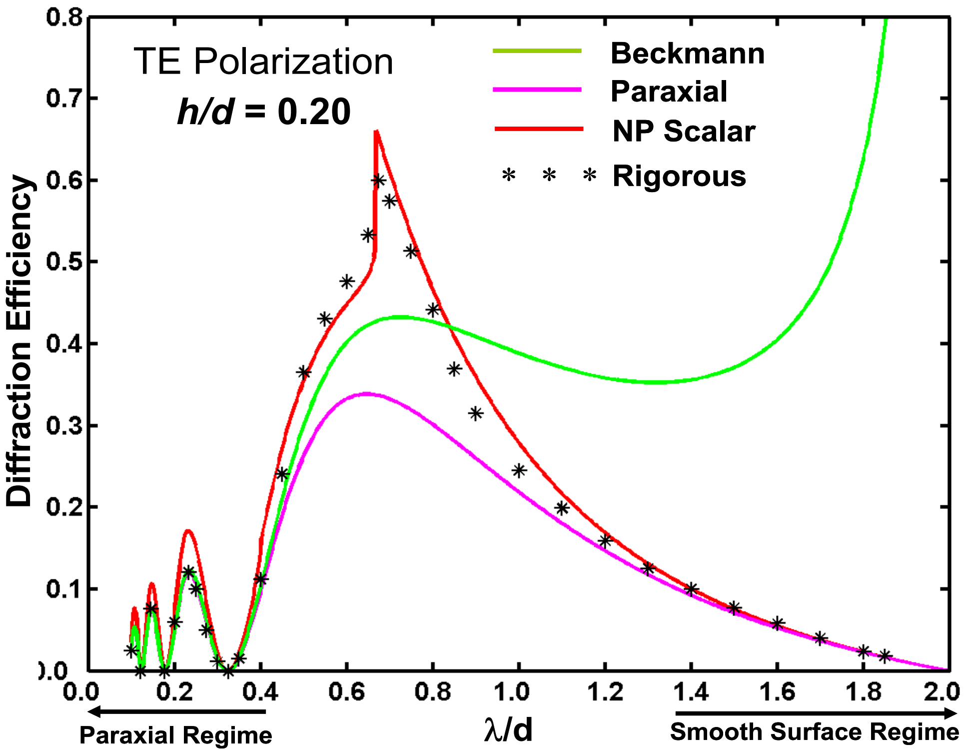
$$K = \frac{\displaystyle\int_{\alpha=-\infty}^{\infty}\int_{\beta=-\infty}^{\infty} L(\alpha,\beta-\beta_o)\,d\alpha\,d\beta}{\displaystyle\int_{\alpha=-1}^{1}\int_{\beta=-\sqrt{1-\alpha^2}}^{\sqrt{1-\alpha^2}} L(\alpha,\beta-\beta_o)\,d\alpha\,d\beta} \equiv \text{Normalization Constant} \qquad \textbf{(2)}$$

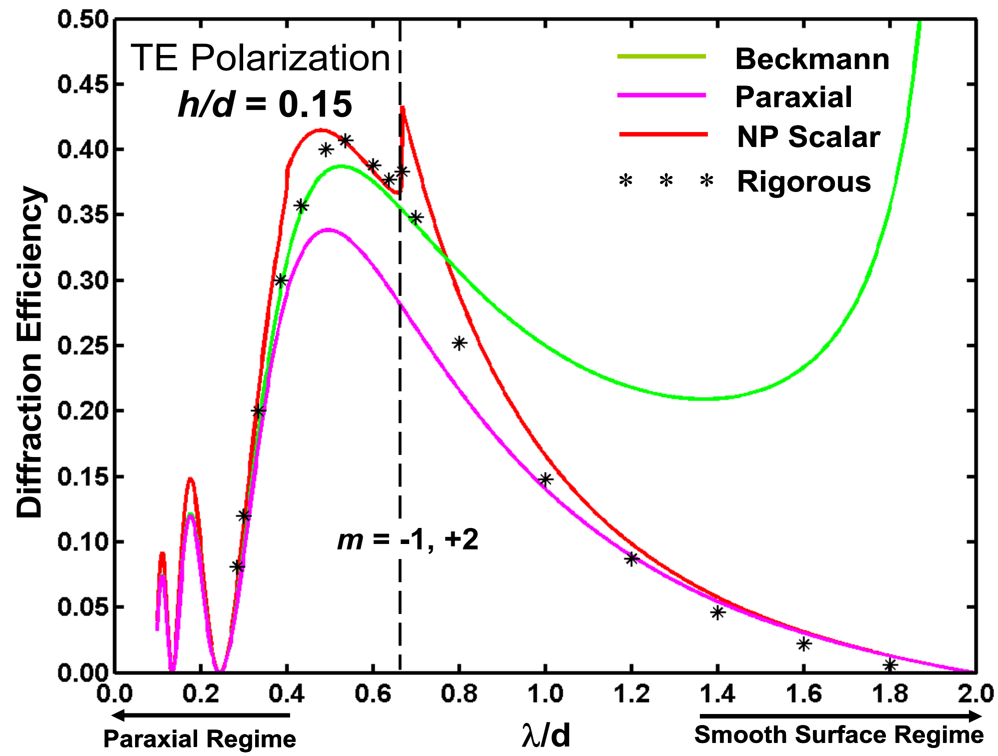
*** J. E. Harvey, et.al., "Diffracted Radiance: A Fundamental Quantity in Non-Paraxial Scalar Diff. Theory", Appl. Opt. 38, 6469 (1999).**

Diffraction Efficiency of a Perfectly Conducting Sinusoidal Phase Grating*

The diffraction efficiency for a perfectly conducting sinusoidal phase grating using our non-paraxial linear systems model of scalar diffraction theory is given by:

$$\eta_m = \frac{P_m}{P_T} = \frac{J_m^2(a/2)}{\sum_{m=\min}^{\max} J_m^2(a/2)} \quad (3)$$





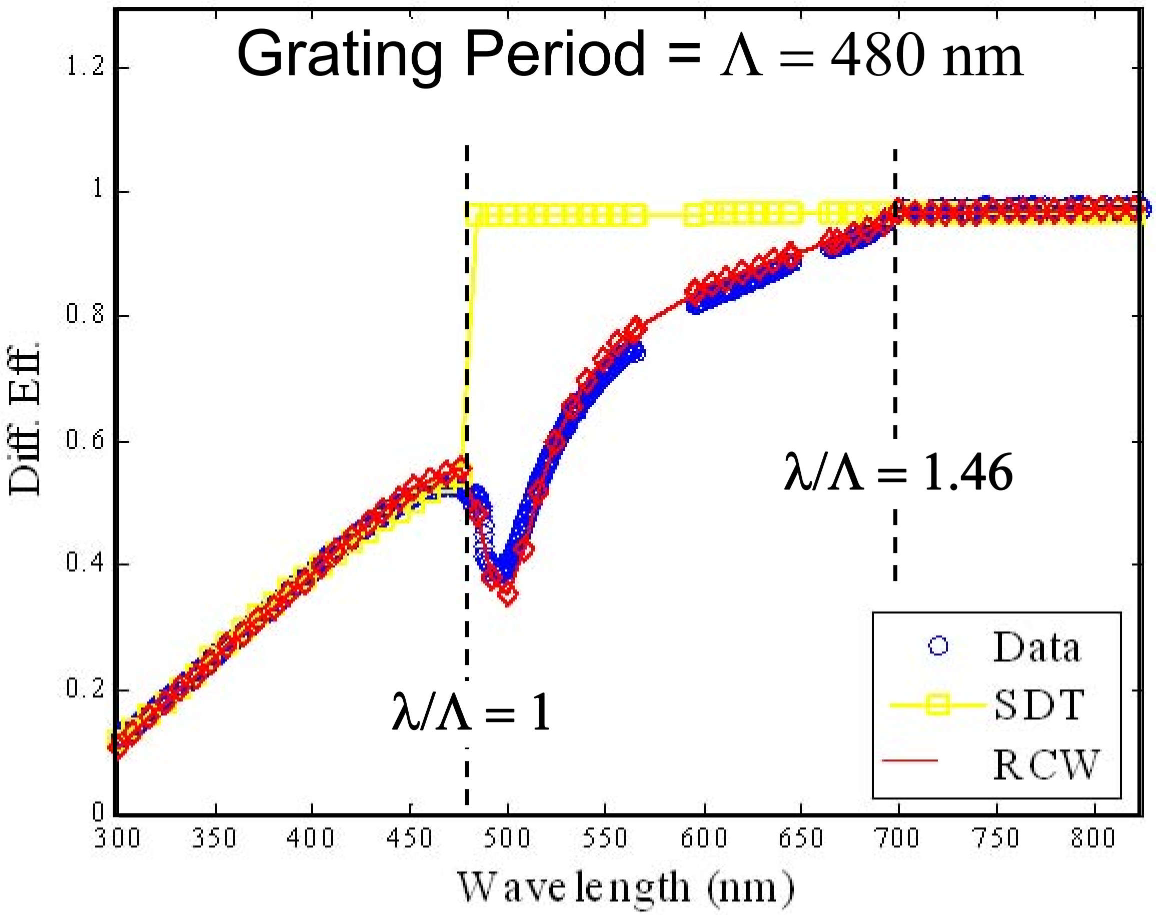
These figures show that using our non-paraxial scalar diffraction theory is able to accurately predict diffraction efficiencies over a much larger range than previously thought possible.

*** J. E. Harvey, A. Krywonos and D. Bogunovic, "Non-paraxial Scalar Treatment of Sinusoidal Phase Gratings", JOSA A 23 (2006).**

Grating Characterization using Scatterometry*

Harvey's renormalized scalar diffraction theory makes it possible to extend the useful range of scalar diffraction theory from $\lambda/\Lambda \leq 0.1$ to $\lambda/\Lambda \leq 1.0$ and for $\lambda/\Lambda > 1.4$.

Using the SDT as a seed function for grating characterization results in a fast and robust two-step hybrid method that is a factor of eight (8) faster than a pure vector calculation code.



* P.- E. Hansen and L. Neilsen, "Combined optimization and hybrid scalar-vector diffraction method for grating topography parameters determination", Materials Science and Engineering B 165, 165-168 (December 2009).

Empirically Modified Beckmann-Kirchhoff Scattering Model*

Our new understanding of non-paraxial scalar diffraction theory, and our knowledge that diffracted radiance is shift-invariant in direction cosine space led us to make the following empirical modifications:

- **Throw away the "F" factor.**
- **Equate to "Radiance".**
- **Apply the re-normalization factor, K.**
- **Multiply by Lambert's cosine function.**

Classical Beckmann-Kirchhoff Theory

$$D\{\rho\} = \frac{\pi\,\ell_c^2\,F^2}{A_s v_z^2 \sigma_s^2}\exp\left[-\frac{v_{xy}^2\,\ell_c^2}{4 v_z^2 \sigma_s^2}\right] \quad (4)$$

$$F = \left[\left(\frac{1}{\cos\theta_i}\right)\frac{1+\cos(\theta_i+\theta_s)}{\cos\theta_i+\cos\theta_s}\right]^2$$

$$v_{xy} = k\sqrt{\sin^2\theta_s + \sin^2\theta_i}$$

A = Illuminated Surface Area $\quad \ell_c$ = Correlation Length

Modified Beckmann-Kirchhoff Theory

$$I(\theta,\phi) = K\,\frac{\pi\,\ell_c^2\cos\theta}{v_z^2\sigma_s^2}\exp\left[-\frac{v_{xy}^2\,\ell_c^2}{4 v_z^2 \sigma_s^2}\right] \quad (5)$$

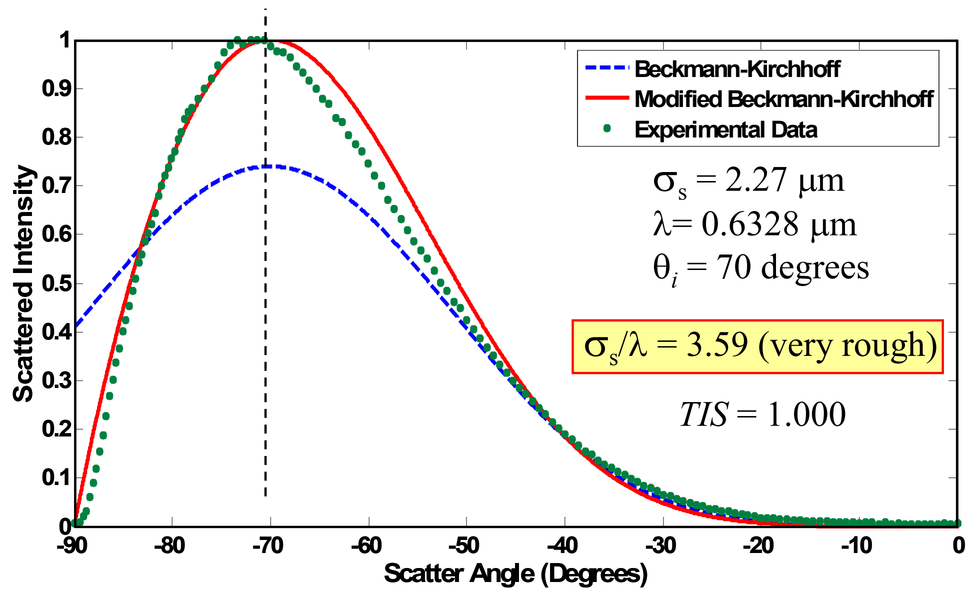
K = Re−normalization Factor

(Assures Conservation of Energy)

$I = L\cos\theta$

(Lambert's Cosine Law)

Experimental Validation



* J. E. Harvey, A. Krywonos, and C. Vernold, "Modified Beckmann-Kirchhoff Scattering Model", Opt. Eng. 46, Art. No. 078002, 1-10 (July 2007).

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Total Integrated Scatter *

The fraction of the total radiant power contained in the specular beam after reflection from a moderately rough surface is given by

$$A = \exp[-(4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2] \qquad (6)$$

and the fraction of the total reflected radiant power that is scattered out of the specular beam, or total integrated scatter (*TIS*) is defined as

$$B = TIS = 1 - \exp[-(4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2] \qquad (7)$$

where σ_{rel} is the bandlimited *relevant* roughness for $1.22/D < f < 1/\lambda$.

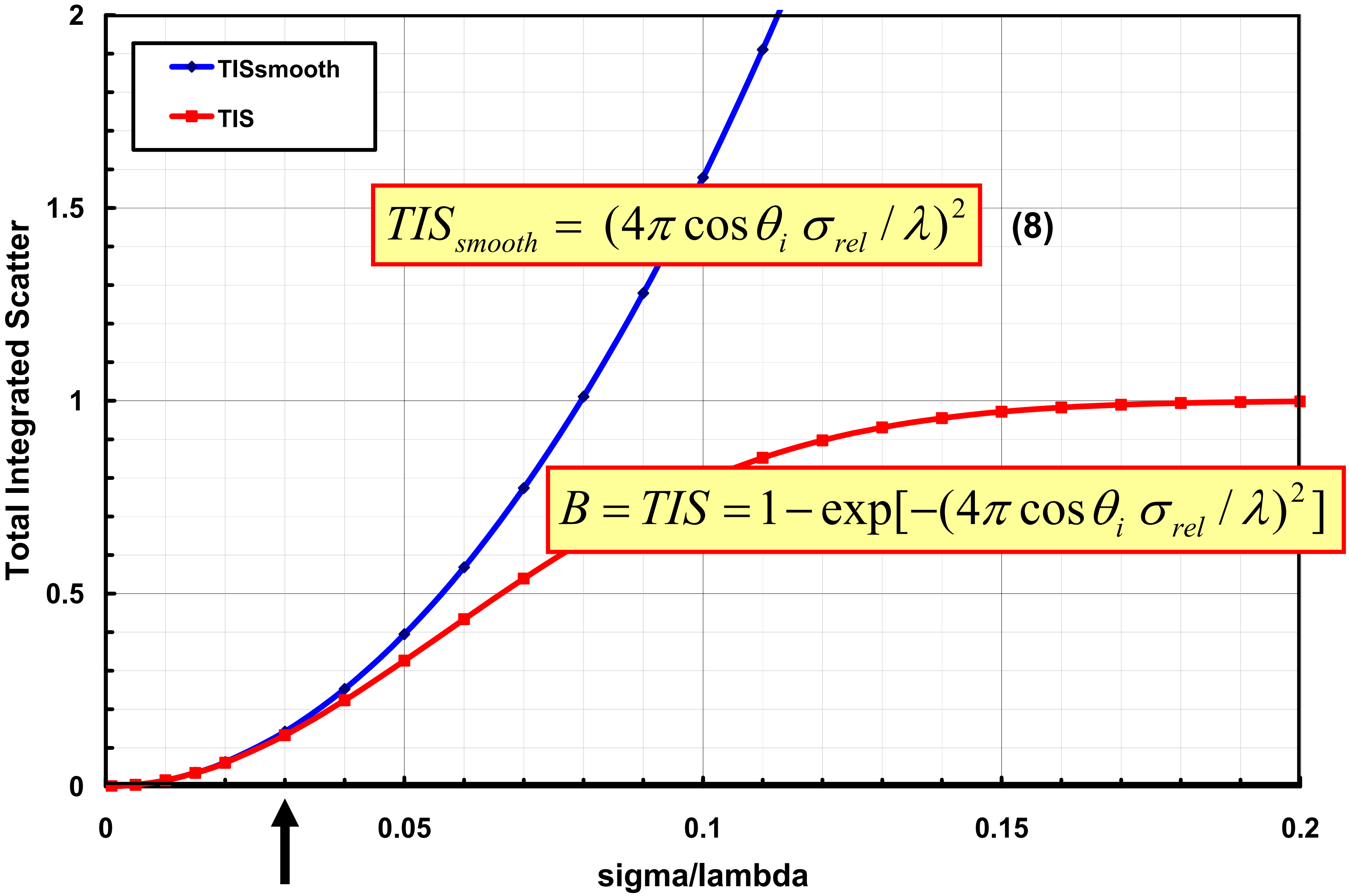
For smooth surfaces ($\sigma \ll \lambda$), the total integrated scatter (TIS_{smooth}) can thus be approximated as

$$TIS_{smooth} = (4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2 \qquad (8)$$

However, one needs to be careful in using this approximate expression as this quantity can quickly exceed unity for moderately rough surfaces.

How Smooth is a Smooth Surface?

This graph shows how the smooth-surface approximation for TIS continues to grow exponentially for large σ/λ, providing an unrealistically large value for moderately rough surfaces.

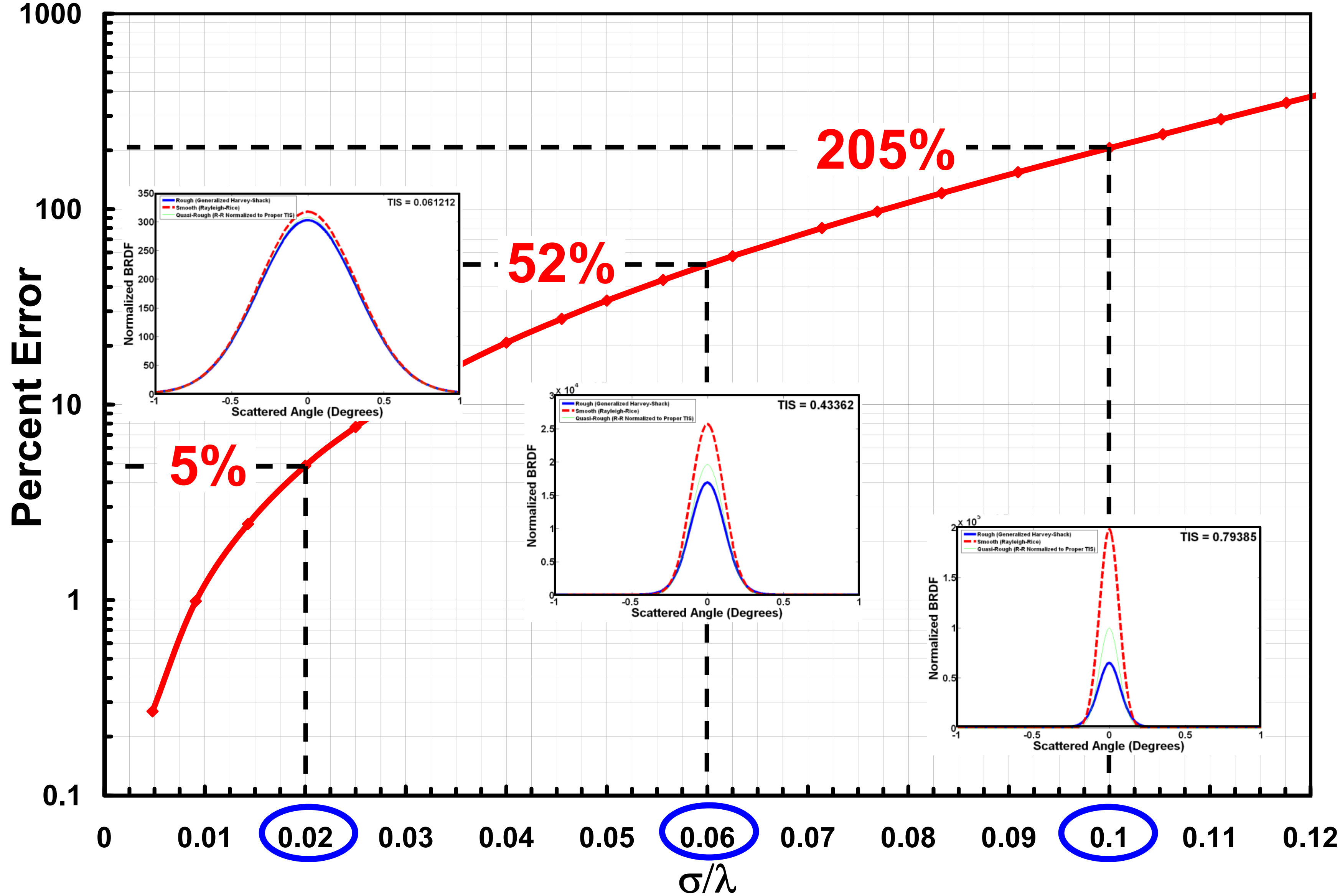


$$TIS_{smooth} = (4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2 \quad (8)$$

$$B = TIS = 1 - \exp[-(4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2] \quad (7)$$

How Smooth is a Smooth Surface?

The smooth-surface approximation is a *very severe limitation* in predicting the BRDF as illustrated below for a Gaussian surface PSD. The percent error in the predicted peak value of the BRDF is illustrated below as a function of σ/λ.



Outline

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- Non-paraxial Scalar Diffraction Theory.
  - Scalar Treatment of Sinusoidal Phase Grating,
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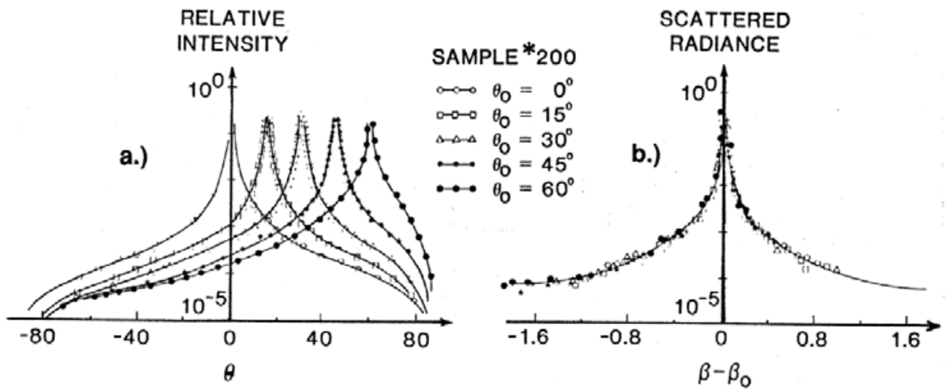
- Results and Conclusions.

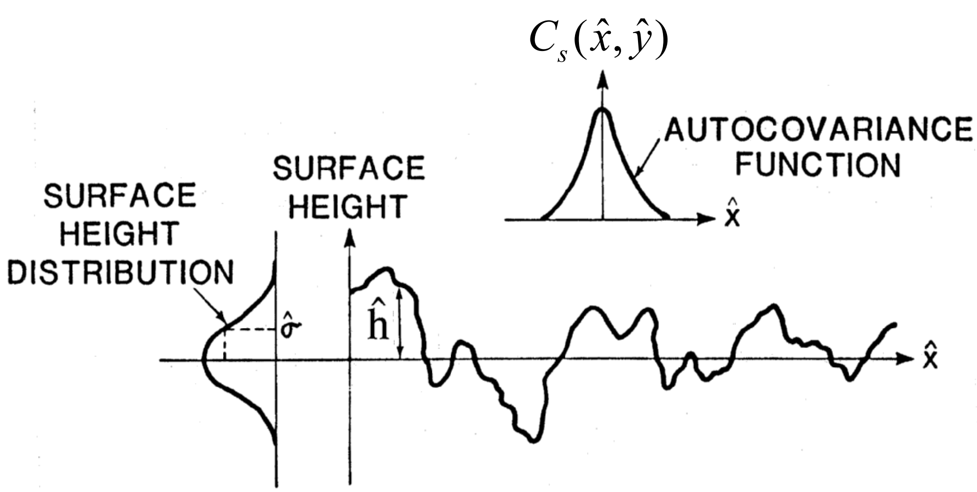
Transfer Function Characterization of Surface Scatter*

In 1976 Harvey and Shack formulated a scattering theory in a linear systems format resulting in a surface transfer function (STF) that relates scattering behavior to surface topography. Surface scatter phenomena was modeled as a simple scalar diffraction process, where the diffracting "aperture" is a random phase "aperture" rather than the conventional binary amplitude aperture. The rough surface merely imparts phase variations onto the incident wavefront upon reflection. *No explicit "smooth surface" approximations were made.*

Experimental Scattered Data



Surface Characteristics



Surface Transfer Function

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

$$H_s(\hat{x},\hat{y}) = A + B\,Q(\hat{x},\hat{y}) \qquad \textbf{(9)}$$

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

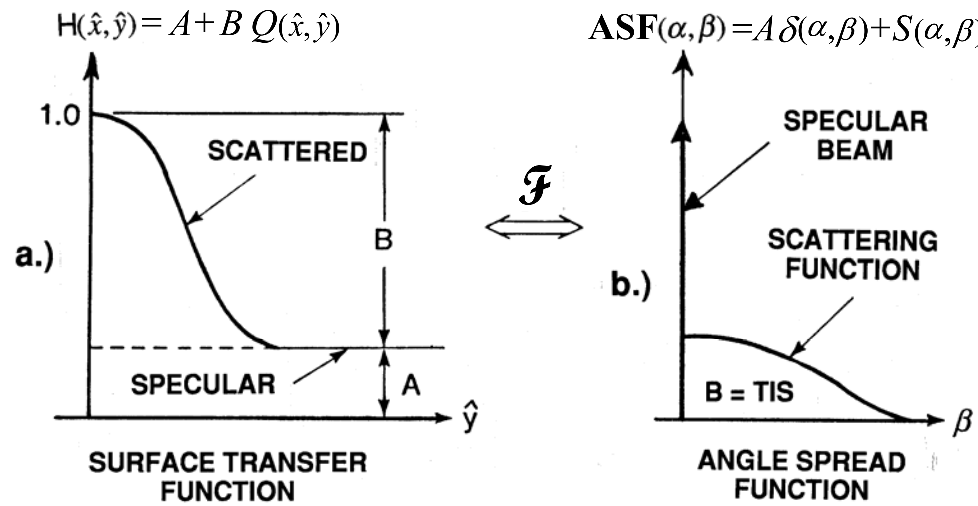
$$B = 1 - \exp[-(4\pi\,\hat{\sigma}_s)^2]$$

* J. E. Harvey, "Light-Scattering Characteristics of Optical surfaces", Ph.D. Dissertation, Univ. of Arizona (1976).

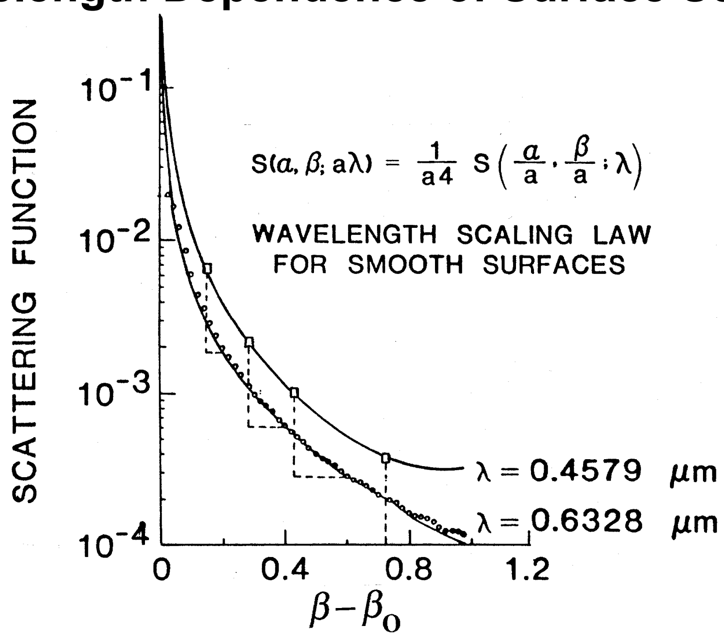
The Associated Angle Spread Function*
(Scattered Radiance)

Insight into the scattering process was inferred by considering the nature of the surface transfer function, and its Fourier transform, the angle spread function (*ASF*). Note that this *ASF* is scattered *radiance*, not irradiance or intensity. Of particular interest was the inverse scattering problem, and the wavelength dependence of the scattered light behavior. It was also convenient that the scattering function for optical surfaces polished by conventional techniques upon ordinary materials exhibited an inverse power law (fractal) behavior.

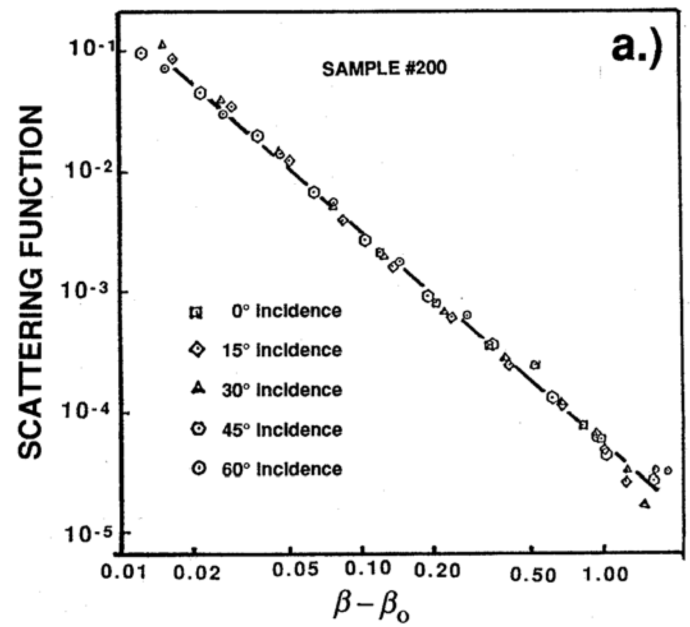
The Associated Angle Spread Function



Wavelength Dependence of Surface Scatter



Inverse Power Law Behavior



∗ J. E. Harvey, "Light-Scattering Characteristics of Optical surfaces", Ph.D. Dissertation, Univ. of Arizona (1976).

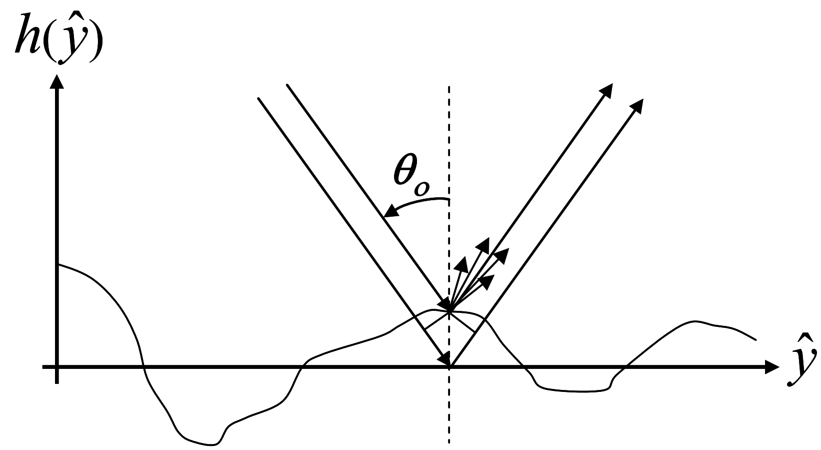
Harvey-Shack Surface Scatter Model*

* R. P. Breault, "Users Manual for APART/PADE Version 6B",Breault Research Organization, Tucson Arizona (1980).

Modified Harvey-Shack Surface Scatter Theory*

During the 1980's the STF was generalized to include the extremely large incident angles inherent to grazing incidence Wolter Type I X-ray telescopes. The optical path difference (OPD) due to reflection from an irregular surface is illustrated here, and the assumed phase variation in the plane of the surface when the Kirchhoff approximation is invoked is presented. We have still made no explicit smooth surface approximation!

Optical Path Difference (OPD) upon Reflection



$$OPD(\hat{x},\hat{y}) = 2\, h(\hat{x},\hat{y}) \cos(\theta_o), \;\; \sigma_w = 2\,\sigma_s \cos(\theta_o)$$

By Invoking the Kirchhoff Approximation

We can write the two-dimensional phase variation in the plane of the surface due to reflection from a rough surface at an arbitrary angle of incidence.

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

Of course, we must add to this the linear phase variation that results from the specularly reflected plane wavefront.

$$\phi_o = 2\pi\beta_o \hat{y}$$

Note that $\beta_o = \sin\theta_o$ and $\gamma_o = \cos\theta_o$.

Modified Surface Transfer Function

$$H_S(\hat{x},\hat{y}) \;=\; \exp\left\{-(4\pi\,\gamma_o\hat{\sigma}_s)^2\left[1 - C_s\left(\frac{\hat{x}}{\hat{\ell}},\frac{\hat{y}}{\hat{\ell}}\right)/\sigma_s^{\,2}\right]\right\} \quad (10)$$

$$H_S(\hat{x},\hat{y}) \;=\; A + B\, Q(\hat{x},\hat{y})$$

where

$$A = \exp[-(4\pi\,\gamma_o\hat{\sigma}_s)^2], \;\; B = 1 - \exp[-(4\pi\,\gamma_o\hat{\sigma}_s)^2]$$

and

$$Q(\hat{x},\hat{y}) = \frac{\exp\left\{(4\pi\,\gamma_o\hat{\sigma}_s)^2\left[C_s\left(\frac{\hat{x}}{\hat{\ell}},\frac{\hat{y}}{\hat{\ell}}\right)/\sigma_s^2\right]\right\} - 1}{\exp(4\pi\,\gamma_o\hat{\sigma}_s)^2 - 1}$$

* J. E. Harvey, et. al., "Transfer Function Characterization of Grazing Incidence Optical Systems", Appl. Opt. 27, 1527-1533 (15 April 1988).

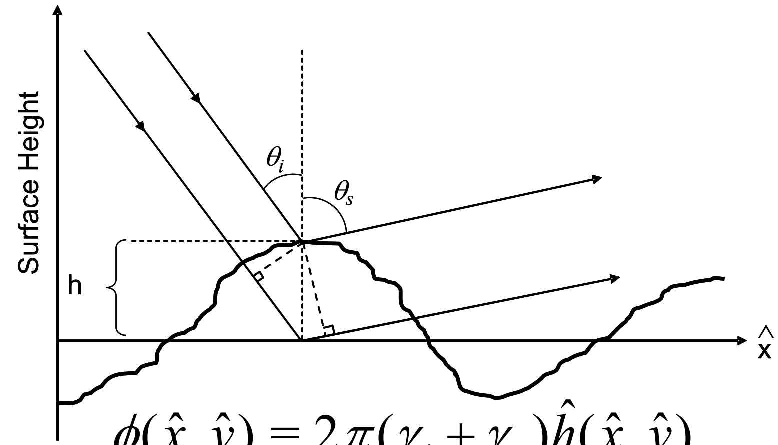
Generalized Harvey-Shack Surface Scatter Theory[1-3]

(Arbitrarily Rough Surfaces, Large Incident and Scatter Angles)

Original Harvey-Shack Theory

- **Scalar theory (no polarization effects).**
- **BRDF shift-invariant in direction cosine space.**
- **Surface transfer function has inherent paraxial limitation.**
- **Does not account for redistribution of energy from evanescent to propagating waves.**

Phase Variation Depends on Scattering Angle



$$\phi(\hat{x},\hat{y}) = 2\pi(\gamma_i + \gamma_s)\hat{h}(\hat{x},\hat{y})$$

2-parameter Family of Transfer Functions

$$H_s(\hat{x},\hat{y};\gamma_i,\gamma_s) = \exp\left\{-\left[2\pi\sigma_{rel}(\gamma_i+\gamma_s)\right]^2\left[1 - C_s(\hat{x},\hat{y})/\sigma_s^2\right]\right\} \quad (11)$$

$$\hat{x} = x/\lambda, \qquad \hat{y} = y/\lambda, \qquad \hat{\sigma} = \sigma/\lambda$$

$$\gamma_i = \cos\theta_i \qquad \gamma_s = \sqrt{1-\alpha_s^2-\beta_s^2} = \cos\theta_s$$

$C_s(\hat{x},\hat{y}) \equiv$ **Surface Autocovariance Function**

$$TIS = 1 - \exp\left\{-\left[2\pi\hat{\sigma}_{rel}(\gamma_i+\gamma_s)\right]^2\right\}$$

$$BRDF = Q\,\mathfrak{F}\left\{H_s(\hat{x},\hat{y};\gamma_i,\gamma_s)\right\} \quad (12)$$

Generalized Harvey-Shack Theory

The system is no longer shift invariant (requires a different transfer function for each incident and scattering angle).

This is similar to imaging systems with field-dependent aberrations, where a different MTF is necessary for each field angle.

This new surface scatter model has been quasi-vectorized by merely substituting the polarization reflectance factor, *Q*, for the reflectance, *R*, in the scalar treatment.

1. A. Krywonos, *Predicting Surface Scatter using a Linear Systems Formulation of Non-paraxial Scalar Diffraction*, PhD Dissertation, UCF (2006).
2. J. Harvey, et.al., "Unified Scatter Model for Rough Surfaces at Large Incident and Scattered Angles", Proc. SPIE 6672-12 (2007).
3. A. Krywonos, J. Harvey and N. Choi, "A Linear systems Formulation of Scattering Theory for Rough Surfaces with Arbitrary Incident and Scattering Angles", in preparation for publication in JOSA A.

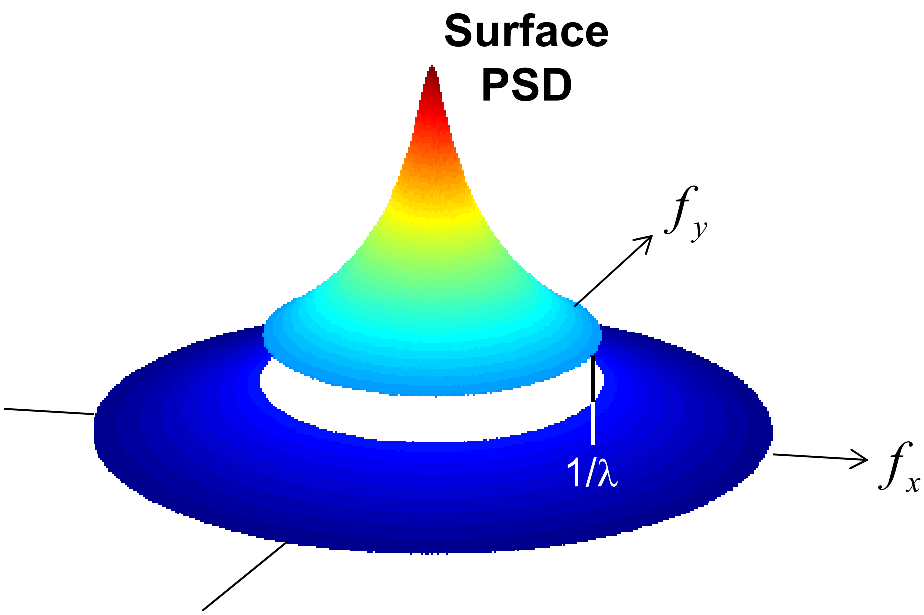
The Relevant Surface PSD for Normal Incidence

(Band-limited rms Surface roughness)

Today most of us recognize that is the "relevant" or "effective" band-limited surface roughness that determines scattered light behavior. Since surface scatter phenomena is a diffraction process, scatter angles are related to discrete spatial frequencies in the surface PSD by the hemispherical grating equation

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

For normal incidence spatial frequencies greater than 1/λ do not scatter light.



For isotropic roughness and normal incidence, the square of the *relevant band-limited surface roughness* is given by the following integral.

$$\sigma_{rel}^2(\lambda) = 2\pi \int_{f=0}^{1/\lambda} PSD(f)\, f\, df\, d\phi \qquad (13)$$

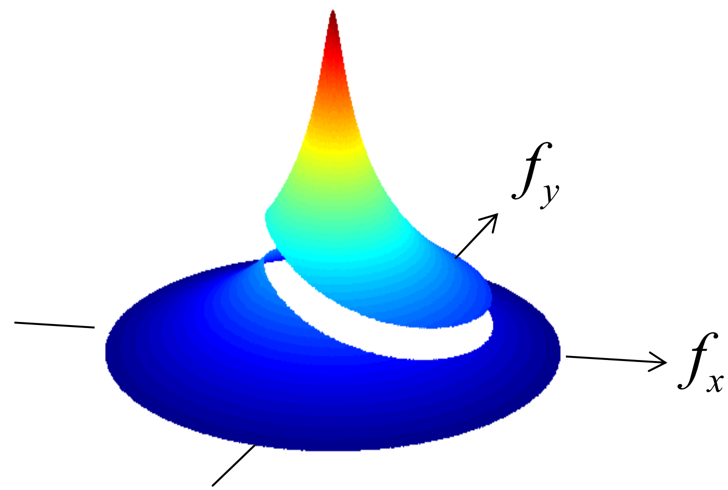
Surface roughness with spatial frequencies greater than 1/λ is irrelevant in that it does not result in scattered radiation.

σ_{rel} for Arbitrary Incident Angle and Wavelength

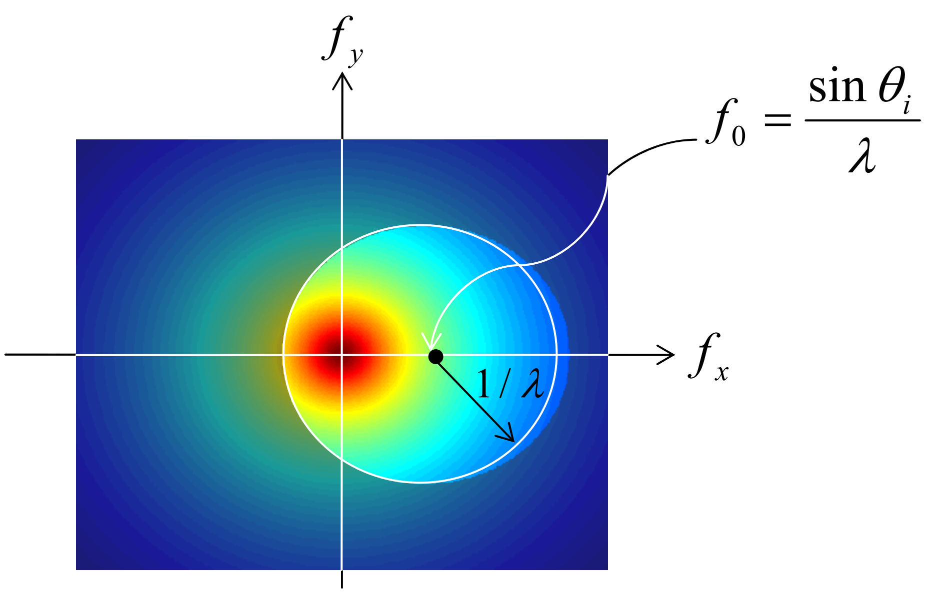
The grating equation for an arbitrary incident angle dictates that the relevant portion of the surface PSD with regard to surface scatter is a shifted circular portion with a radius of 1/λ cut out of the surface PSD with a cookie-cutter.

$$f_x = \frac{\sin\theta_s \cos\varphi_s - \sin\theta_i}{\lambda}, \; f_y = \frac{\sin\theta_s \sin\varphi_s}{\lambda} \quad (14)$$

Relevant Portion of Surface PSD



Center-shifted Circle in *f*-domain

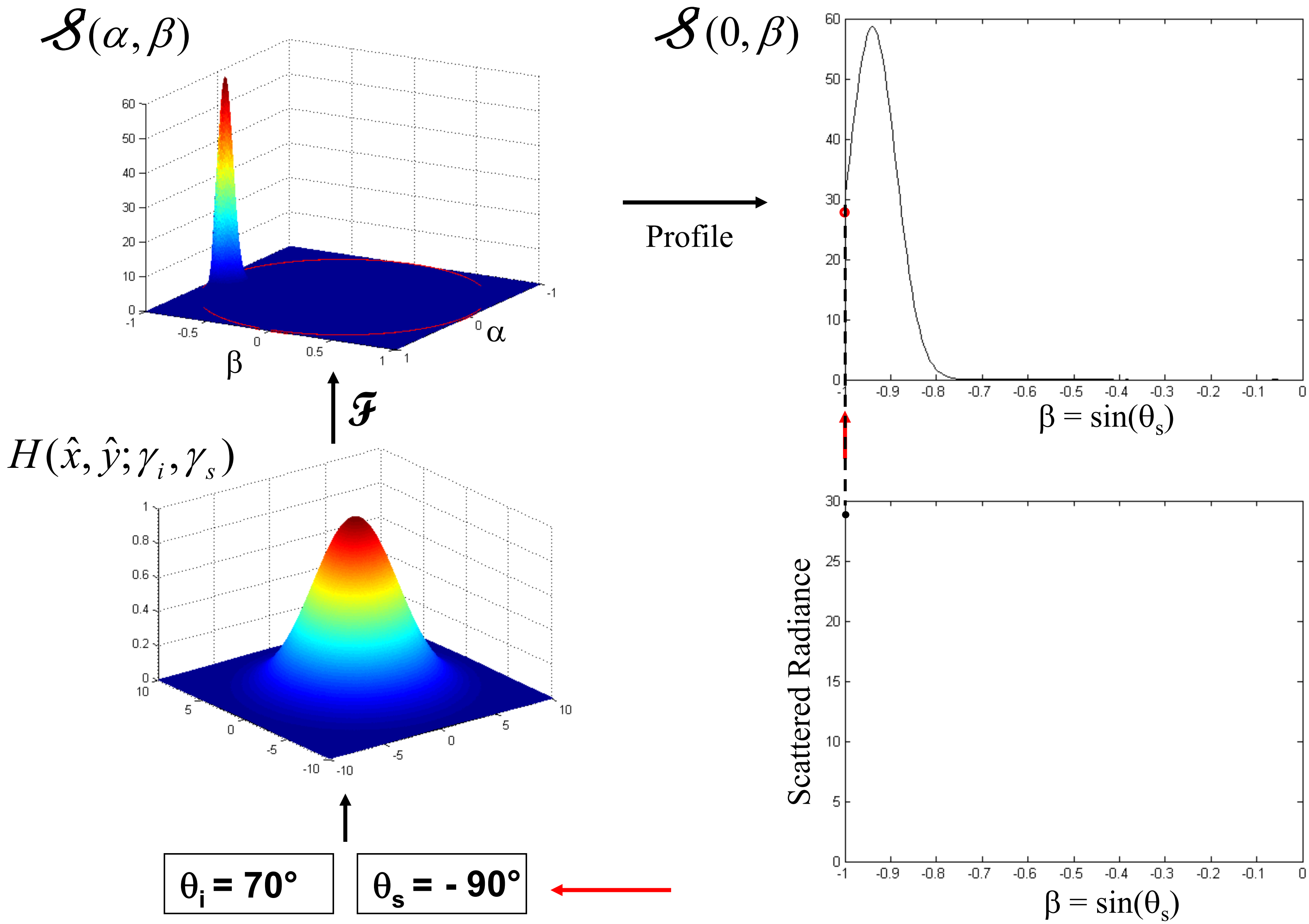


Band-limited Relevant rms Surface Roughness

- Rms surface roughness is obtained by integrating surface PSD over this shifted circle of radius 1/λ.
- It is thus a function of both incident angle and wavelength.

$$\sigma_{rel}^2(\lambda) = \int_{-1/\lambda+f_0}^{1/\lambda+f_0} \int_{-\sqrt{1/\lambda^2-(f_x-f_0)^2}}^{+\sqrt{1/\lambda^2-(f_x-f_0)^2}} PSD(f_x, f_y)\, df_x\, df_y \quad (15)$$

Description of Generalized Harvey-Shack Calculations



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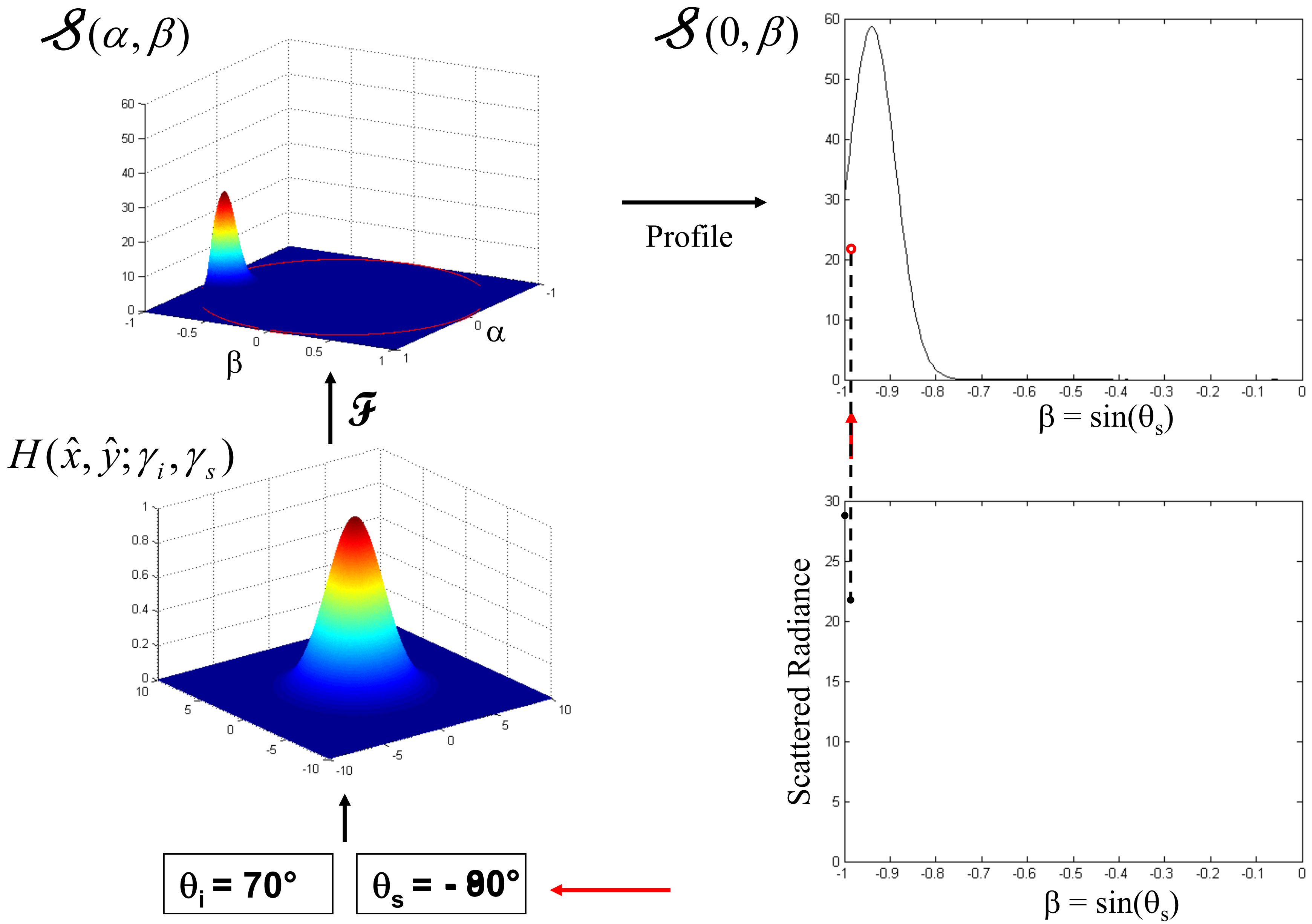

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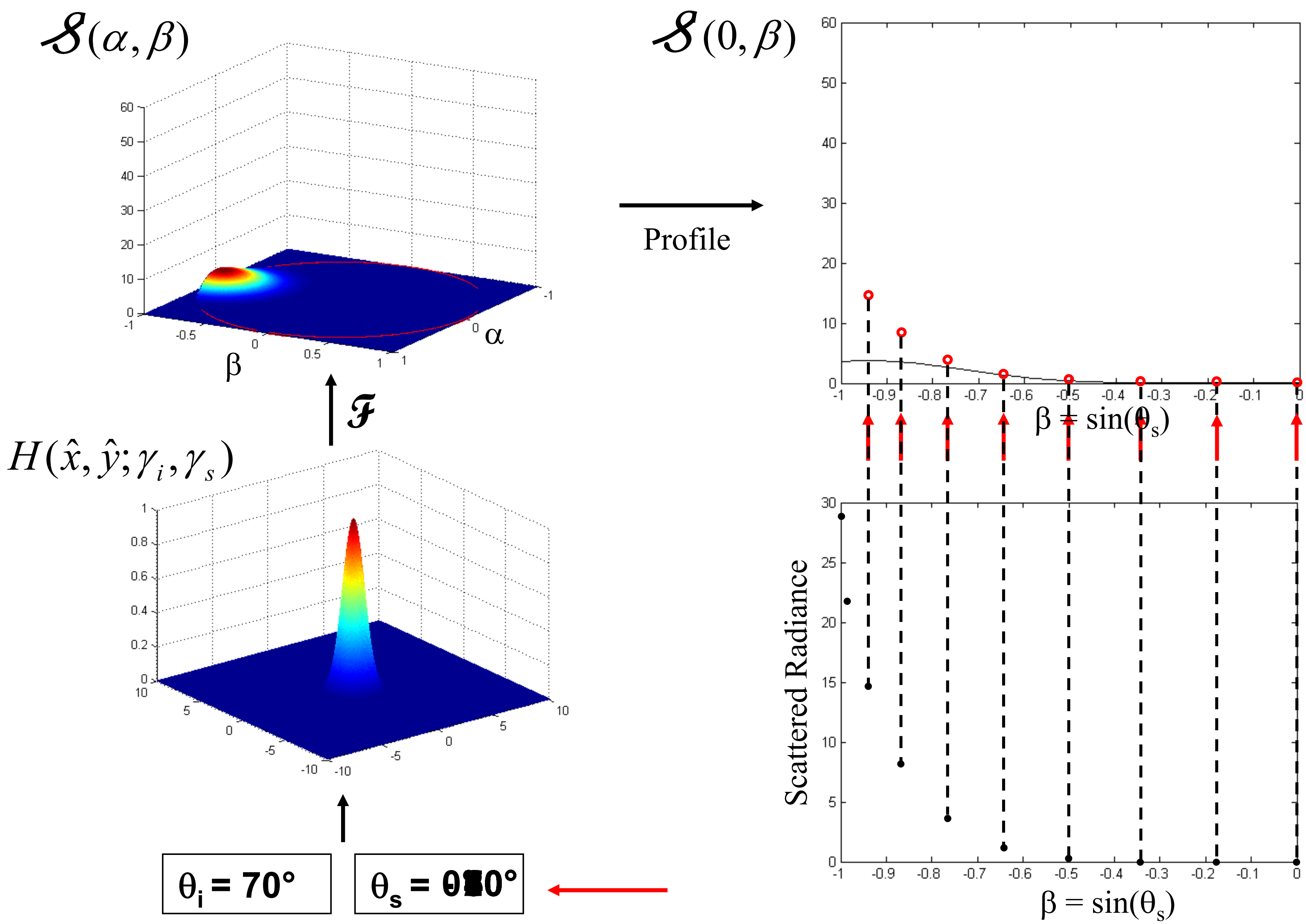

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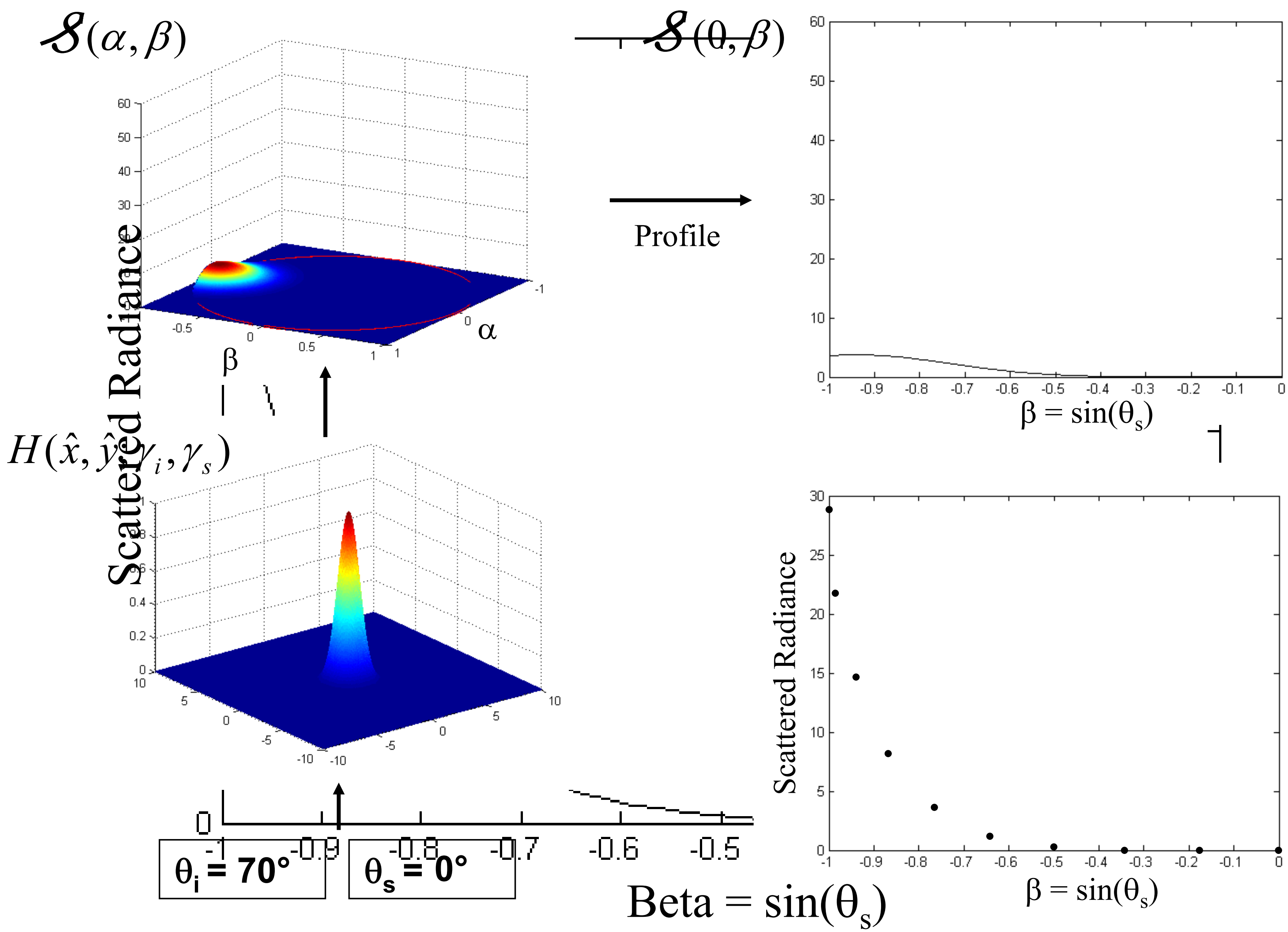
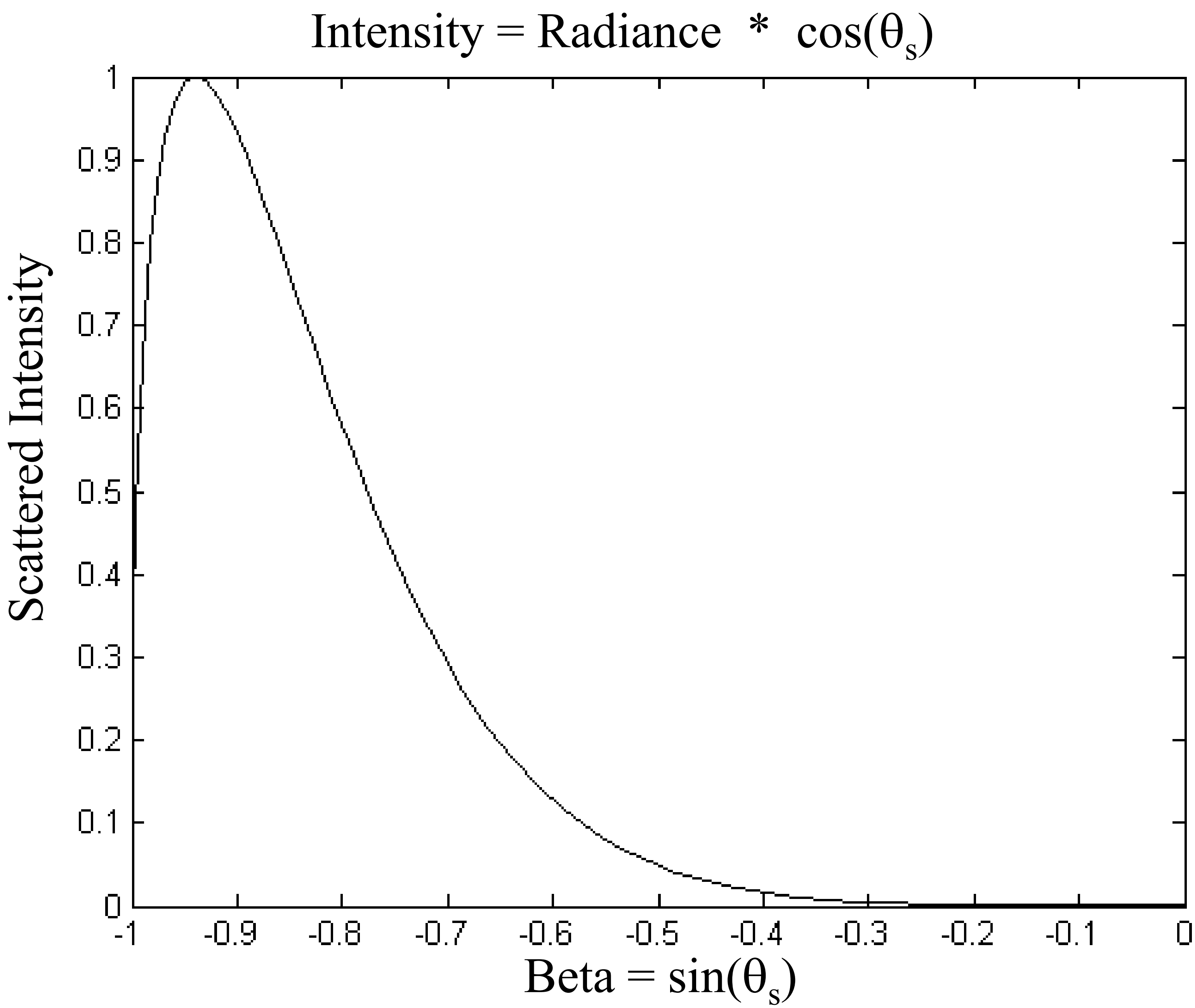


Description of Generalized Harvey-Shack Calculations



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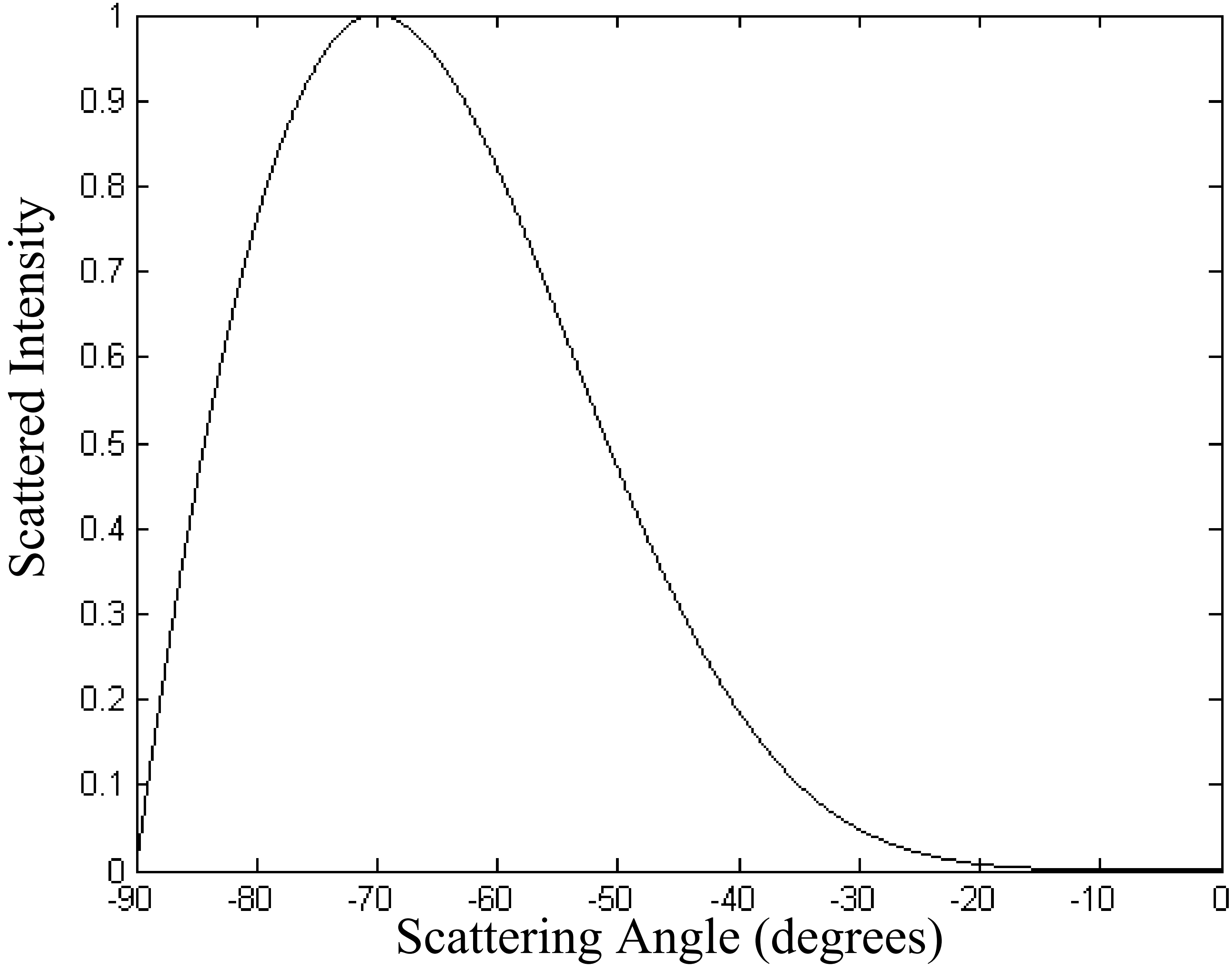

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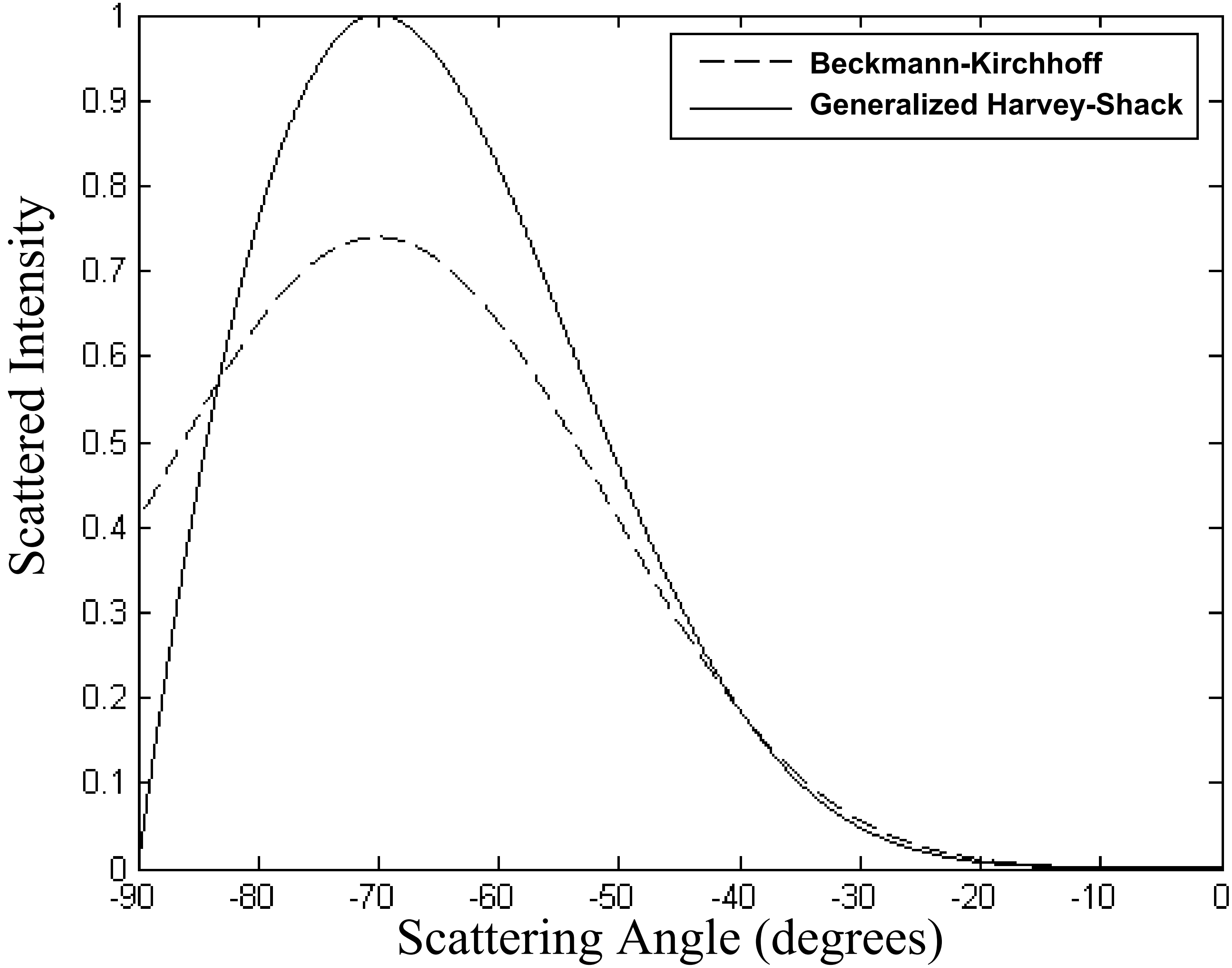
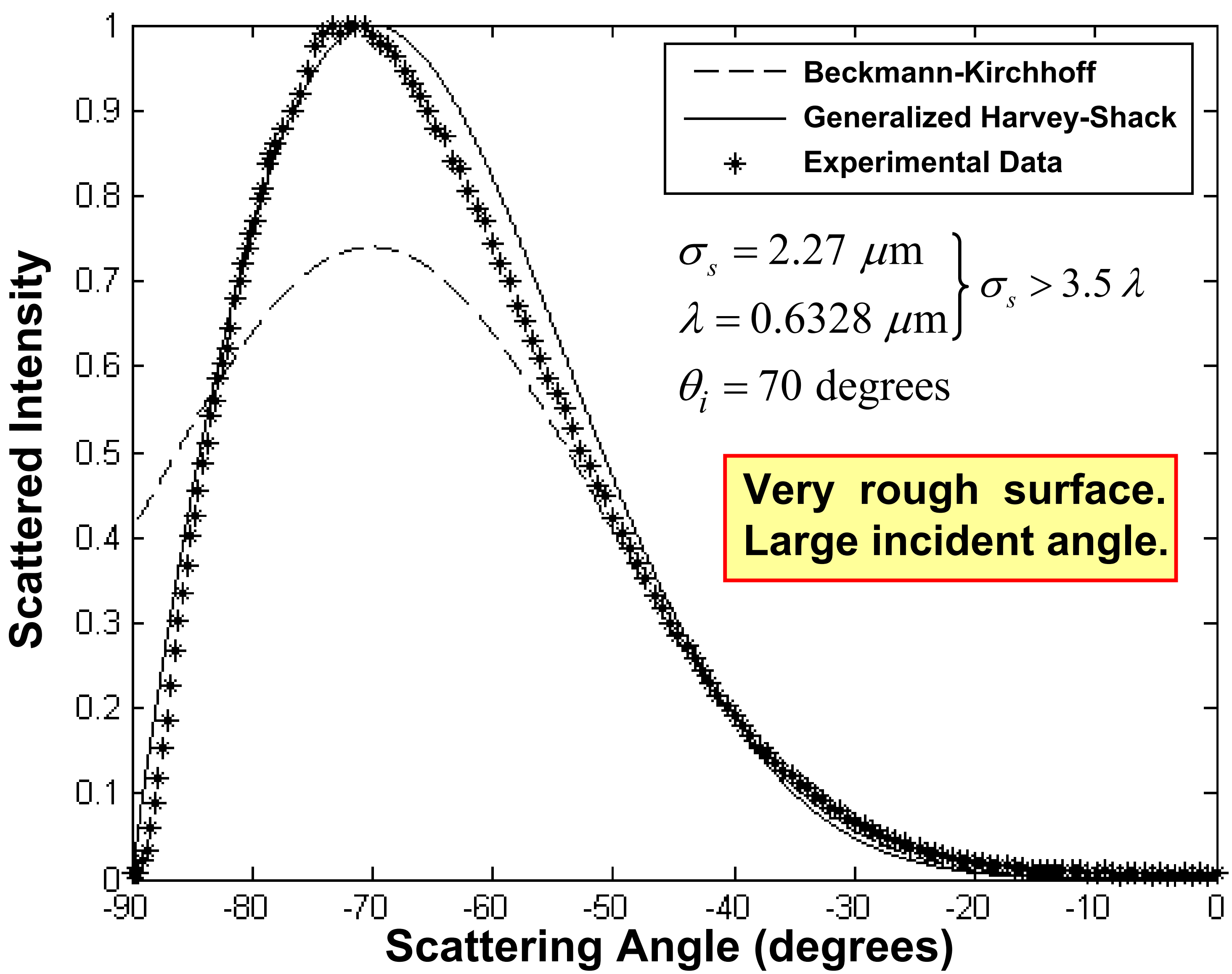


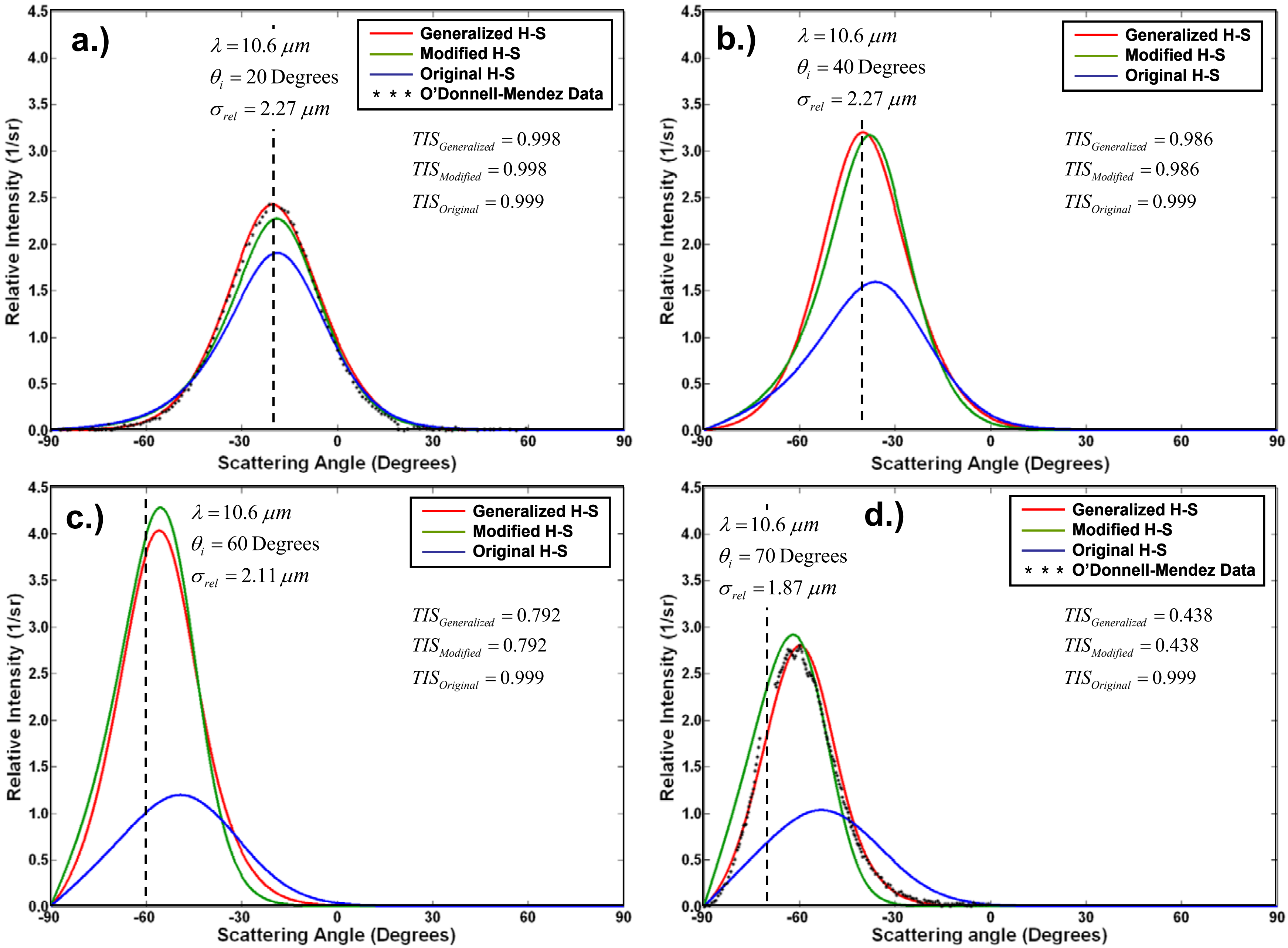
Generalized Harvey-Shack Scatter Theory

(Experimentally Validated by O'Donnell-Mendez Data) *



* K. A. O'Donnell and E. R. Mendez, "Experimental study of scattering from characterized random surfaces", J. Opt. Soc. Am. A, 4, 1194-1205 (1987).

Additional Experimental Validation



Smooth-surface Approximation to GHS Theory*

(Obliquity Factor Differs from Rayleigh-Rice Theory)

Generalized Harvey-Shack

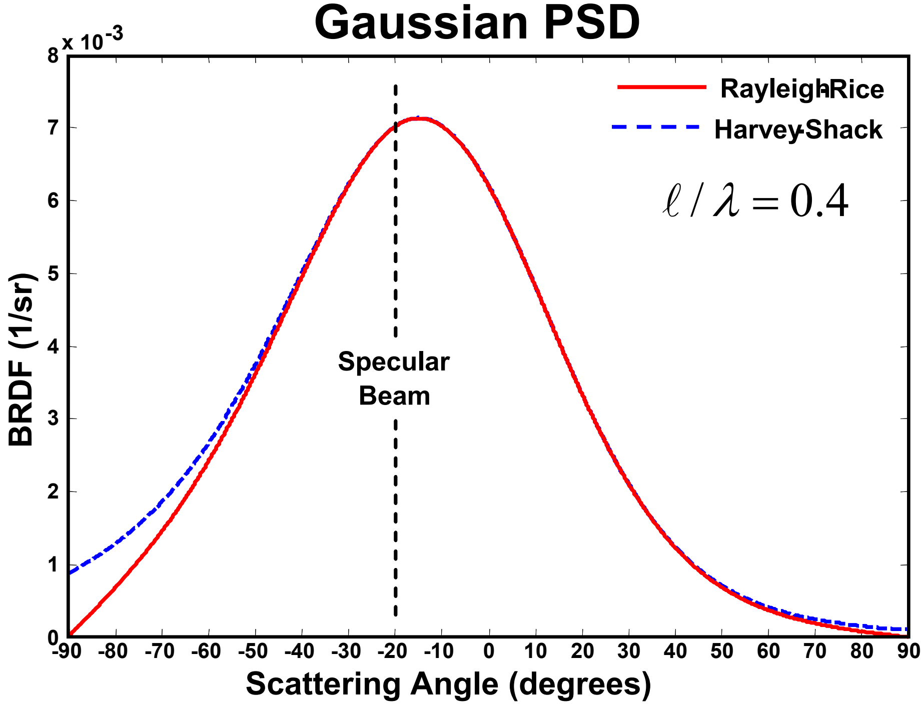
$$BRDF = \frac{4\pi^2}{\lambda^4}(\cos\theta_o + \cos\theta_s)^2\, Q\, PSD(f_x, f_y) \quad (16)$$

Rayleigh-Rice

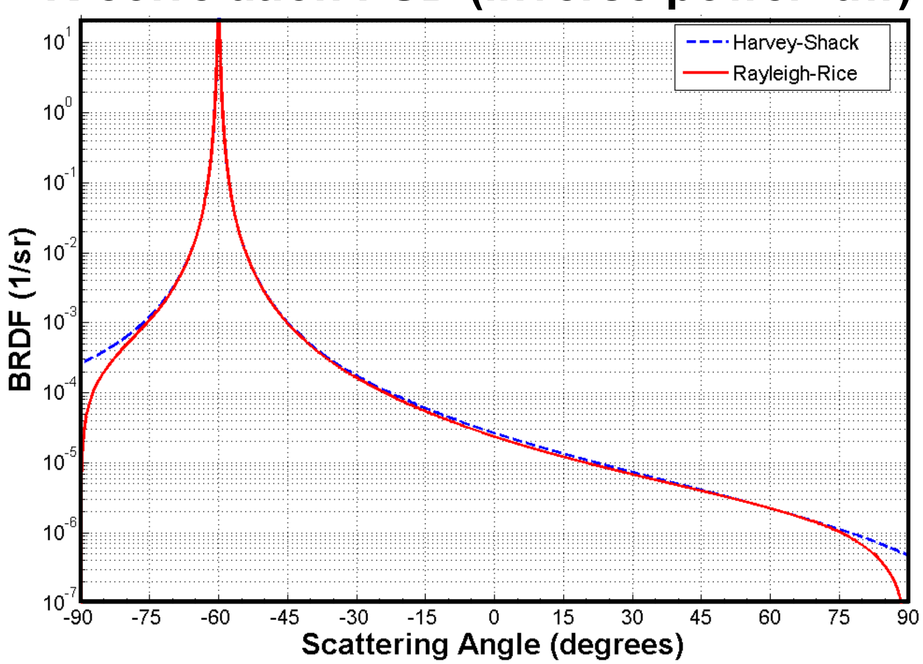
$$BRDF = \frac{16\pi^2}{\lambda^4}\cos\theta_o \cos\theta_s\, Q\, PSD(f_x, f_y) \quad (17)$$

The above two equations are equivalent for small incident and scattered angles; however, the Rayleigh-Rice expression drives the BRDF to zero at ± 90 degrees regardless of the form of the surface PSD. In general, *BRDF* 's *do not go to zero* at ± 90 degrees (a Lambertian surface is an obvious counter-example). Furthermore the Rayleigh-Rice expression results in undesirable artifact in the predicted PSD when solving the inverse scattering problem (the ubiquitous "hook" at high spatial frequencies).

Gaussian PSD



K-correlation PSD (inverse power law)



* J. E. Harvey and A. Krywonos, "Improved Characterization of Optical Surfaces from Scattered Light Measurements", presented at OSA Topical Meeting on Optical Interference Coatings, Tucson, AZ, June 4-7, 2007; Summary published in Conference Proceedings.

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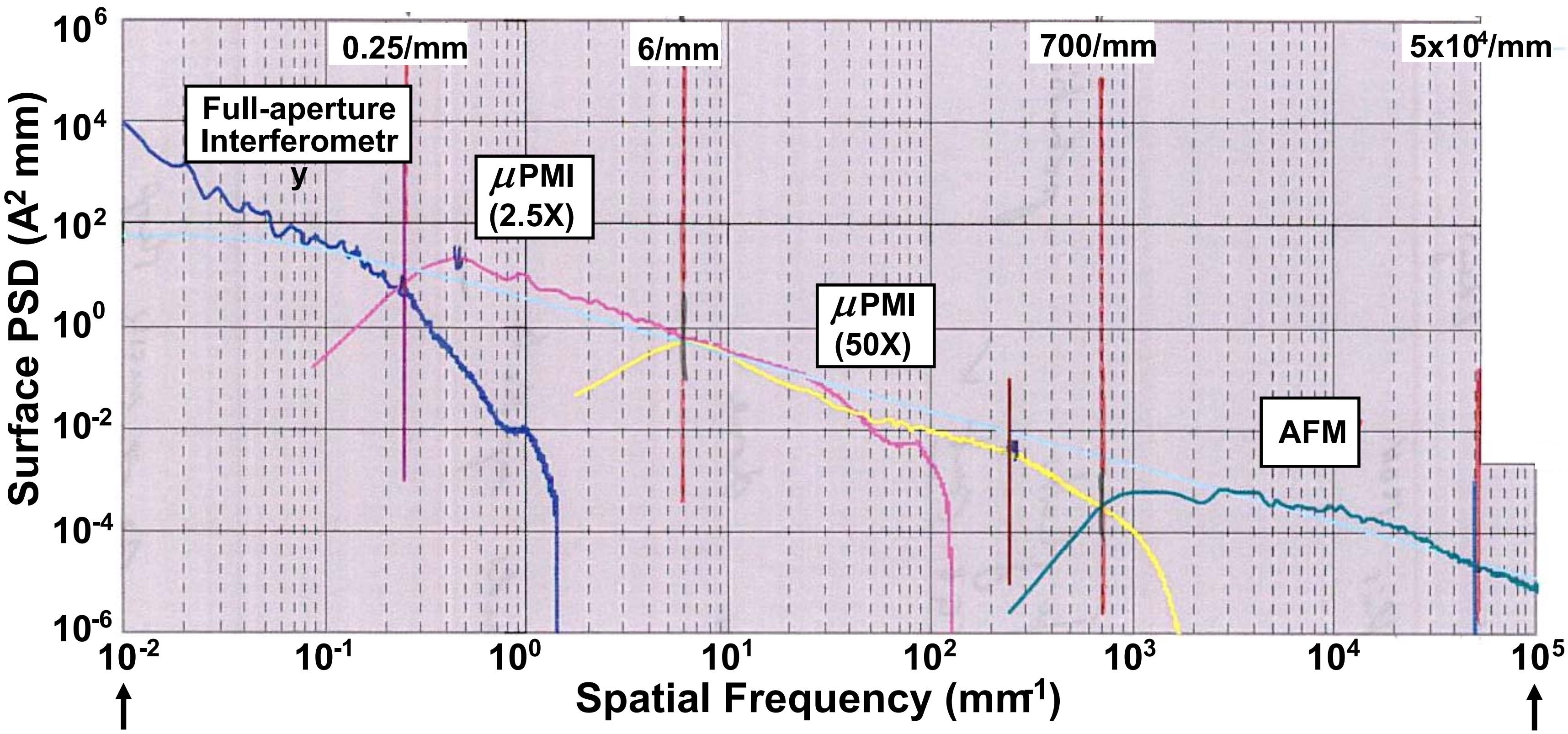
Example of Measured Metrology Data
(Including the very real "Mid" Spatial Frequencies)

It often takes three, or even four different metrology instruments to measure the surface characteristics over the entire range of relevant spatial frequencies for a given application.



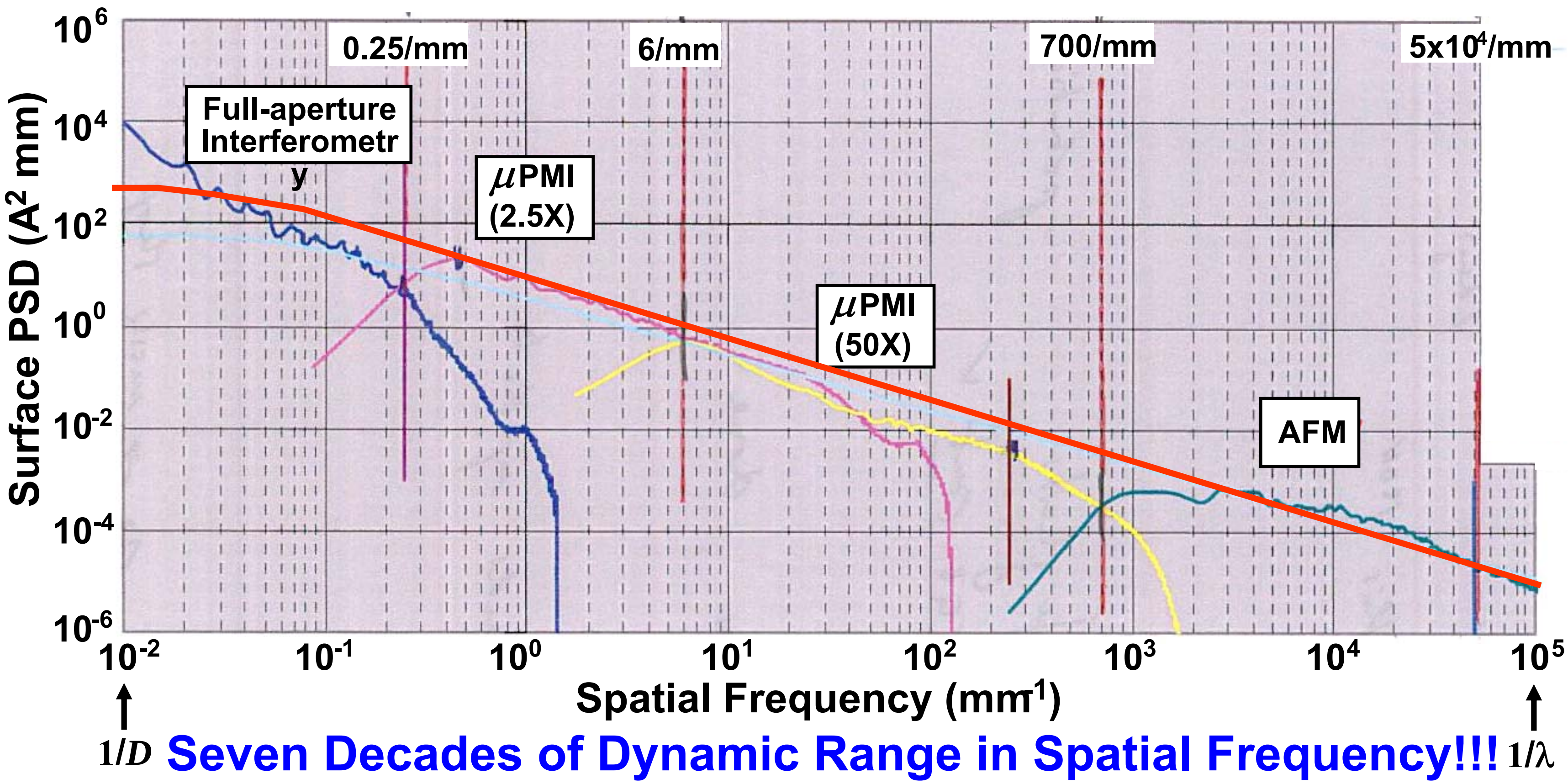
Seven Decades of Dynamic Range in Spatial Frequency!!!

This metrology data can then be fit with an appropriate fitting function that can be used for making BRDF predictions, and then calculating image degradation. Note 7 decades of dynamic range in spatial frequency for $D = 100mm$ and $\lambda = 100$ A.

ABC, or *K*-Correlation Function Fit to Metrology Data*

Here we have fit the measured metrology data with an ABC or K-Correlation Function of the following form. The advantages of using a fitting function of this form is shown on the next slide.

$$PSD(f_x)_{1-D} = \frac{A}{\left[1+(B\,f_x)^2\right]^{C/2}} \qquad (18)$$



Seven Decades of Dynamic Range in Spatial Frequency!!!

* E. L. Church and P. Z. Takacs, "The optimal estimation of finish parameters", Proc. SPIE 1530, p. 71-78 (1991).

Properties of *ABC* or *K*-Correlation Functions*

The *ABC*, or *K*-correlation function expressed by Eq.(19) has several very useful properties. The 2-D surface PSD (assuming isotropic roughness) can be obtained from the 1-D surface profile measurements by using Eq.(20). The total volume under the 2-D surface PSD is given by Eq.(21), and the Fourier transform of the 2-D K-correlation function is given by Eq.(22).

$$PSD(f_x)_{1-D} = \frac{A}{\left[1+(B\,f_x)^2\right]^{C/2}}$$ 3-parameter K-correlation function or ABC function. **(19)**

$$PSD(f)_{2-D} = K\frac{A\,B}{\left[1+(B\,f)^2\right]^{(C+1)/2}}\ ,\quad K = \frac{1}{2\sqrt{\pi}}\frac{\Gamma\big((C+1)/2\big)}{\Gamma\big(C/2\big)}$$ 2-D surface PSD. **(20)**

$$f = \sqrt{f_x^2 + y_y^2}$$

$$\sigma^2_{Total} = \frac{2\pi K A}{(C-1)B}$$ Total volume under 2-D surface PSD. **(21)**

$$ACV_s(r) = \sqrt{2\pi}\,\frac{A}{B}\,\frac{2^{-C/2}}{\Gamma(C/2)}\left(\frac{2\pi r}{B}\right)^{(C-1)/2}\mathcal{K}_{(C-1)/2}\left(\frac{2\pi r}{B}\right)$$ Surface Autocovariance Function. **(22)**

Where $\mathcal{K}_{(C-1)/2}$ is the modified Bessel function of the 2nd kind and $r = \sqrt{x^2 + y^2}$

E. Church and P. Takacs, "The optimal estimation of finish parameters", in *Optical Scatter: Applications, Measurement, and Theory*, J. C. Stover, Ed., Proc. SPIE **1530,** p. 71-78 (1991).
J, M. Elson, J. M. Bennett, and J. C. Stover, "Wavelength and angular dependence of light scattering from beryllium: comparison of theory and experiment", Appl. *Opt.* **32** (1993).
M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, New York: Dover (1965).

The *FFTLog* Hankel Transform Algorithm*

- ***FFTLog*** **is a set of subroutines that compute the fast Fourier or Hankel (i.e., Fourier-Bessel) transform of a periodic sequence of logarithmically spaced data points.**

- ***FFTLog*** **can be regarded as a natural analogue to the standard Fast Fourier Transform (FFT), in the sense that, just as the normal FFT gives the exact (to machine precision) Fourier transform of a linearly spaced periodic sequence of data points, so also** ***FFTLog*** **gives the exact Fourier or Hankel transform, of arbitrary order, of a logarithmically spaced periodic sequence of data points.**

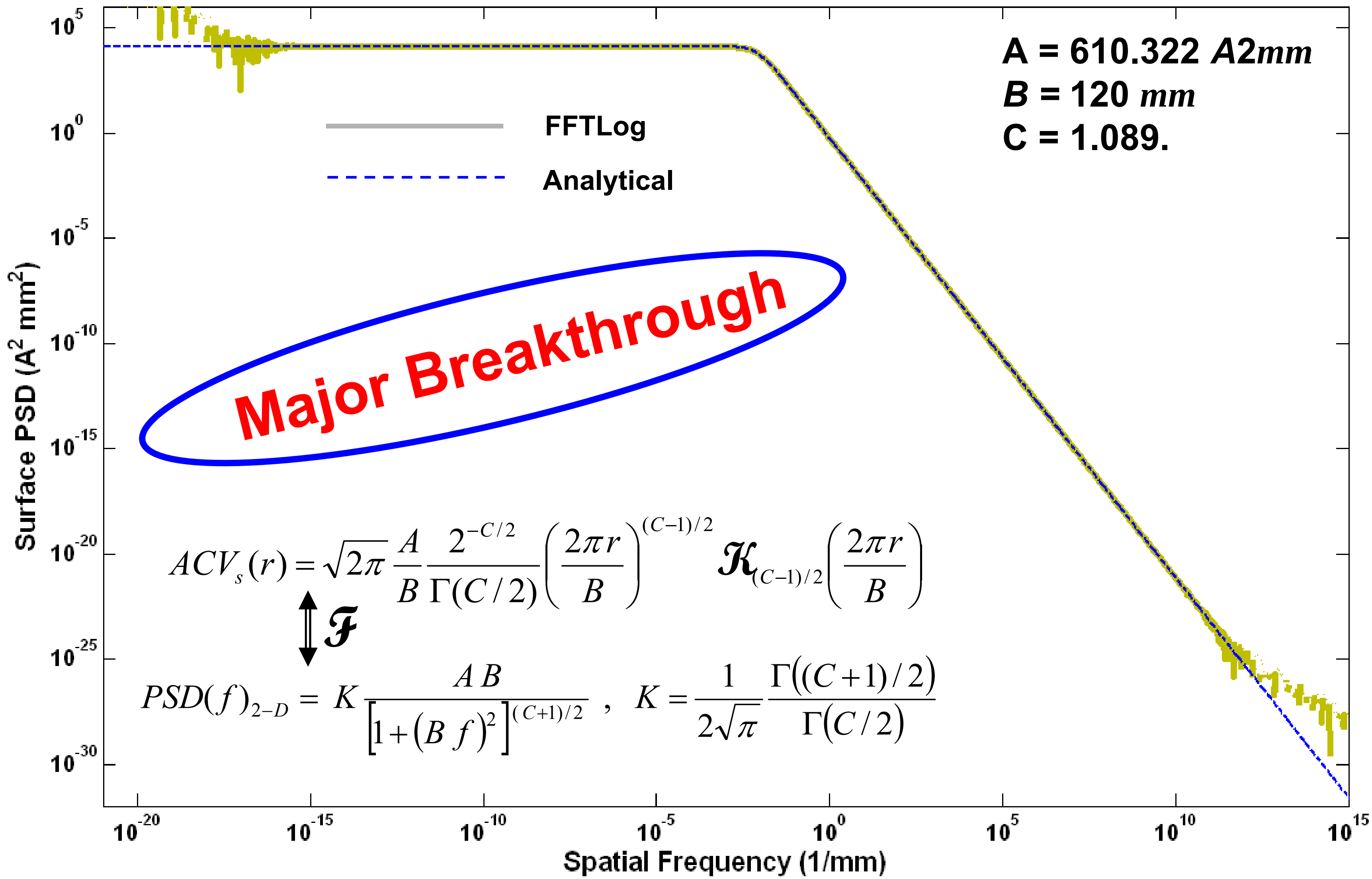
- ***FFTLog*** **shares with the normal FFT the problems of ringing (response to sudden steps) and aliasing (periodic folding of frequencies), but under appropriate circumstances** ***FFTLog*** **may approximate the results of a continuous Fourier or Hankel transform.**

- **The** ***FFTLog*** **algorithm is particularly useful for applications where the power spectrum extends over many orders of magnitude in wavenumber** ***k*****, and varies smoothly in ln*****k*****.**

*** A. J. S. Hamilton, "Uncorrelated Modes of Nonlinear Power spectrum", Mon.Not.Roy.Astron.Soc. 312 (2000) 257-284.**

Numerical Validation of the *FFTLog* Algorithm

For well-behaved functions, the *FFTLog* algorithm is accurate over 25 decades of variation in spatial frequency (Note that the "ringing" and "aliasing" effects inherent to numerical Fourier transform calculations).



$$ACV_s(r) = \sqrt{2\pi}\,\frac{A}{B}\,\frac{2^{-C/2}}{\Gamma(C/2)}\left(\frac{2\pi r}{B}\right)^{(C-1)/2} \mathcal{K}_{(C-1)/2}\left(\frac{2\pi r}{B}\right)$$

$$\Updownarrow \mathcal{F}$$

$$PSD(f)_{2-D} = K\,\frac{A\,B}{\left[1+(B\,f)^2\right]^{(C+1)/2}}\;,\quad K = \frac{1}{2\sqrt{\pi}}\,\frac{\Gamma((C+1)/2)}{\Gamma(C/2)}$$

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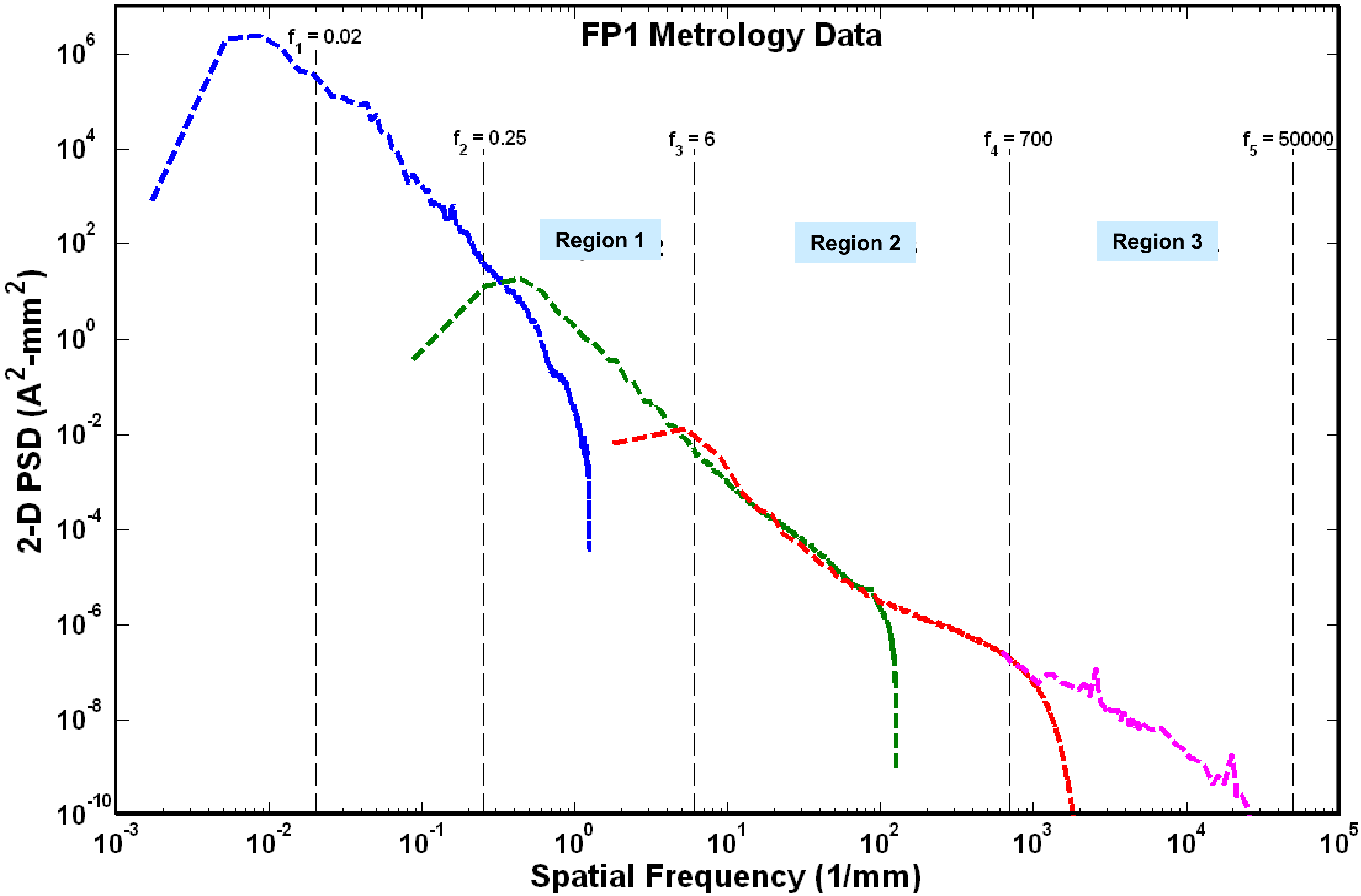
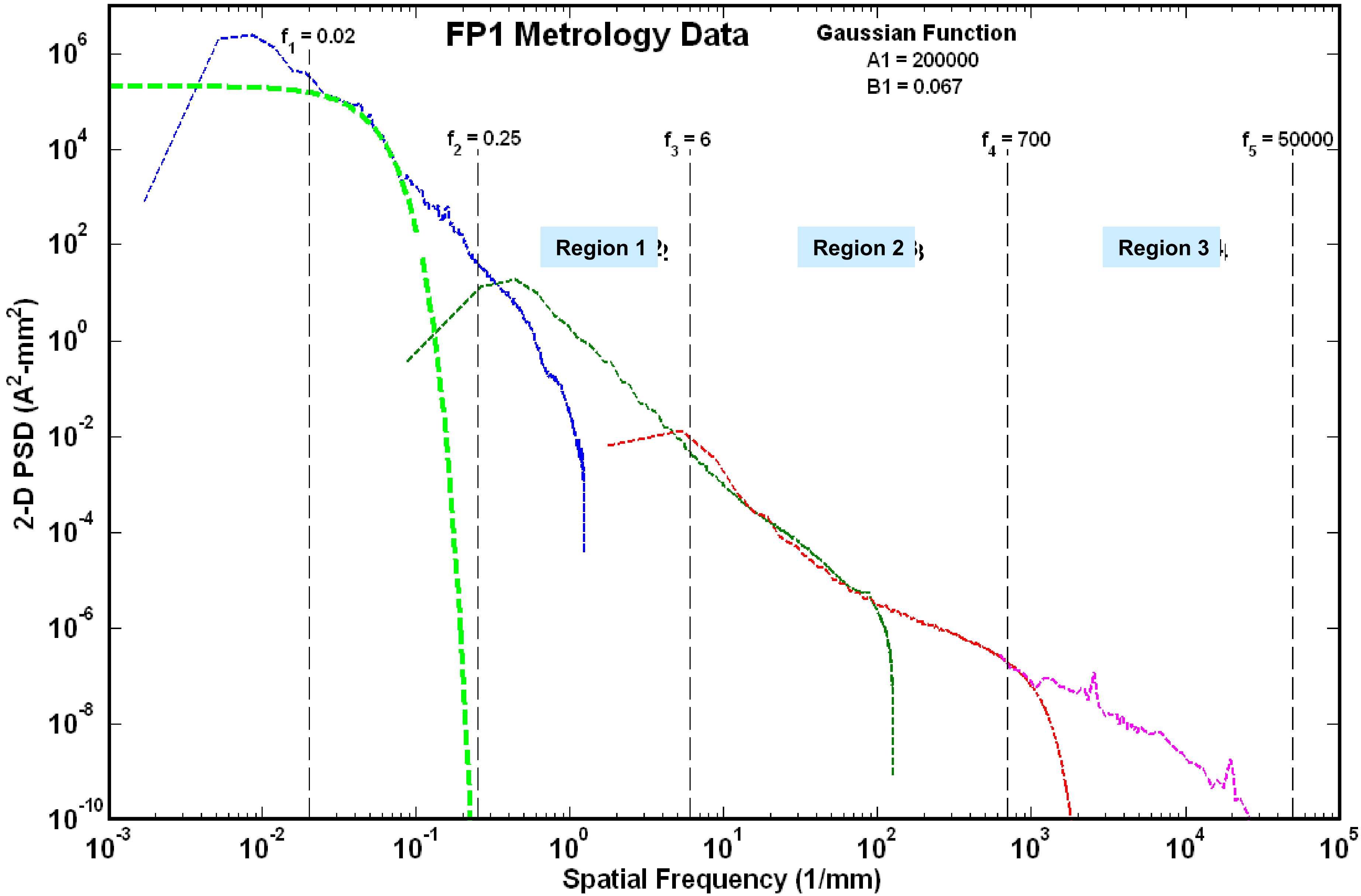
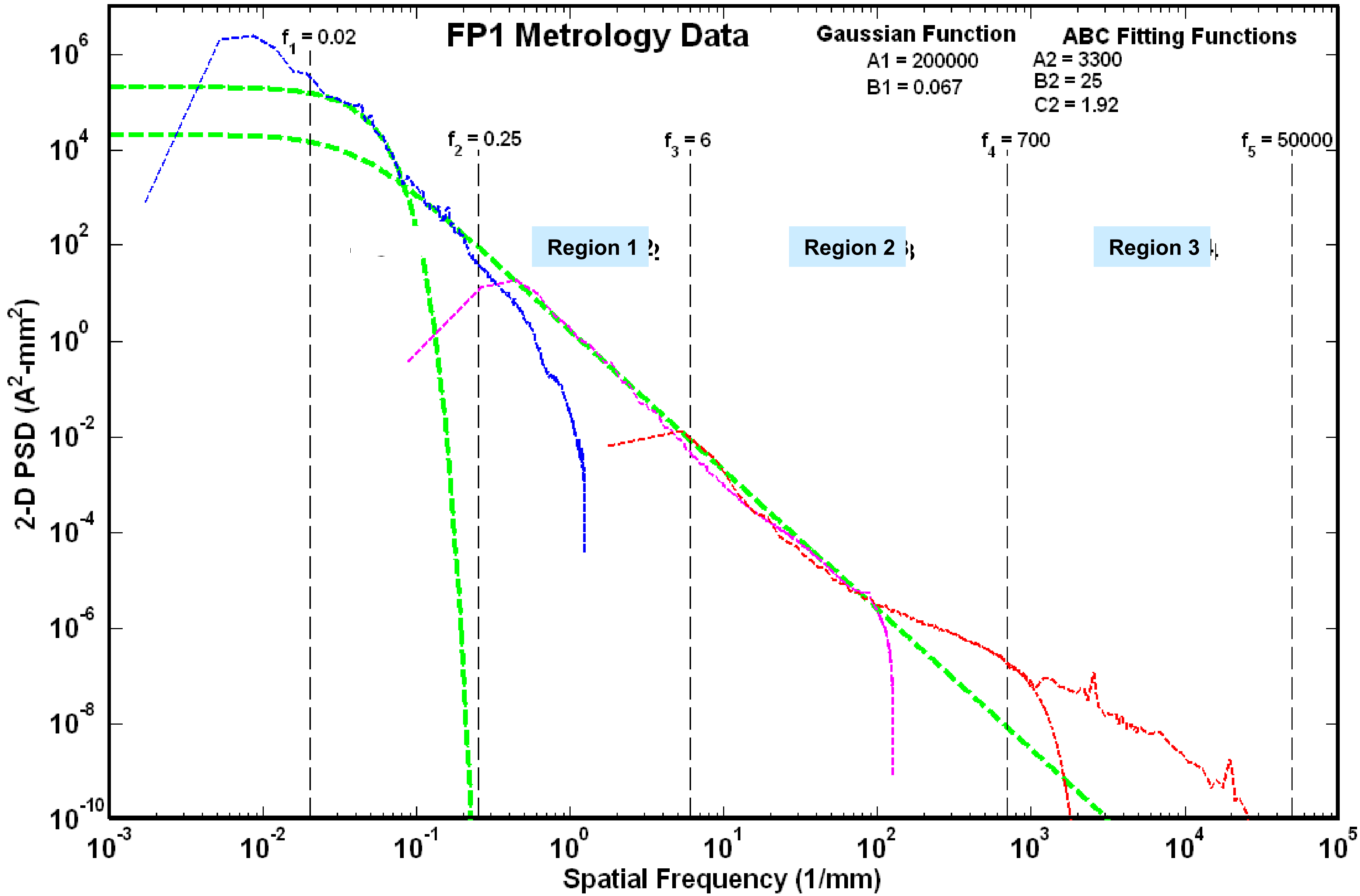
SUVI FP1 Metrology Data
(SUVI Primary Mirror)



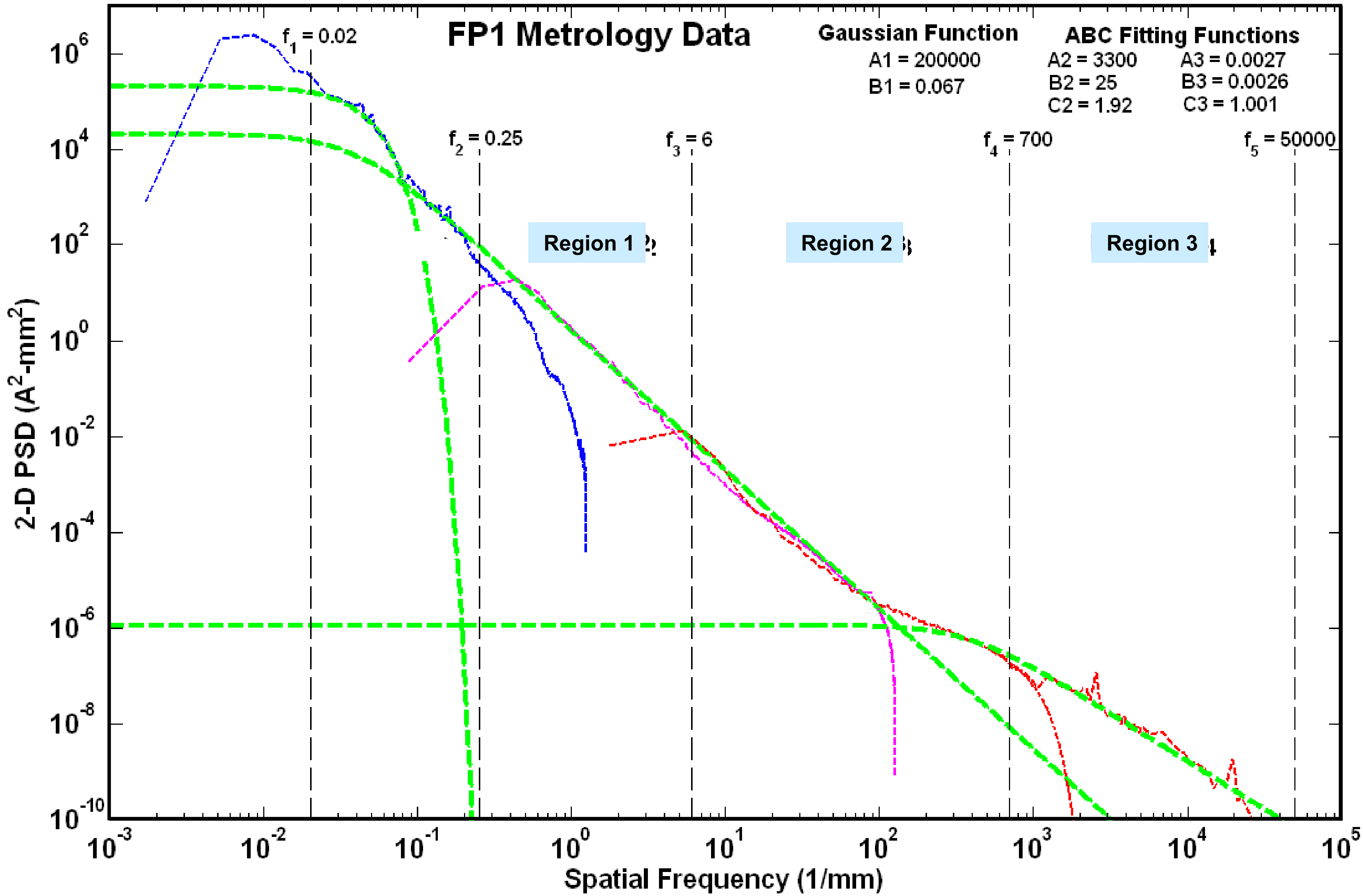
1st Fitting Function to FP1 Metrology Data



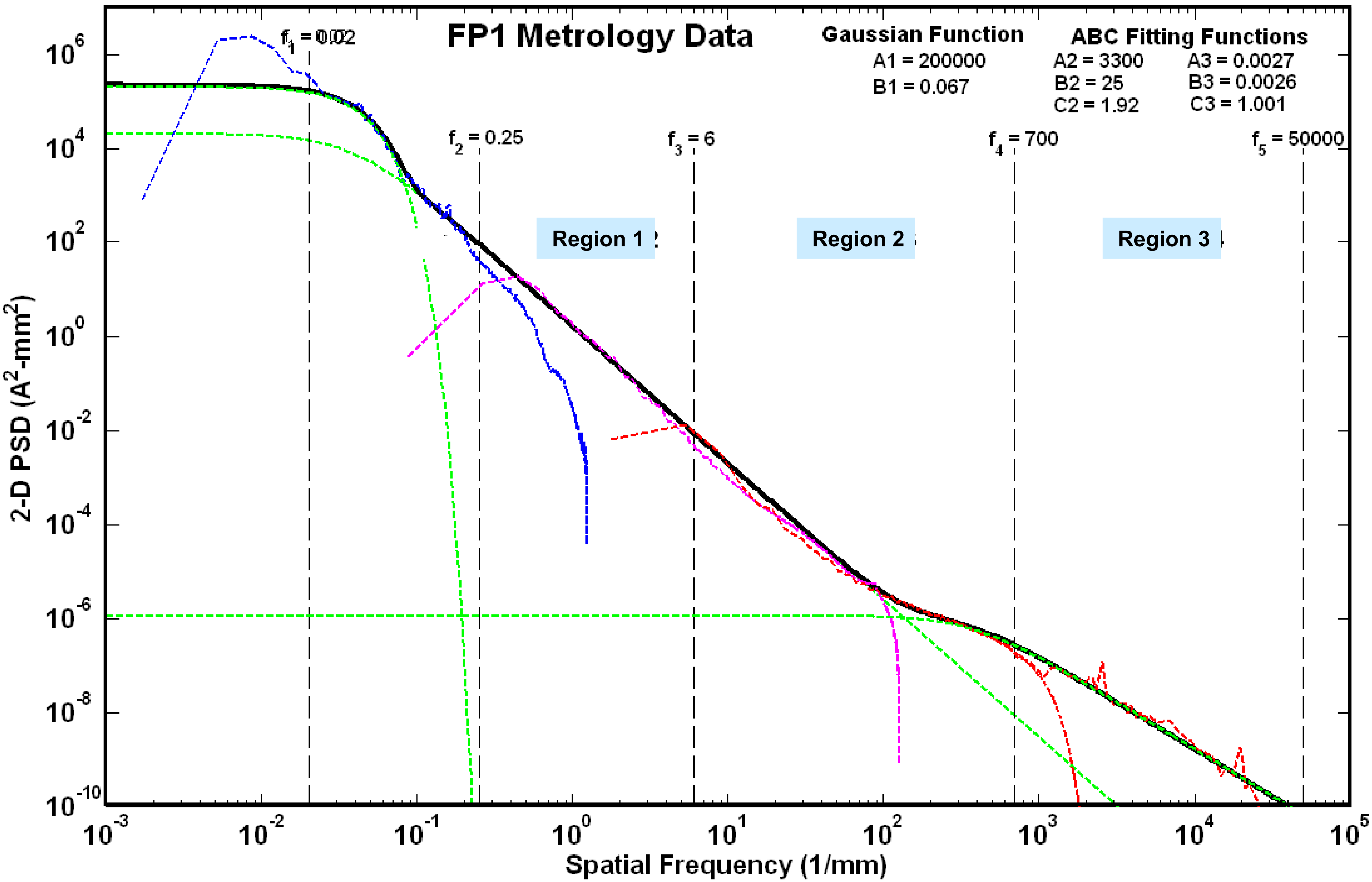
2nd Fitting Function to FP1 Metrology Data



3rd Fitting Function to FP1 Metrology Data



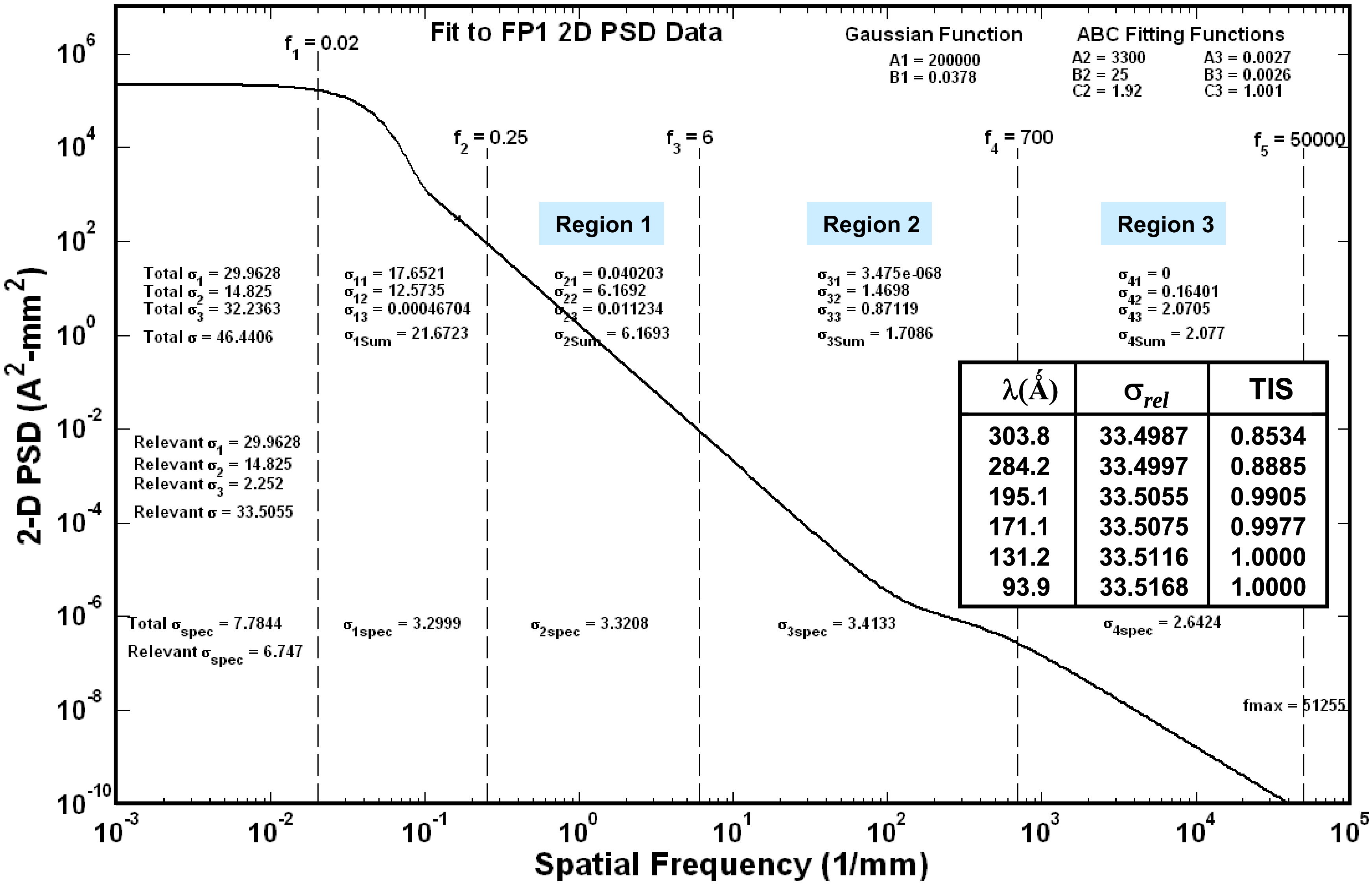
Sum of three Fitting Functions



FP1 2-D PSD Metrology Data

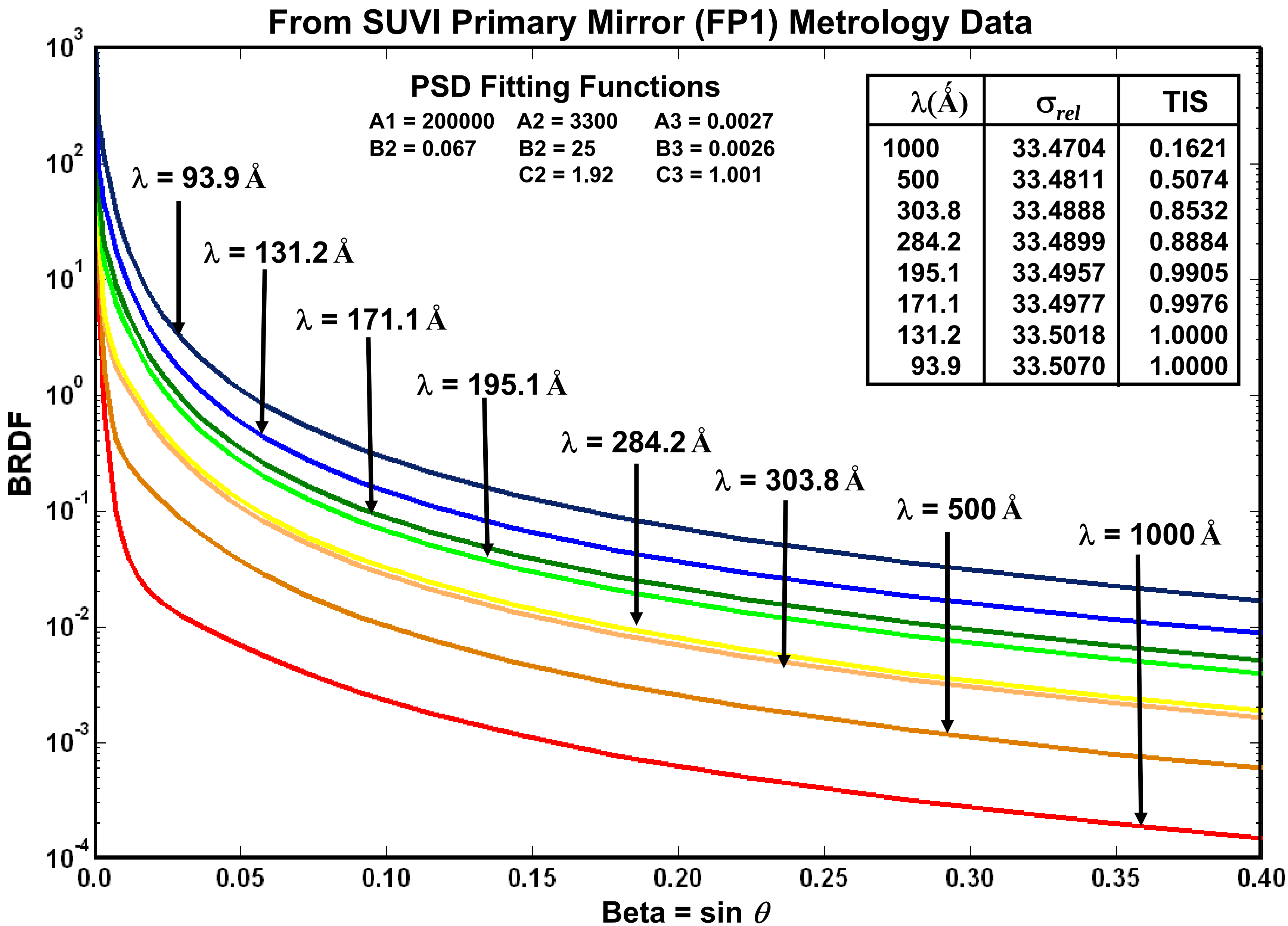
(With Band-limited Roughness Values)

One Gaussian + Two ABC Functions



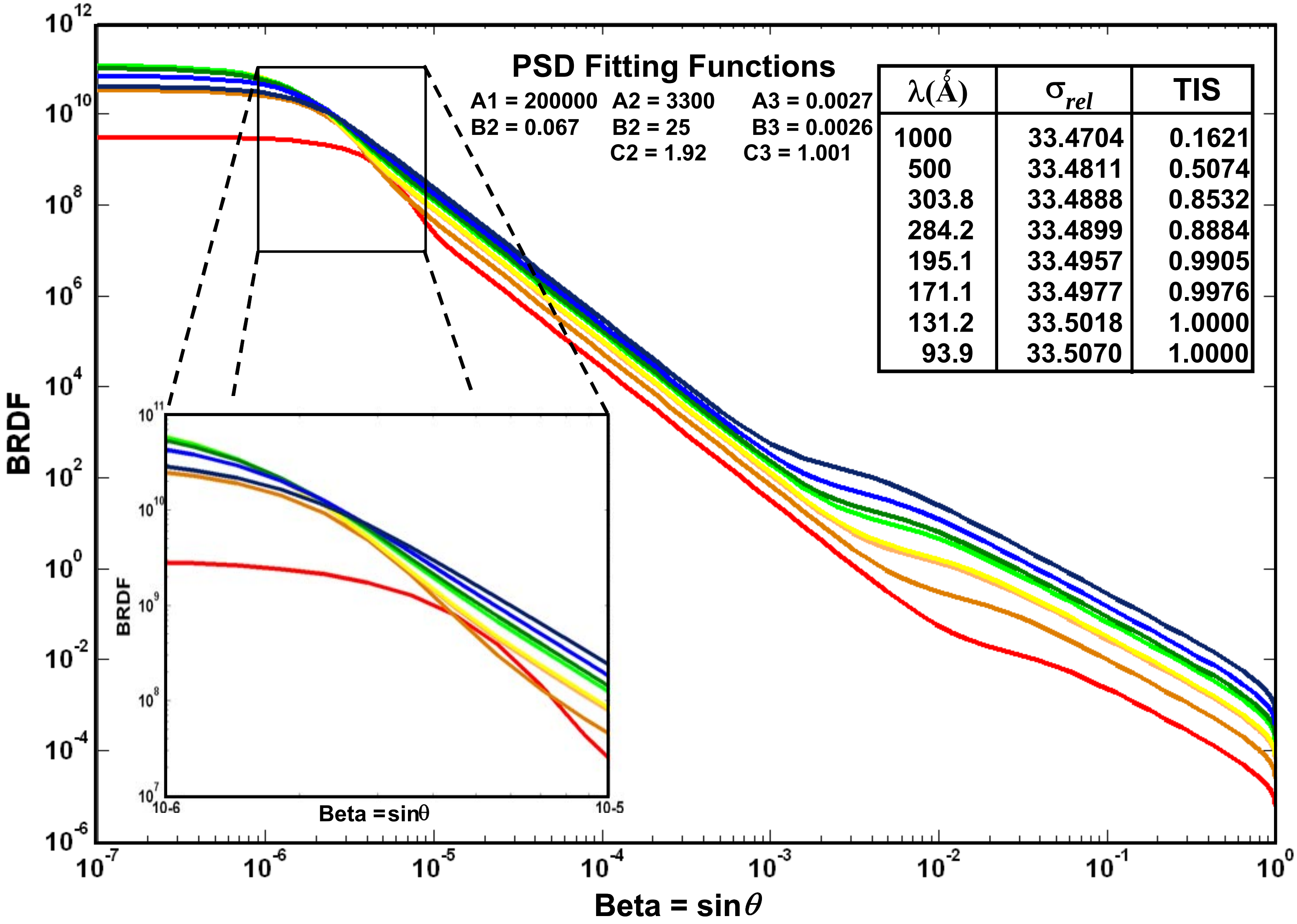
λ(Å)	σ_{rel}	TIS
303.8	33.4987	0.8534
284.2	33.4997	0.8885
195.1	33.5055	0.9905
171.1	33.5075	0.9977
131.2	33.5116	1.0000
93.9	33.5168	1.0000

BRDF Predictions from FP1 Metrology Data



λ(Å)	σ_{rel}	TIS
1000	33.4704	0.1621
500	33.4811	0.5074
303.8	33.4888	0.8532
284.2	33.4899	0.8884
195.1	33.4957	0.9905
171.1	33.4977	0.9976
131.2	33.5018	1.0000
93.9	33.5070	1.0000

BRDF Predictions from FP1 Metrology Data



Outline

- Historical Review of Surface Scatter Theory.
- Statement of the EUV Imaging Problem (Summary of Results).
- Non-paraxial Scalar Diffraction Theory.
  - o Scalar Treatment of Sinusoidal Phase Grating,
  - o Modified Beckmann-Kirchhoff Surface Scatter Model.
- Total Integrated Scatter (TIS) for Moderately Rough Surfaces.
- Generalized Harvey-Shack (GHS) Scatter Theory.
  - o Two-parameter Family of Surface Transfer Functions.
  - o Very Computationally Intense Calculations.
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  - o Solution: FFTLog Numerical Hankel Transform Algorithm.
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Analytic Expression for In-field Scattered Irradiance in Imaging Systems*

Although optical systems are complex, the distribution of scattered light from their elements is not. The halo of scattered light that surrounds a bright source image is merely the sum of the contributions from each element. Furthermore, the scattered-light irradiance distribution from any one element has the form of that element's BSDF, and its magnitude and scale depend only upon the size of the beam that passes through that element.

Most in-field scattered light distributions are obtained by very computationally-intensive calculations; i.e, by tracing millions of rays on a computer. However, the analytic formulas presented in Reference 1 makes all of this unnecessary. In addition, the analytic formulas provide insight and understanding that is totally absent from the conventional brute-force ray-tracing approaches. Design trades can now be performed, and limits on system performance assessed, without the need for complex computer calculations.

Gary Peterson, "Analytic Expressions for In-field Scattered Light Distribution", Proc SPIE 5178-01, 184-193 (2004).
Gary Peterson, *Analytic Expressions for In-field Stray Light Irradiance in Imaging Systems*, Master's Report, OSC/UA (2003).

Analytic Expression for In-field Scattered Irradiance in Imaging Systems*

Making use of the Lagrange invariant of 1st-order imaging systems and the brightness theorem (conservation of radiance), the scattered irradiance in the focal plane of an imaging system from the j^{th} element for an in-field point source was derived by Peterson

$$E_{sj}(r) = E_{ent}\pi(na)^2 T \frac{s_{ent}^2}{s_j^2} BRDF\left((na)\frac{r}{s_j}\right) \qquad \textbf{(23)}$$

where r is the distance from the point source image on the detector, na is the numerical aperture of the system, T is the system transmittance, s_{ent} is the radius of the entrance pupil, s_j is the radius of the beam on the j^{th} element, and E_{ent} is the irradiance in the entrance pupil of the system. ***This formulation is based upon both a smooth-surface and a paraxial assumption.*** **For a two-mirror telescope, we can thus write**

$$E_s(r) = E_{ent}\pi\,(na)^2\,T\,s_{ent}^2\left[\frac{BRDF_P\left((na)\,r/s_p\right)}{s_p^2} + \frac{BRDF_s\left((na)\,r/s_s\right)}{s_s^2}\right] \qquad \textbf{(24)}$$

Since $s_{ent} = s_p$, $na = \dfrac{1}{2F^{\#}} = \dfrac{s_p}{f'}$, **and** $P_T = E_{ent}\pi\, s_p{}^2\, T \quad \left(f' = \text{system focal length}\right)$

$$\frac{E_s(r)}{P_T} = \left(\frac{1}{f'}\right)^2\left[BRDF_P\left(r/f'\right) + \left(\frac{s_p}{s_s}\right)^2 BRDF_s\left((s_p/s_s)(r/f')\right)\right] \qquad \textbf{(25)}$$

* **G. Peterson, "Analytic expressions for in-field scattered light distributions", Proc SPIE 5178 (2004).**

Generalized Peterson Analytical Scattering Model

Since Peterson's elegant and insightful treatment is limited by both a *paraxial* and a *smooth-surface* assumption, it must be generalized to include scattering from moderately rough surfaces before applying to the NOAA Solar UV Imager (SUVI) Program. We have thus:

- **Removed the "smooth-surface" limitation by including "scattered-scattered" radiation from the two-mirror SUVI telescope.**

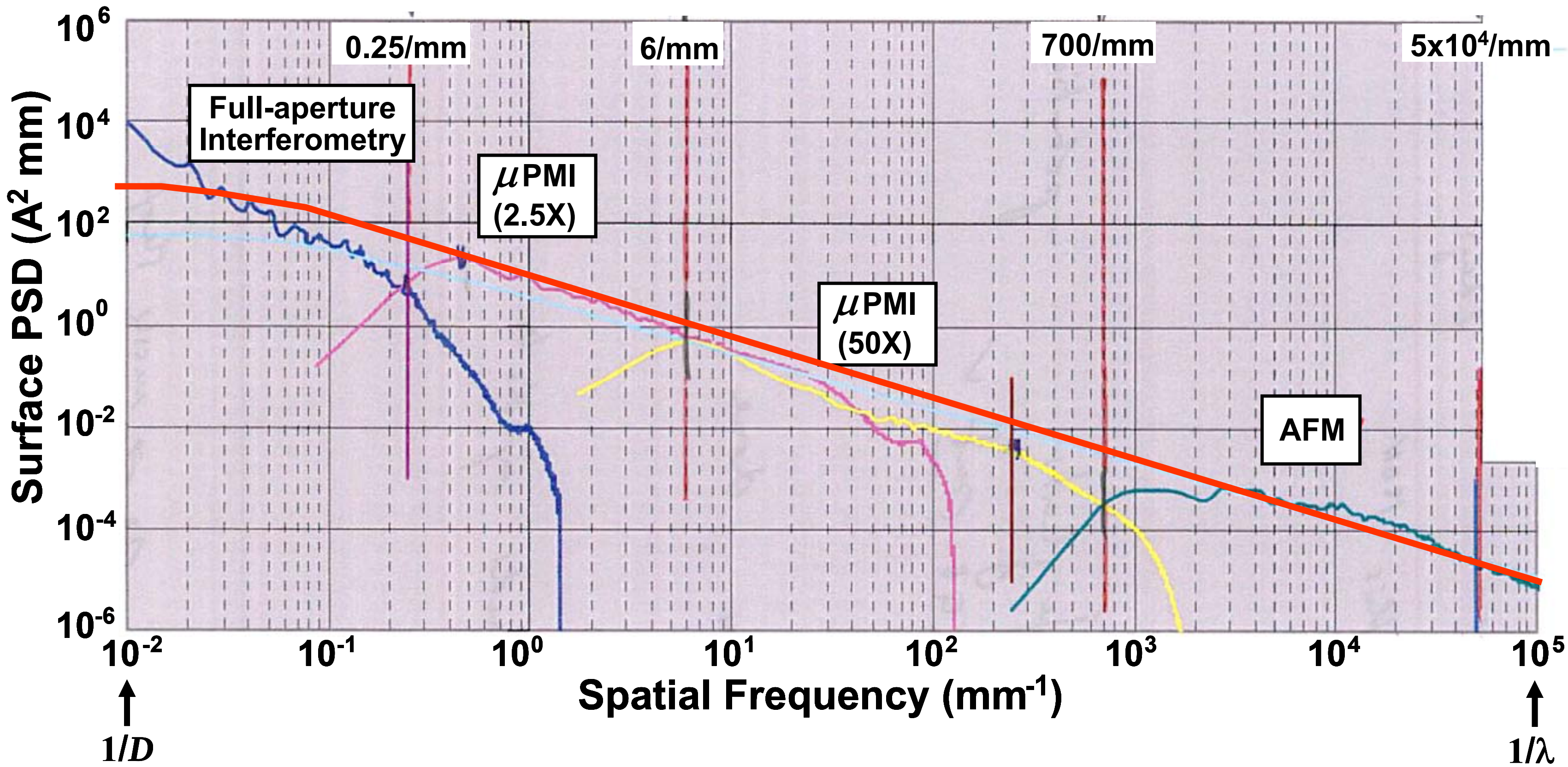
- **Verified that the SUVI application is indeed paraxial.**

- **The simple analytical model has then been numerically validated by comparing the results with the very computationally-intensive commercially-available ZEMAX and ASAP codes.**

Gary Peterson, "Analytic Expressions for In-field Scattered Light Distribution", Proc SPIE 5178-01, 184-193 (2004).
Gary Peterson, *Analytic Expressions for In-field Stray Light Irradiance in Imaging Systems*, Master's Report, OSC/UA (2003).

The SUVI Spec Surface PSD

(Scattered-Scattered Light will be Very Substantial)



PSD Fitting Function

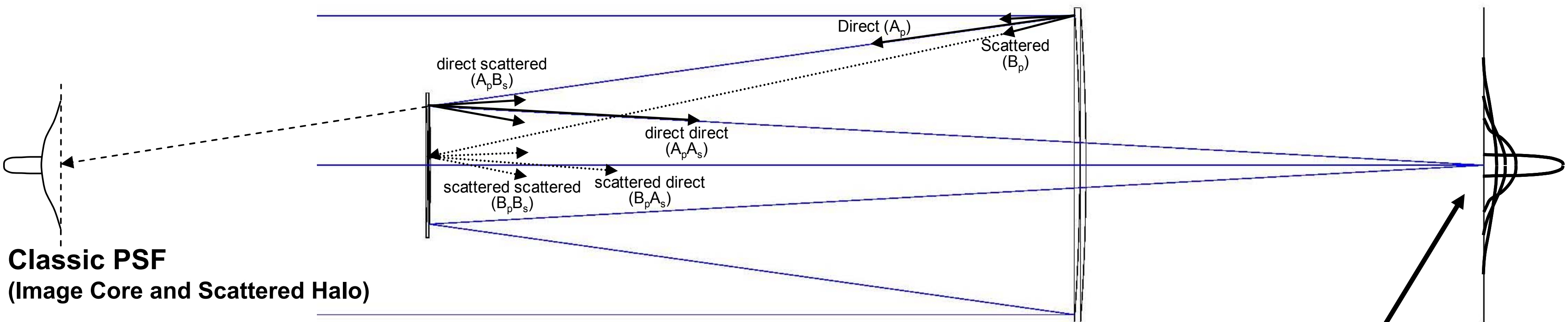
$$PSD(f_x)_{1-D} = \frac{A}{\left[1 + (B\, f_x)^2\right]^{C/2}}$$

A1 = 610.322 Å^2*mm*
B1 = 120 *mm*$^{-1}$
C1 = 1.089

λ(Å)	σ_{rel}	TIS
1000	6.5698	0.0068
500	6.6487	0.0275
303.8	6.7020	0.0740
284.2	6.7089	0.0842
195.1	6.7470	0.1721
171.1	6.7600	0.2185
131.2	6.7857	0.3445
93.9	6.8171	0.5650

Scattering in a Two-mirror EUV Telescope

For a solar EUV telescope surface scatter from the primary and secondary mirrors sometimes dominates both geometrical aberrations and diffraction effects in the degradation of image quality.



$$A = \exp\left[-(4\pi\sigma_{rel}/\lambda)^2\right] = \text{Fraction of total reflected energy in specular beam.}$$
$$B = TIS = 1 - A = \text{Fraction of total reflected energy in scattered halo.} \quad (26)$$

The SUVI point spread function (PSF) consists of four components with an energy distribution given by:

Direct-direct component (Specular) — A_p A_s

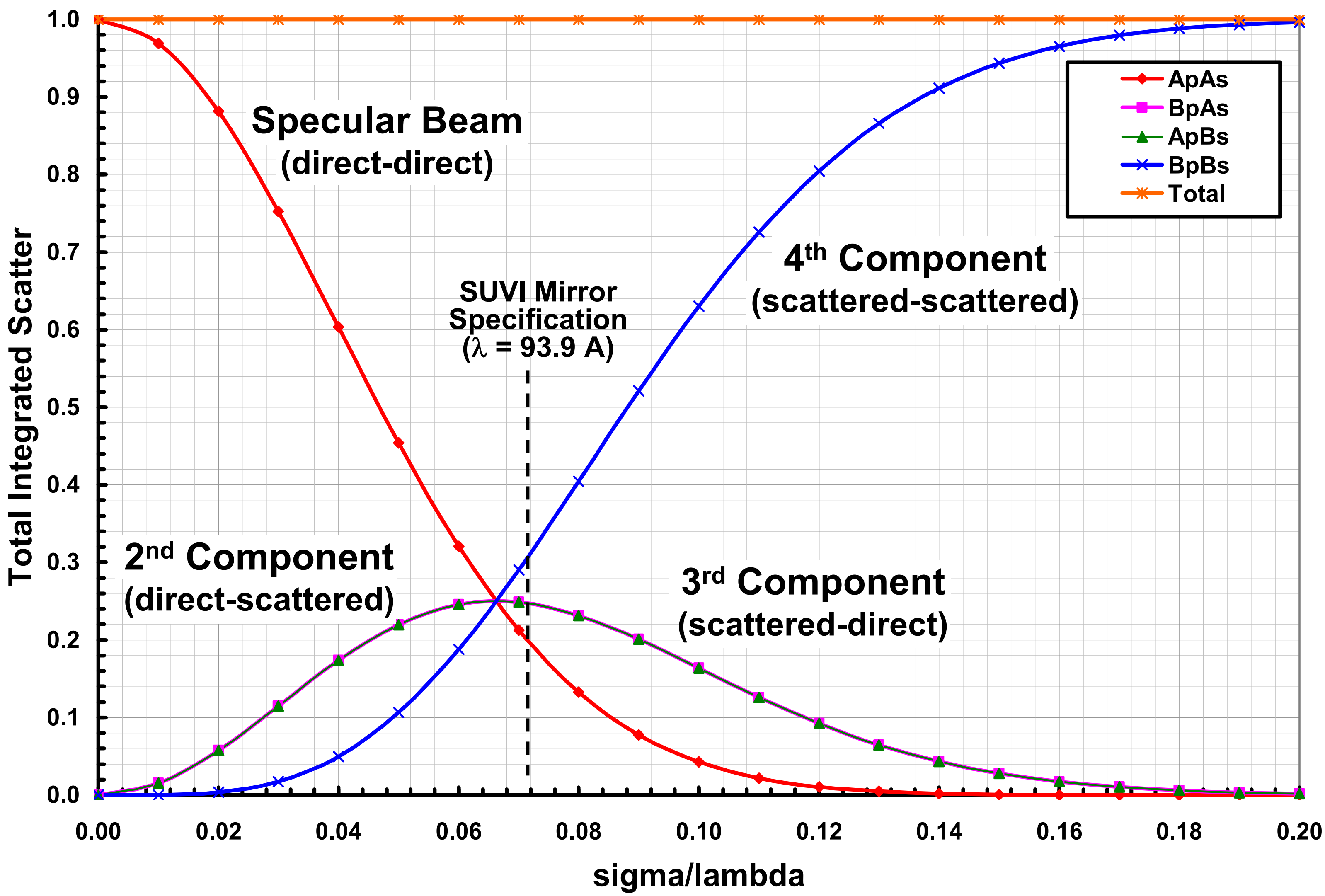
Scattered-direct component — B_p A_s

Direct-scattered component — A_p B_s

Scattered-scattered component — B_p B_s

Energy Distribution between PSF Components

The radiant energy distribution between the four components of the PSF is shown below as a function of σ/λ. The σ is the relevant rms roughness (PSD integrated from $f_{min} < f < 1/\lambda$) . Note that for σ/λ > 0.066, the broad scattered-scattered component becomes dominant.



Including the Scattered-Scattered Light

Since most EUV applications clearly do not satisfy the smooth surface assumption, but are perceived to satisfy the paraxial limitation, we merely construct an expression for each of the four components making up the PSF in the focal plane of the telescope, and substitute it into Eq.(25) of Peterson's analytic treatment

$$PSF = PSF_{dd} + PSF_{sd} + PSF_{ds} + PSF_{ss} \tag{27}$$

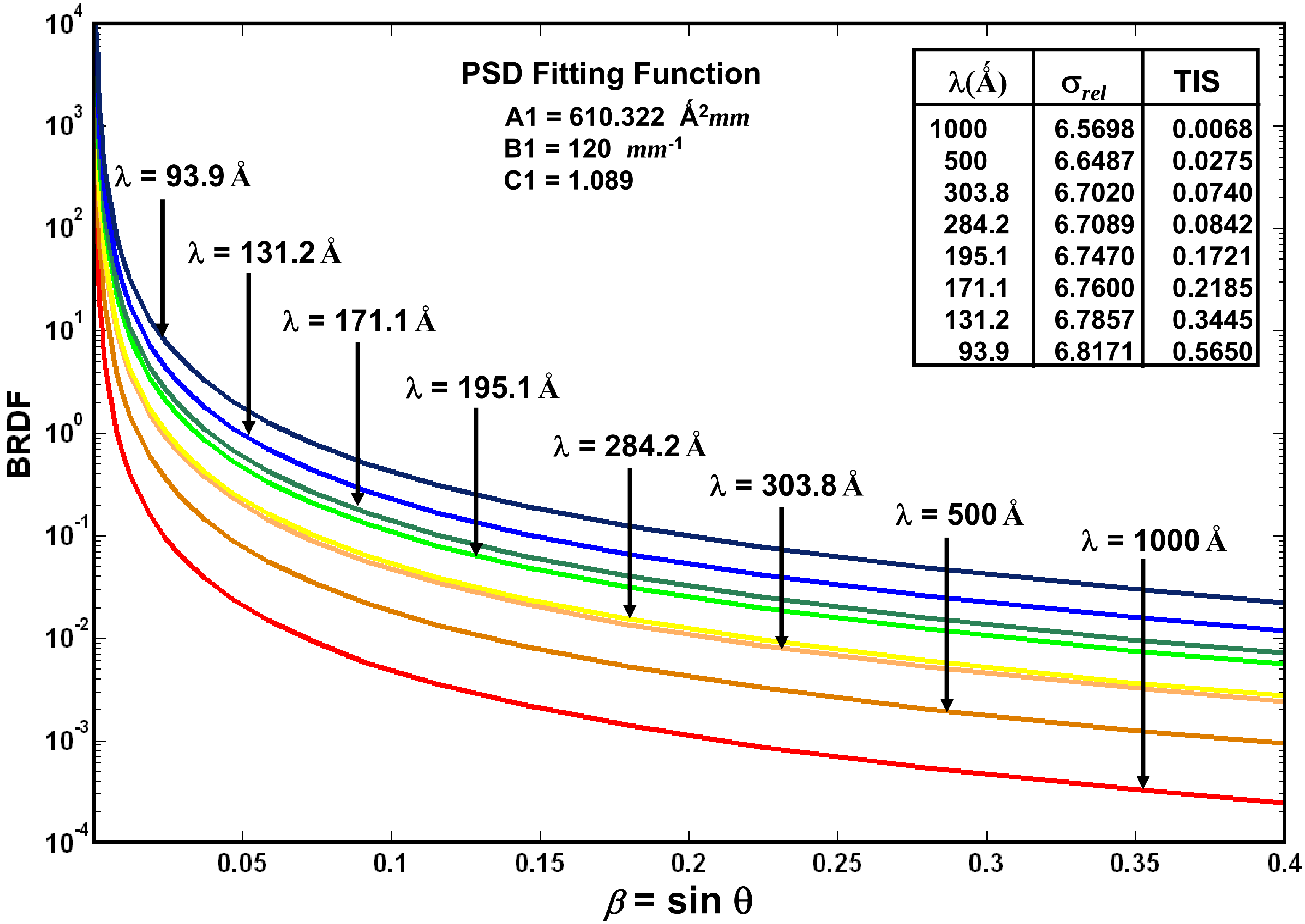
Care is taken to normalize each component such that their respective volumes (fractional total reflected radiant power) will be given by A_pA_s, B_pA_s, A_pB_s, and B_pB_s.

We will assume a 175 cm focal length Ritchey-Chretien telescope design with an aperture diameter of 19 cm and an obscuration ratio of $\varepsilon = 0.4$. There will thus be no geometrical aberrations on-axis; and the specular beam will be the well-known Fraunhofer diffraction pattern produced by the annular aperture of the telescope

$$PSF_{dd}(r) = \frac{1}{\left(1-\varepsilon^2\right)^2}\left[\frac{2J_1(x)}{(x)} - \varepsilon^2\,\frac{2J_1(\varepsilon x)}{\varepsilon x}\right]^2 \quad \text{where} \quad x = \frac{\pi r}{\lambda f/D}. \tag{28}$$

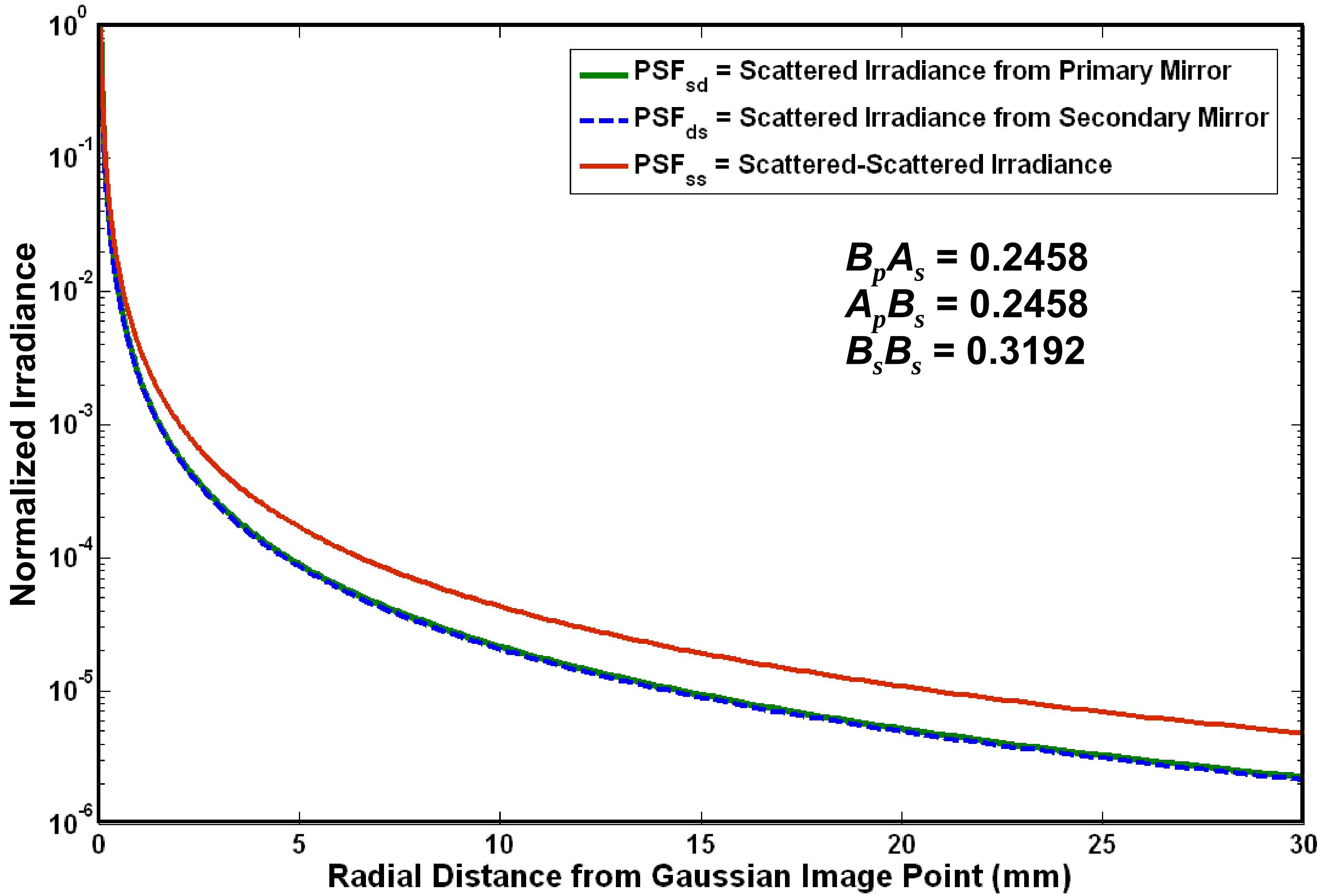
The above expression is normalized to a unit volume. It will thus need to be multiplied by the coefficient A_pA_s in the following analysis.

BRDF Profiles Calculated from SPEC PSD with the GHS Scattering Theory

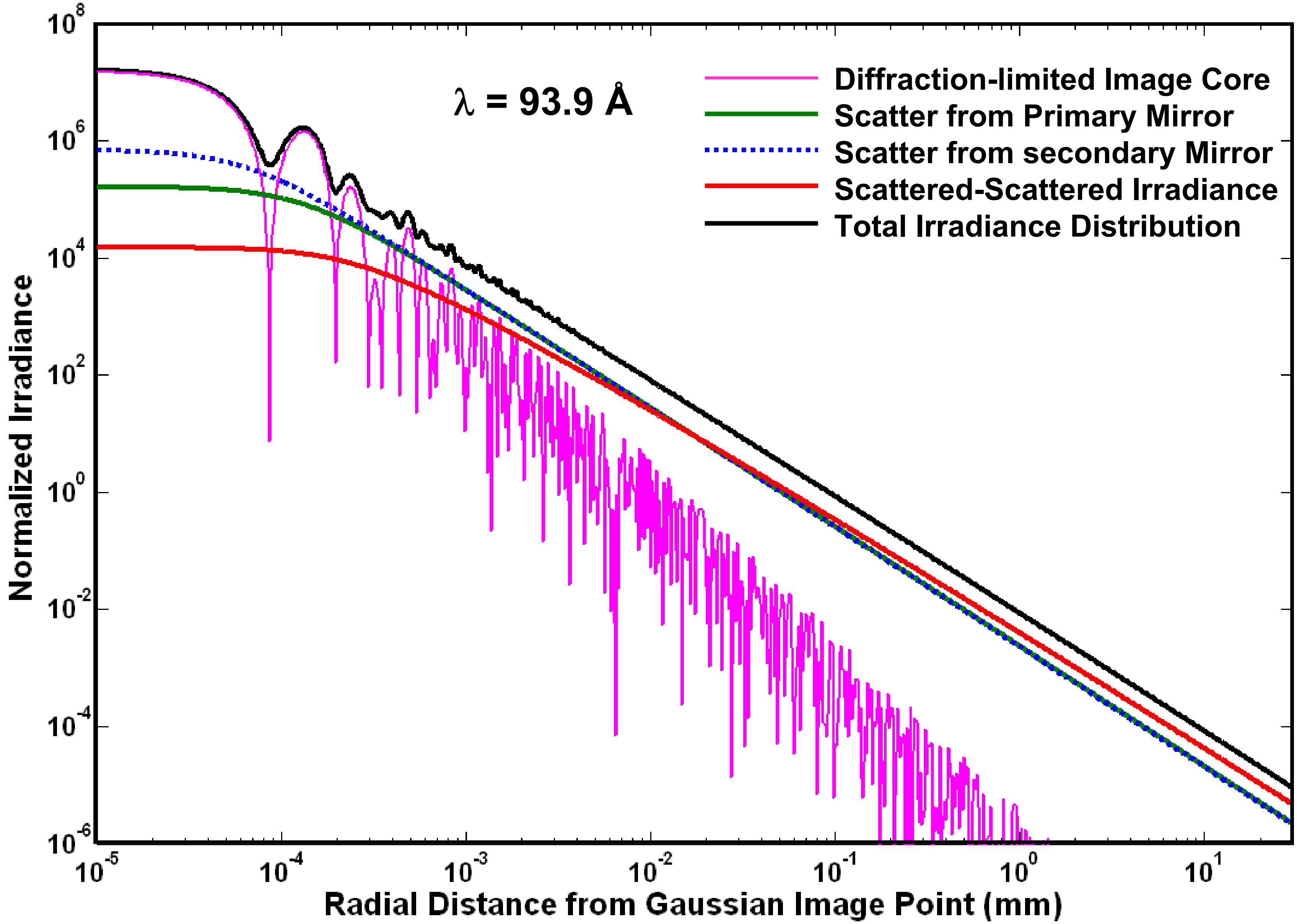


Scattered-Scattered Light Dominates

(λ = 93.9 A)

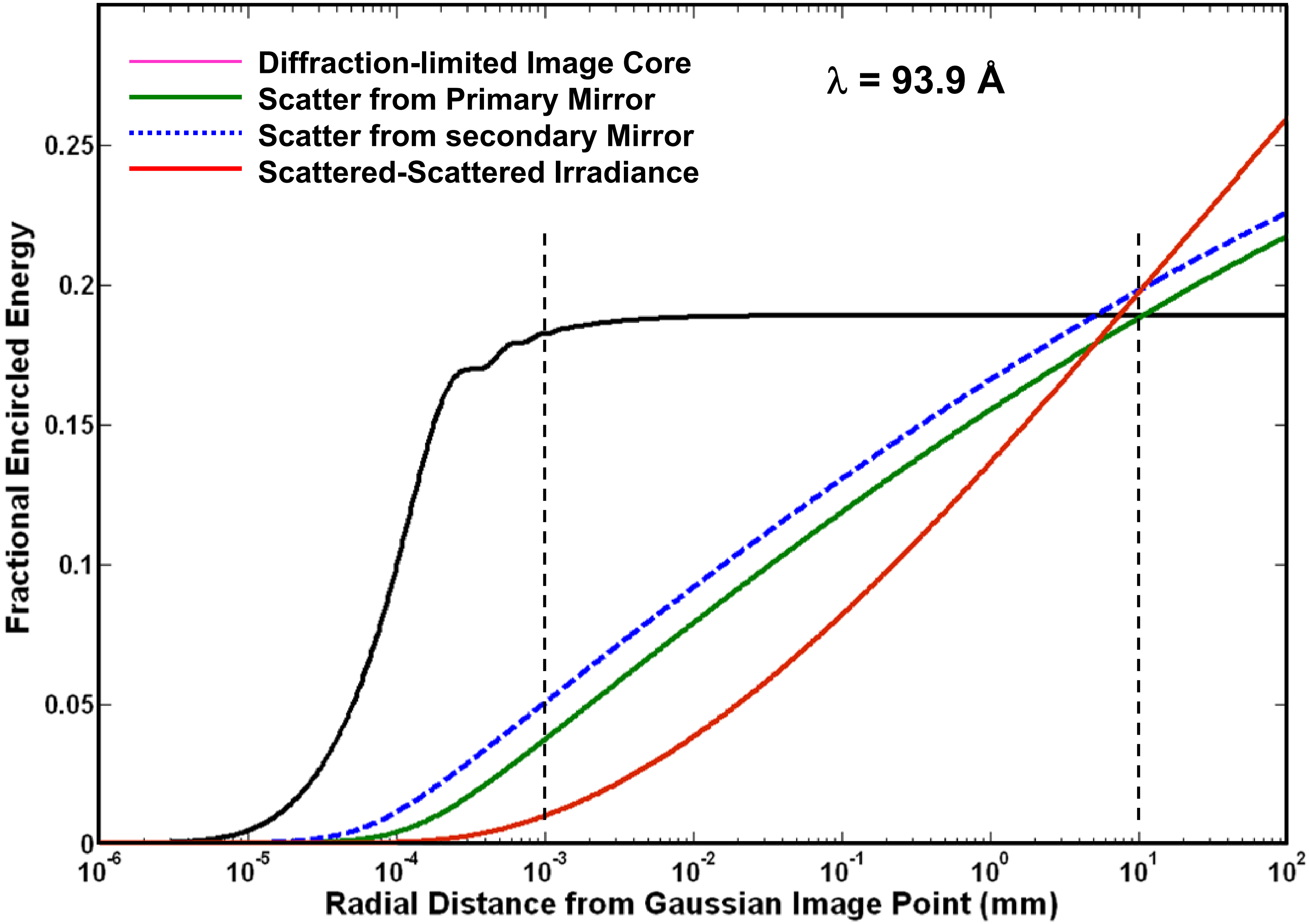


Radial Profiles of Four Components
(λ = 93 A)



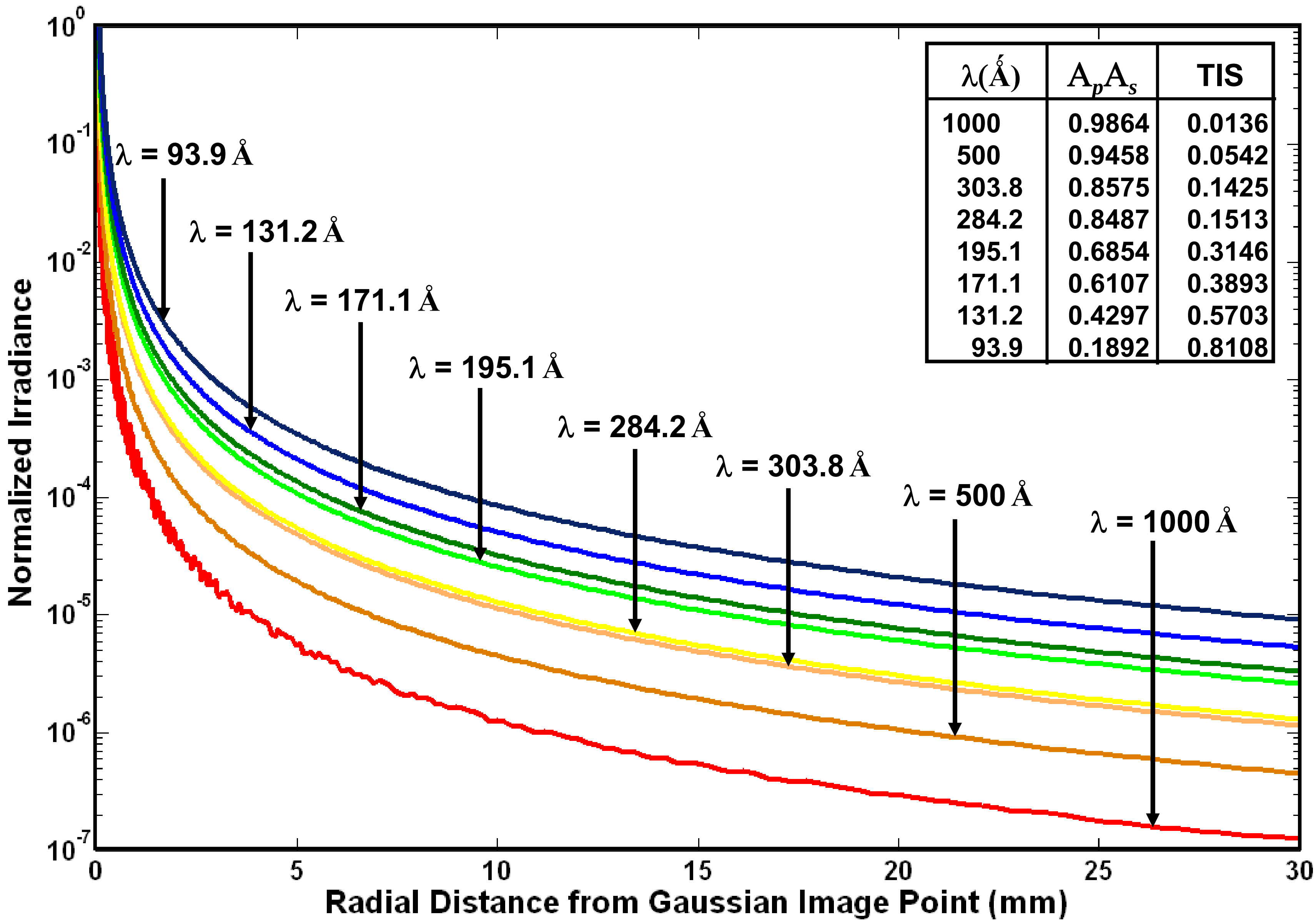
FEE Plots of the 4 Components of PSF

(λ = 93.9 A)

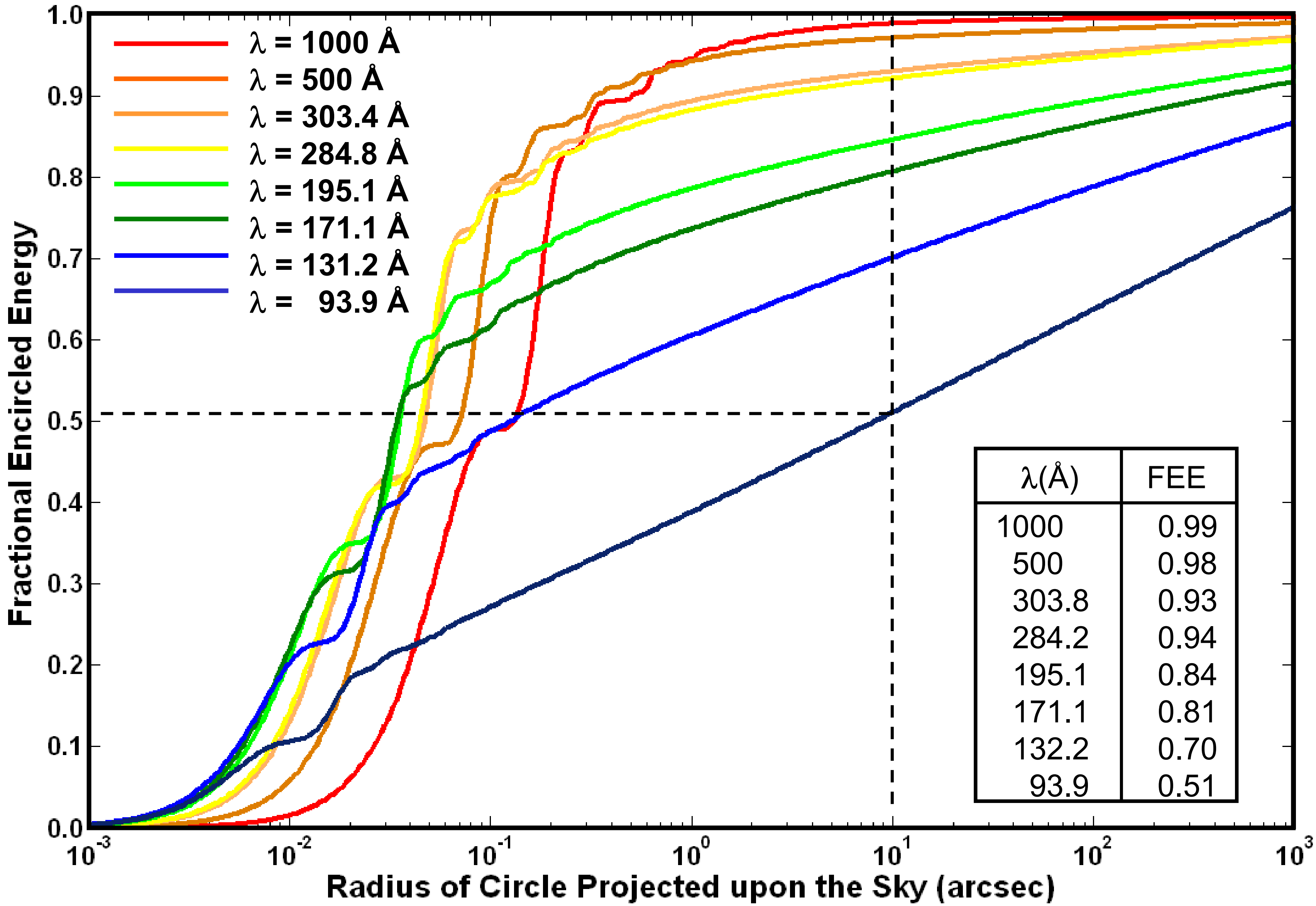


Irradiance Profile in Telescope Focal Plane

(Predicted by Generalized Peterson Model)



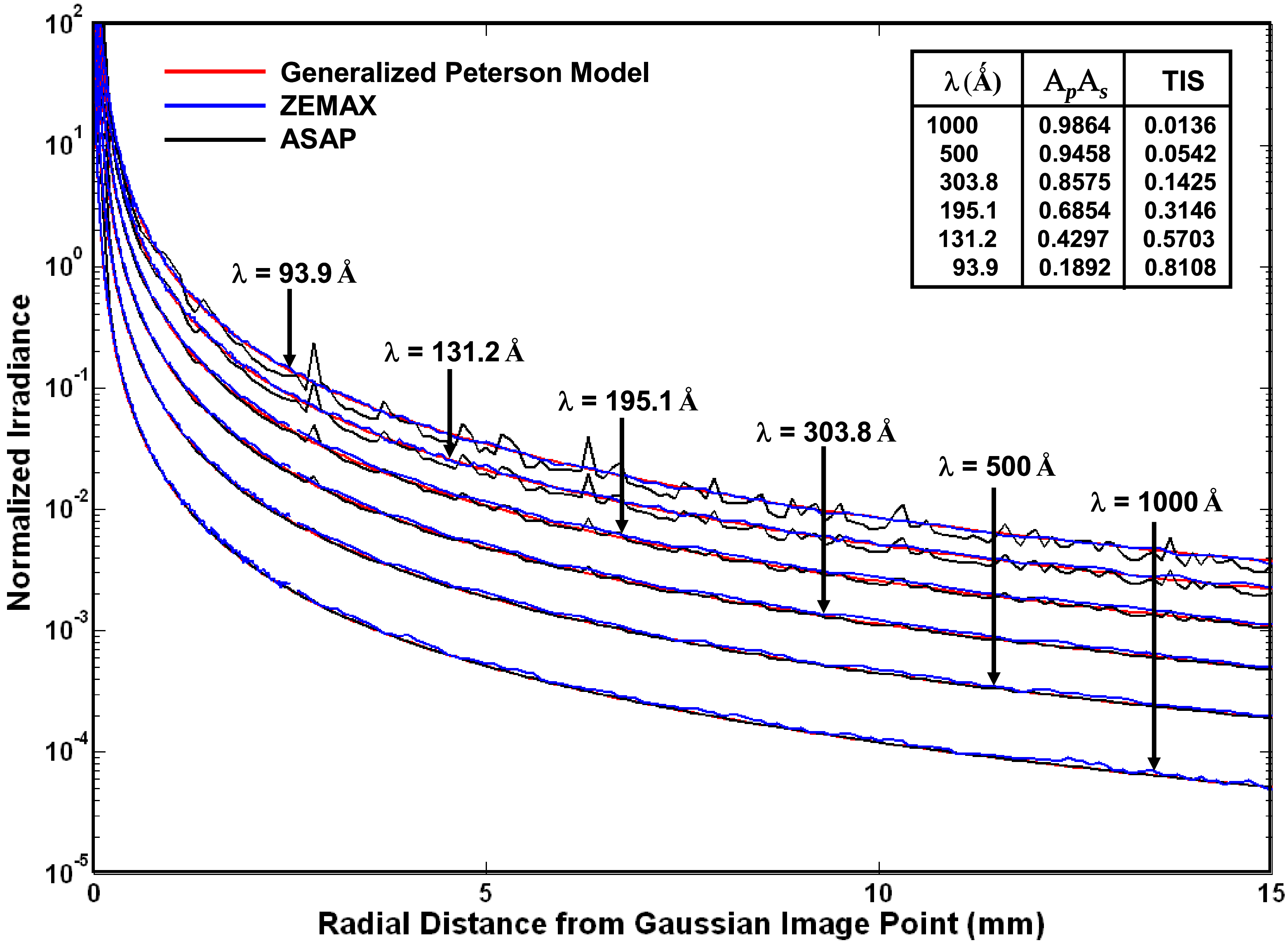
FEE Plots of the Total PSF Projected onto Sky



SUVI Image Quality Requirements
(Fractional Ensquared Energy: Expressed as %)

Square Size (arcsec)	Wavelength					
	93.9	131.2	171.1	195.1	284.2	303.8
7x7	43	50	50	50	50	50
10x10	49	53	59	60	60	60
20x20	57	61	65	65	65	65
40x40	67	69	70	70	70	70
65x65	72	75	75	75	75	75
150x150	78	82	84	85	85	85

Numerical Validation by ASAP and ZEMAX*



* J. E. Harvey, N. Choi, A. Krywonos, G. Peterson, and M. Bruner, “Image Degradation due to Scattering Effects in Two-mirror Telescopes”, Supmited for publication in Opt. Eng. (Mar 2010)

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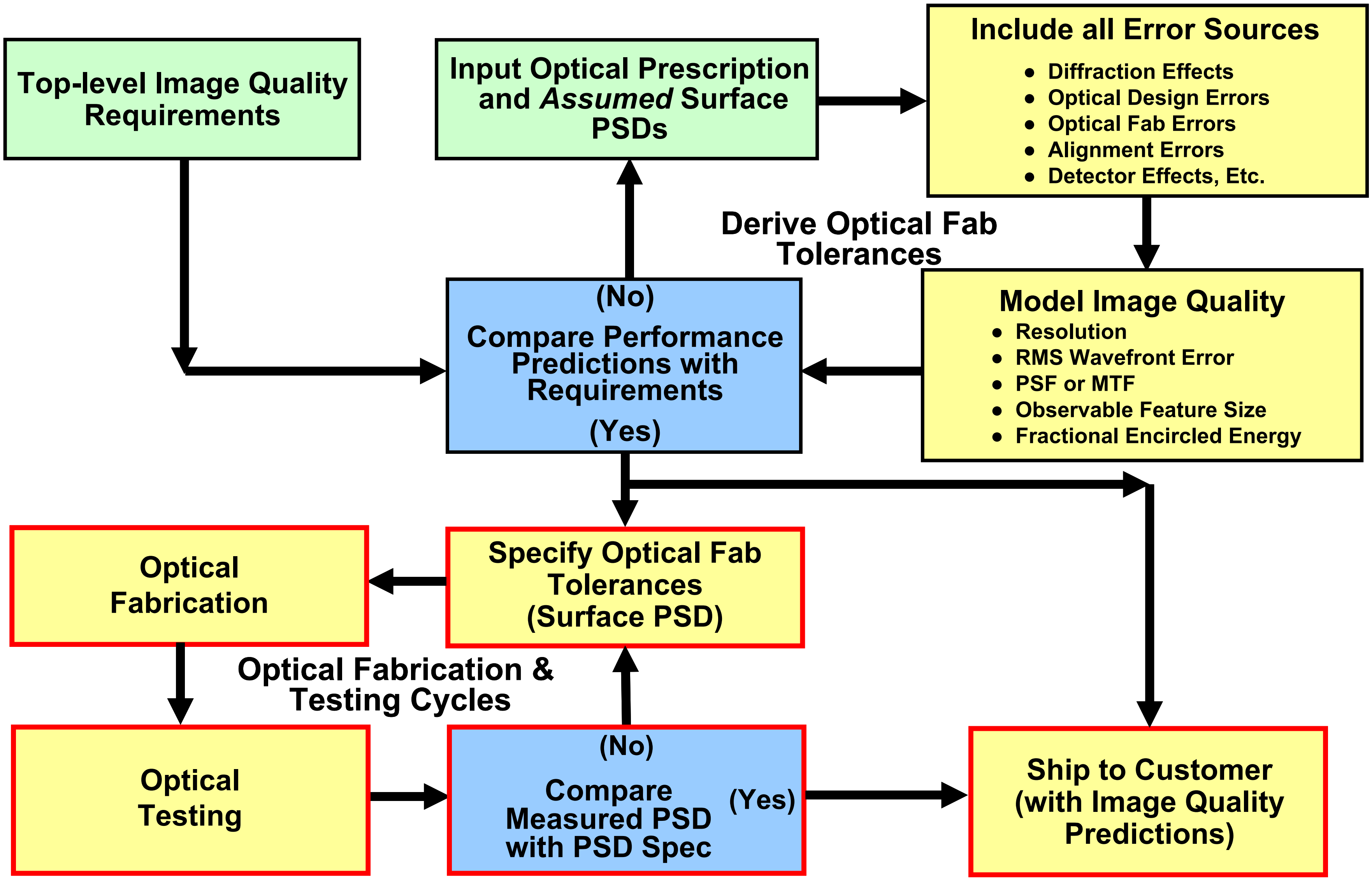
Flow Chart of the "Just-Good-Enough" Optical Fabrication Strategy*



* J. E. Harvey, J. Lentz, and J. B. Houston, Jr., "'Just-Good-Enough' Optical Fabrication", presented at the OSA Topical Meeting on Optical Fabrication and Testing, Rochester, NY (October 2008).

Summary, Results and Conclusions

- Stated a Need for Calculating Image Degradation from Measured Metrology Data.
- Reviewed a Generalized Surface Scatter (GHS) Theory valid for Rough Surfaces at Large Incident and Scattered Angles.
- Discussed Computational Problems for Surface PSDs with Large Dynamic Range in Spatial Frequency.
- Introduced the FFTLog Algorithm as a Solution to the computational Problem.
- Demonstrated BRDFs Calculated from Surface PSDs for increasingly short wavelengths (which violate the smooth-surface approximation).
- Generalized the Peterson Analytical Model for Calculating Image Degradation to include surface scatter from rough surfaces.
- Demonstrated a variety of useful parametric performance predictions provided by the Generalized Peterson Analytical Model.
- Numerically validated the Generalized the Peterson Analytical Model with both ASAP and ZEMAX.
- Showed Flow Chart of "*Just-Good-Enough*" Optical Fabrication Strategy.

The Inverse Scattering Problem

The smooth-surface criterion must be satisfied to perform the inverse scattering problem of predicting surface characteristics from BRDF measurements

$$PSD(f_x, f_y) = \frac{\lambda^4}{16\pi^2} \frac{BRDF}{\cos\theta_o \cos\theta_s \, Q}$$

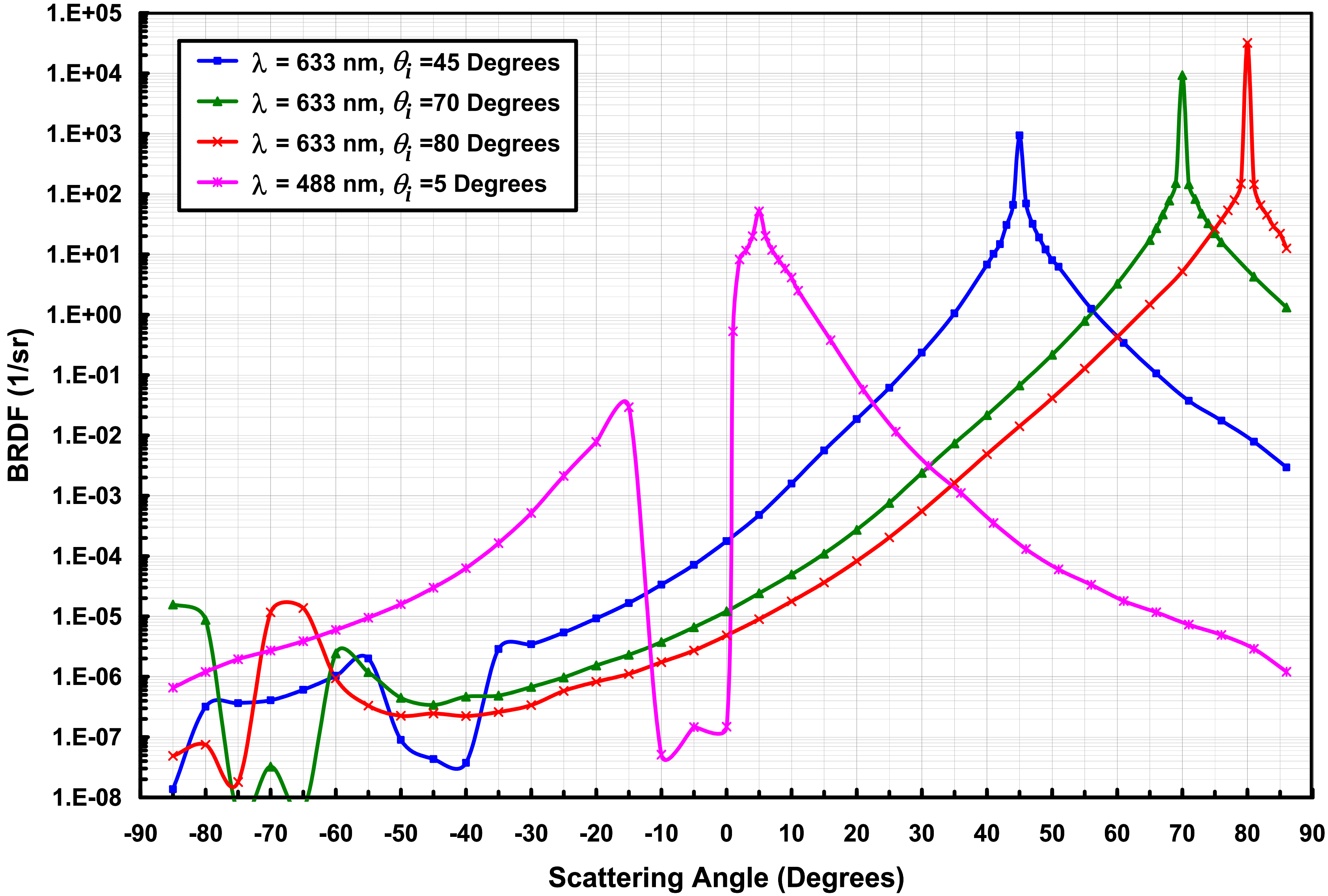
Rayleigh-Rice Inverse Scattering Solution

Recall that the smooth-surface criterion for the Rayleigh-Rice surface scatter theory is given by

$$4\pi\sigma_{rel} \cos\theta_i / \lambda \ll 1$$

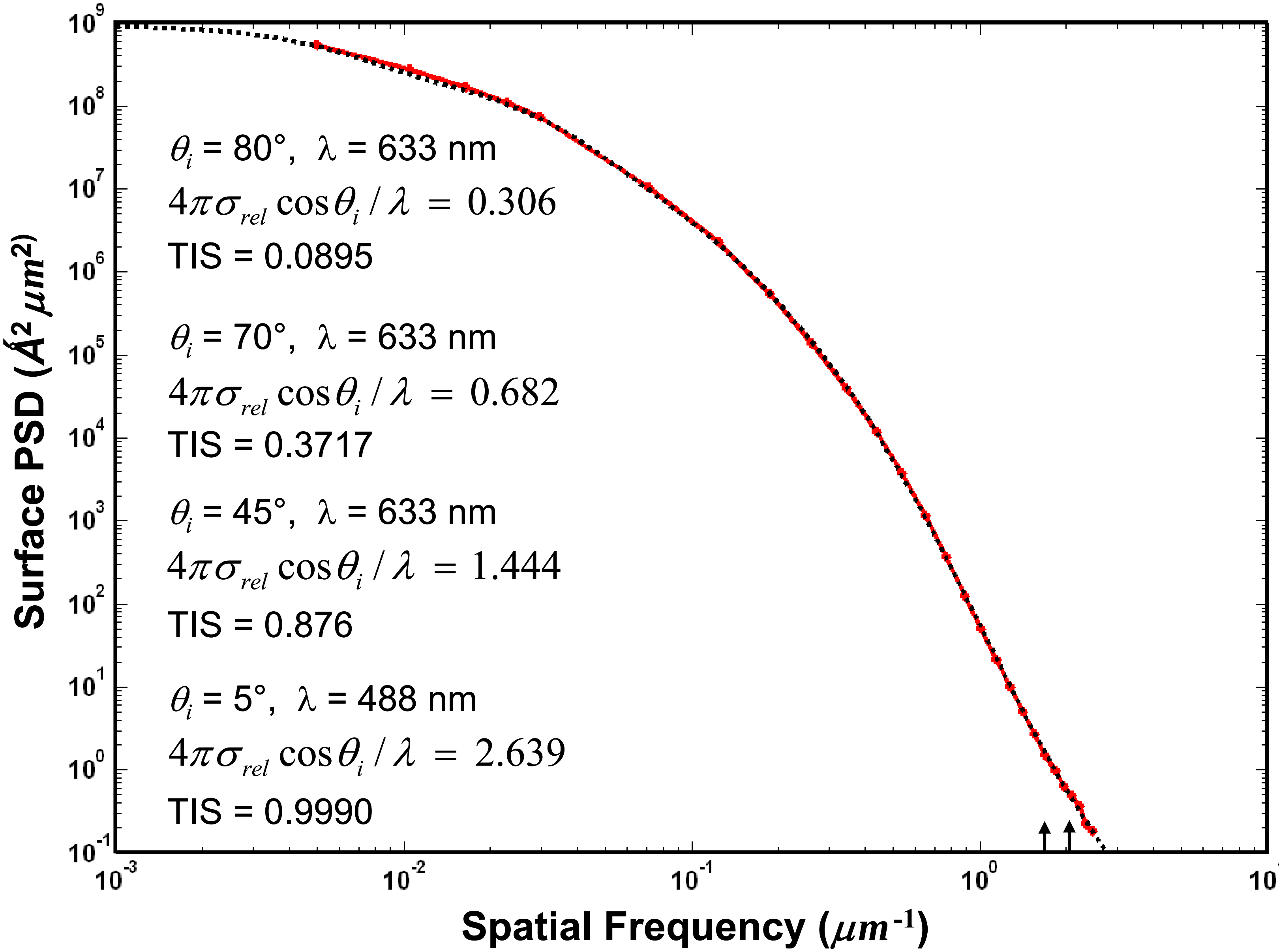
This suggests that a *large incident angle* can compensate for a *moderately rough surface.*

BRDF Data from a Moderately Rough Surface at Different Incident Angles and Wavelengths*

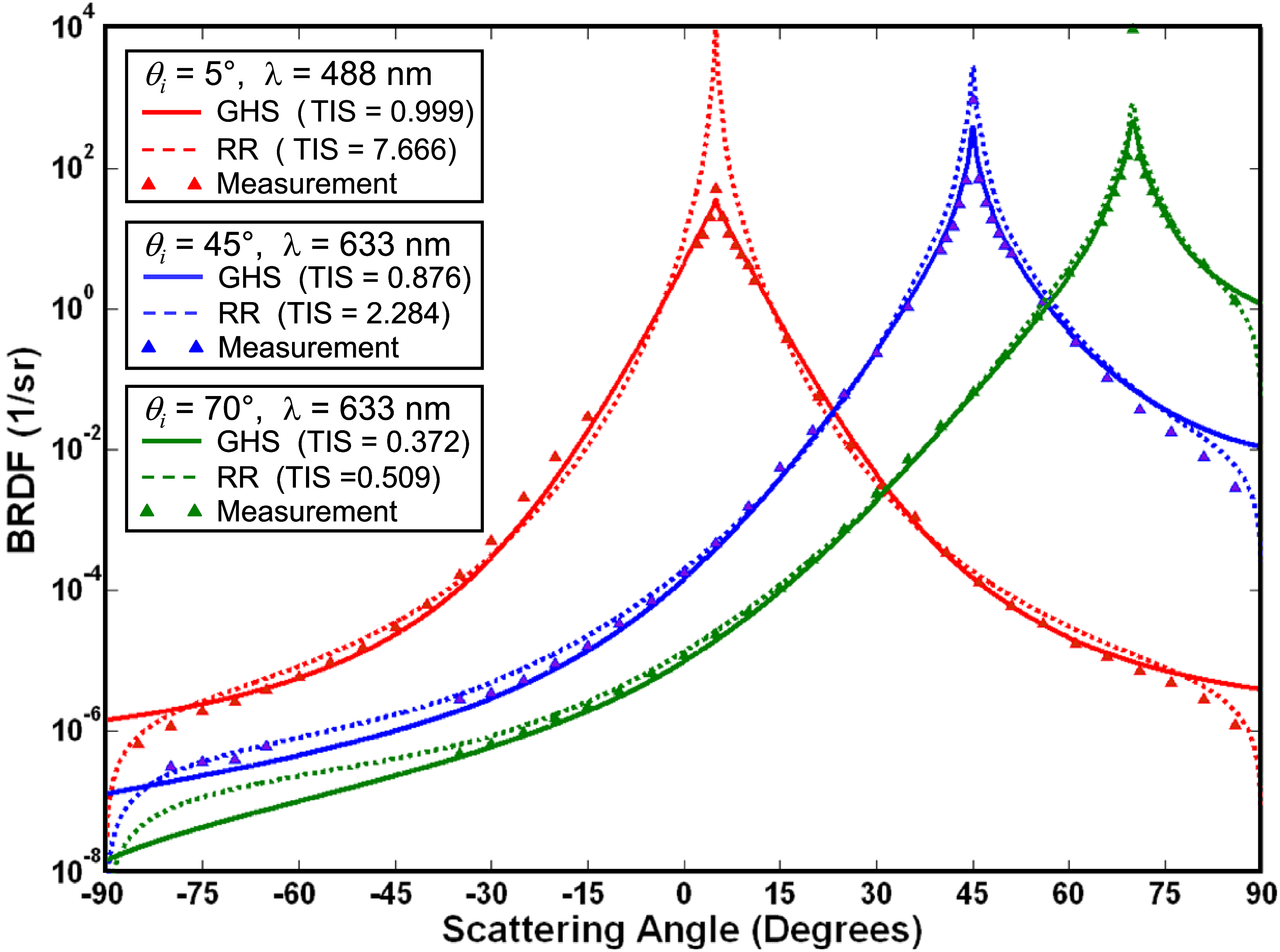


* **Measurements made from the back side of a silicon wafer by John Stover of *The Scatter Works* in Tucson, AZ.**

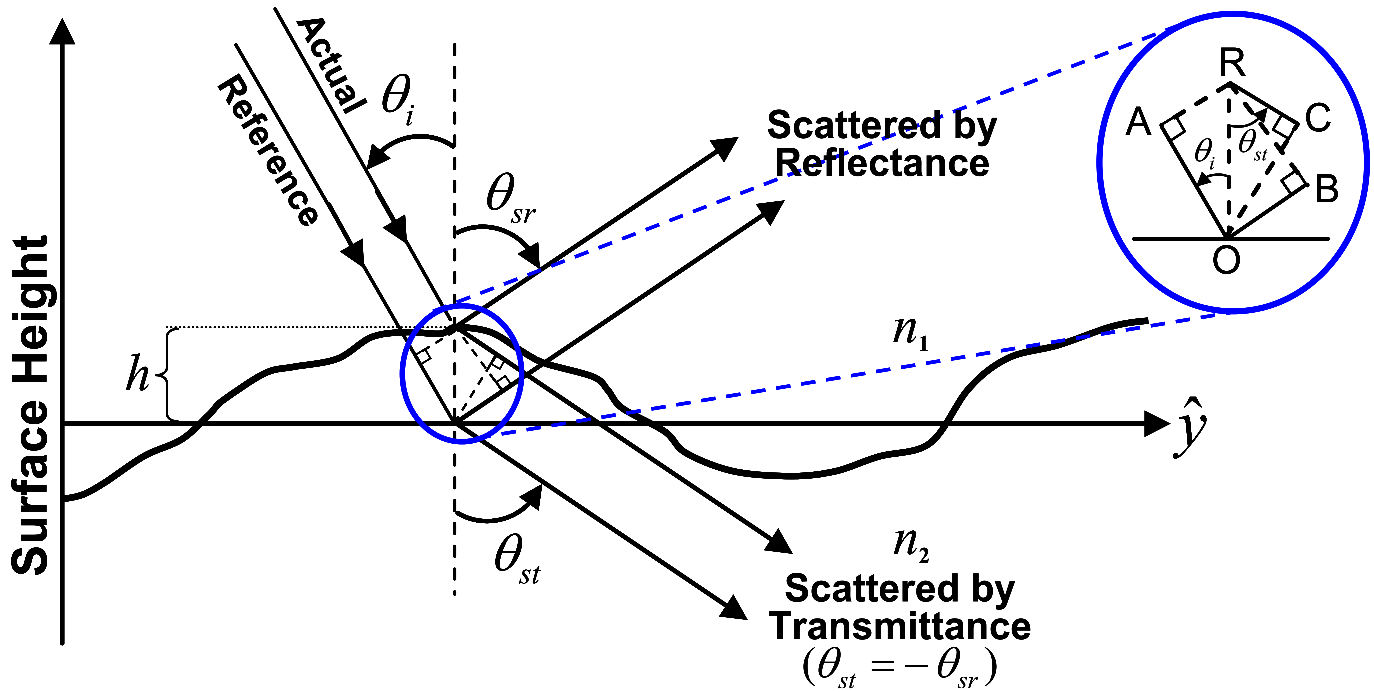
Surface PSD Calculated from the 80° BRDF



GHS and Rayleigh-Rice BRDF Predictions
(at Other Incident Angles and Wavelengths)



Phase Variation Introduced by Scattering from an Interface between Two Arbitrary Media



$$OPD = OPL_{actual} - OPL_{reference}$$

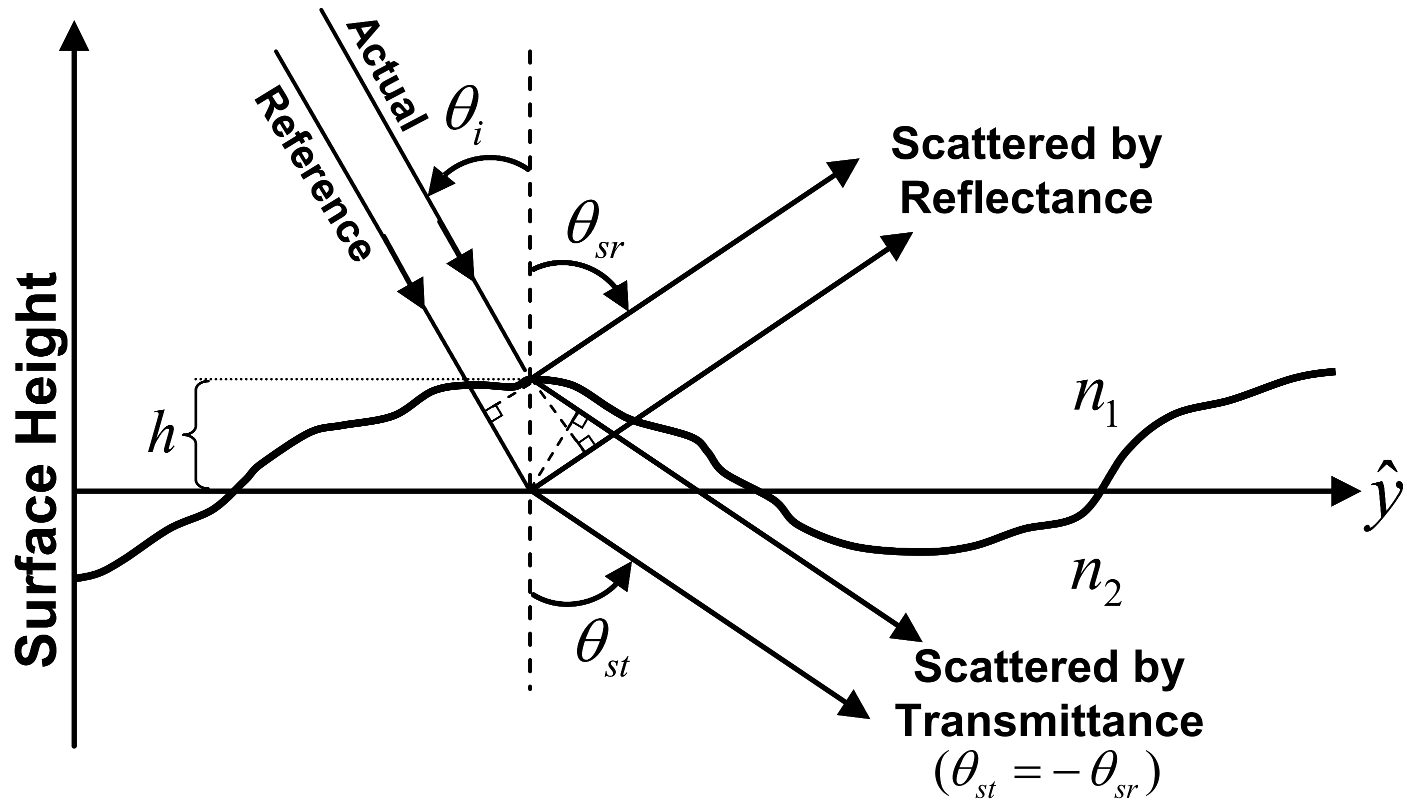
$$OPD_r = -\left(n_1\overline{AO} + n_2\overline{OB}\right)$$

$$OPD_t = -\left(n_1\overline{AO} - n_2\overline{RC}\right)$$

$$OPD = -h\left(n_1 \cos\theta_i - n_2 \cos\theta_s\right)$$

$$\phi(\hat{x},\hat{y}) = (2\pi/\lambda)\,OPD = -2\pi\left(n_1 \cos\theta_i - n_2 \cos\theta_s\right)\hat{h}(\hat{x},\hat{y})$$

Surface Transfer Function Characterizing Scattering from a Rough Interface between Two Arbitrary Media



$$OPD = -h\left(n_1 \cos\theta_i - n_2 \cos\theta_s\right)$$

$$\phi(\hat{x},\hat{y}) = (2\pi/\lambda)\, OPD = -2\pi\left(n_1 \cos\theta_i - n_2 \cos\theta_s\right)\hat{h}(\hat{x},\hat{y})$$

$$H_s(\hat{x},\hat{y};\gamma_i,\gamma_s) = \exp\left\{-\left[2\pi\hat{\sigma}_{rel}(n_1\gamma_i - n_2\gamma_s)\right]^2\left[1 - C_s(\hat{x},\hat{y})/\sigma_{rel}^2\right]\right\}$$

Predicting both the BTDF and the BRDF

$$H_s(\hat{x},\hat{y};\gamma_i,\gamma_s) = \exp\left\{-\left[2\pi\hat{\sigma}_{rel}(n_1\gamma_i - n_2\gamma_s)\right]^2\left[1 - C_s(\hat{x},\hat{y})/\sigma_{rel}^2\right]\right\}$$

Surface Transfer Function of Moderately Rough Interface between Two Arbitrary Dielectric Media