Predicting Image Degradation from Optical Surface Metrology Data

James E. Harvey

Center for Research and Education in Optics and Lasers (CREOL)
The University of Central Florida
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presented at

Fraunhofer IOF

Jena, Germany

March 11, 2010

University of Central Florida

CREOL: College of Optics and Photonics

Generalized Surface Scatter Theory for Moderately Rough Surfaces

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Abstract

Image degradation due to scattered radiation from residual optical fabrication errors is a serious problem in many short wavelength (X-ray/EUV) imaging systems. Most currently-available image analysis codes (ZEMAX, ASAP, FRED, etc.) require the scatter behavior (BRDF data) as input in order to calculate the image quality from such systems. This BRDF data is difficult to measure and rarely available for the operational wavelengths of interest. Since the smooth-surface approximation is often not satisfied at these short wavelengths, the classical Rayleigh-Rice expression that indicates the BRDF is directly proportional to the surface PSD cannot be used to calculate BRDFs from surface metrology data for even slightly rough surfaces. An FFTLog numerical Hankel transform algorithm enables the practical use of the computationally intensive Generalized Harvey-Shack (GHS) surface scatter theory to calculate BRDFs for increasingly short wavelengths that violate the smooth surface approximation implicit in the Rayleigh-Rice surface scatter theory. A generalized Peterson analytical scatter model is then used to make accurate image quality predictions. The generalized Peterson model is numerically validated by both ASAP and ZEMAX.

Applications with Moderately Rough Surfaces

- **Imaging with very Short Wavelengths (X-ray/EUV).**
  - **Predicting BRDFs from Measured or Assumed Surface Metrology Data**
  - **Predicting Image Quality from known Scatter Behavior.**
  - **Deriving Optical Fabrication Tolerances necessary to meet Specific Image Quality Requirements.**

- **Increasing the Efficiency of Thin-film Photovoltaic Solar Cells**
  - **Engineering Enhanced Roughness TCO/Si Interfaces.**
  - **Inducing “light trapping” for Better Absorption of Incident Light.**
  - **Develop a “forward modeling” Capability to Optimize Surface Characteristics.**

Outline

- Historical Review of Surface Scatter Theory.
- Statement of the EUV Imaging Problem (Summary of Results).
- Non-paraxial Scalar Diffraction Theory.
  - Scalar Treatment of Sinusoidal Phase Grating,
  - Modified Beckmann-Kirchhoff Surface Scatter Model.
- Total Integrated Scatter (TIS) for Moderately Rough Surfaces.
- Generalized Harvey-Shack (GHS) Scatter Theory.
  - Two-parameter Family of Surface Transfer Functions.
  - Very Computationally Intense Calculations.
- Example of Measured Metrology Data from an EUV Mirror.
  - Problem: Large dynamic Range of Relevant Spatial Frequencies.
  - Solution: FFTLog Numerical Hankel Transform Algorithm.
- BRDFs from Real Metrology Data from Moderately Rough Surfaces. (that violate the smooth surface approximation).
- Generalized Peterson Analytical Scattering Model.
  - Dealing with the “Scattered-Scattered” Light.
  - Numerical Validation with ASAP and ZEMAX.
- Results and Conclusions.

Historical Review of Surface Scatter Theory

- **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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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."

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* 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.
- Angela Duparre and Sven Schroder: Surface Characterization & Scatter Measurements

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Statement of the Problem

For short wavelength 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:**
    - **Calculate the BRDF from assumed metrology data.**
    - **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 must be 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:

- **Developed a Linear Systems Formulation of Non-paraxial Scalar Diffraction Theory** (Diffracted Radiance, Direction Cosine space).
- **Empirically Modified Beckmann-Kirchhoff Scatter Theory** (non-paraxial).
- **Rigorously Derived a New Unified Surface Scatter Model.**
  - 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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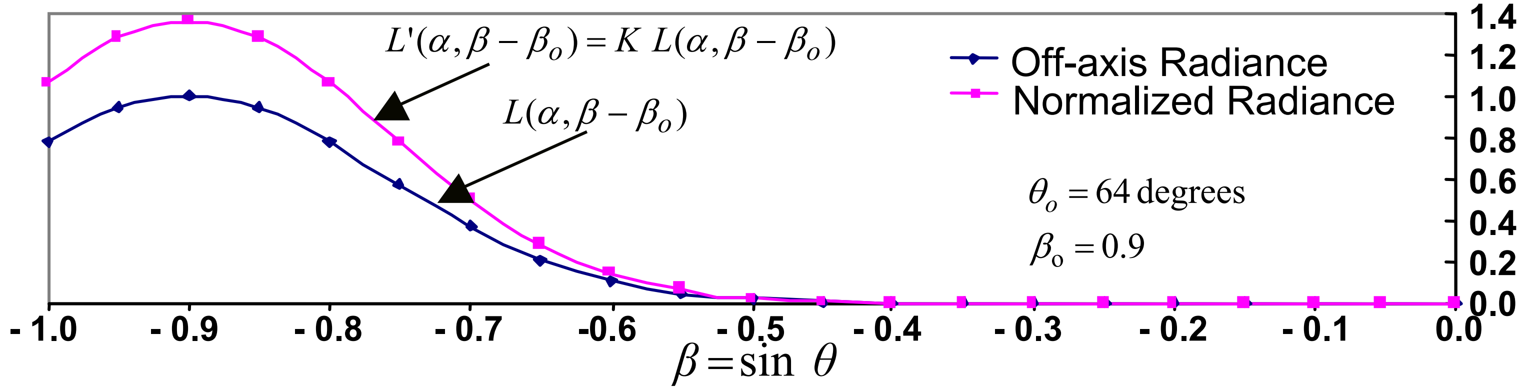
Diffracted Radiance: The Fundamental Quantity Predicted by Scalar Theory *

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.

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

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.

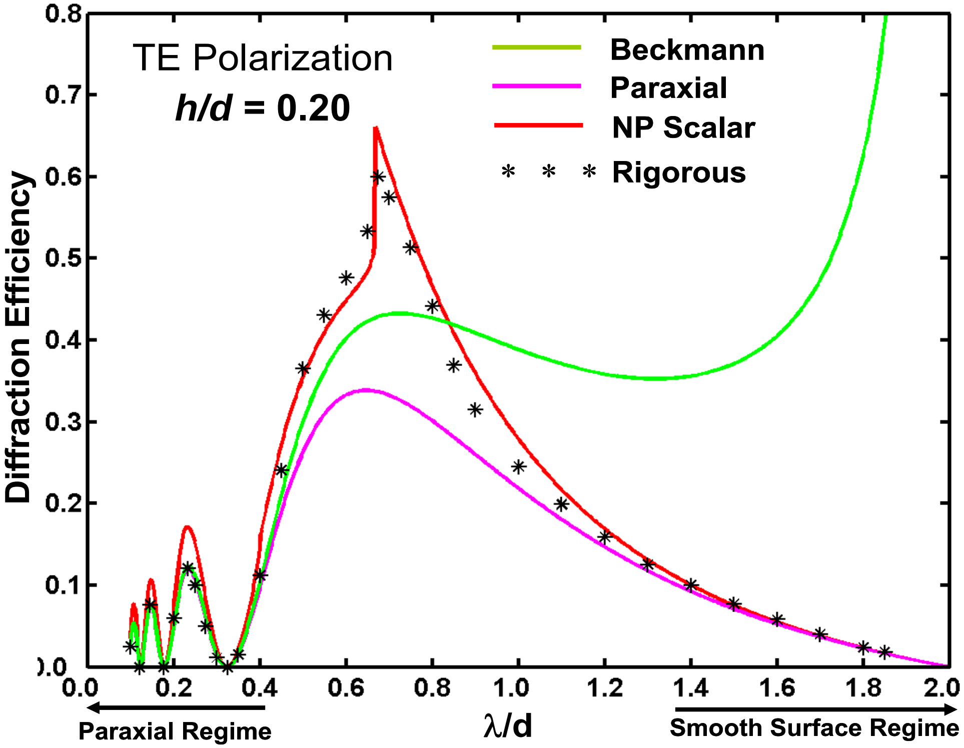
$$K = \frac{\displaystyle\int_{\alpha=-\infty}^{\infty}\int_{\beta=-\infty}^{\infty} L(\alpha,\beta-\beta_o)\,d\alpha\,d\beta}{\displaystyle\int_{\alpha=-1}^{1}\int_{\beta=-\sqrt{1-\alpha^2}}^{\sqrt{1-\alpha^2}} L(\alpha,\beta-\beta_o)\,d\alpha\,d\beta} \equiv \text{Normalization Constant} \qquad (2)$$

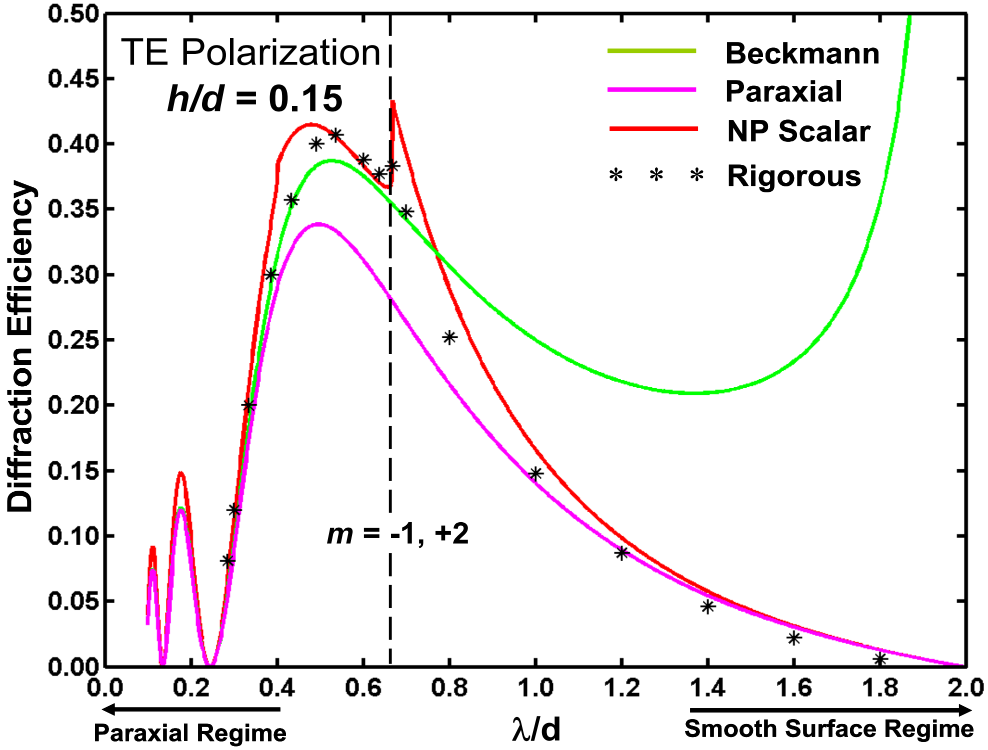
* J. E. Harvey, et.al., "Diffracted Radiance: A Fundamental Quantity in Non-Paraxial Scalar Diff. Theory", Appl. Opt. 38, 6469 (1999).

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:

$$\eta_m = \frac{P_m}{P_T} = \frac{J_m^2\left(a/2\right)}{\sum\limits_{m=\min}^{\max} J_m^2\left(a/2\right)} \tag{3}$$





These figures show that using our non-paraxial scalar diffraction theory is able to predict 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).

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

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

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

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

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

Modified Beckmann-Kirchhoff Theory

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

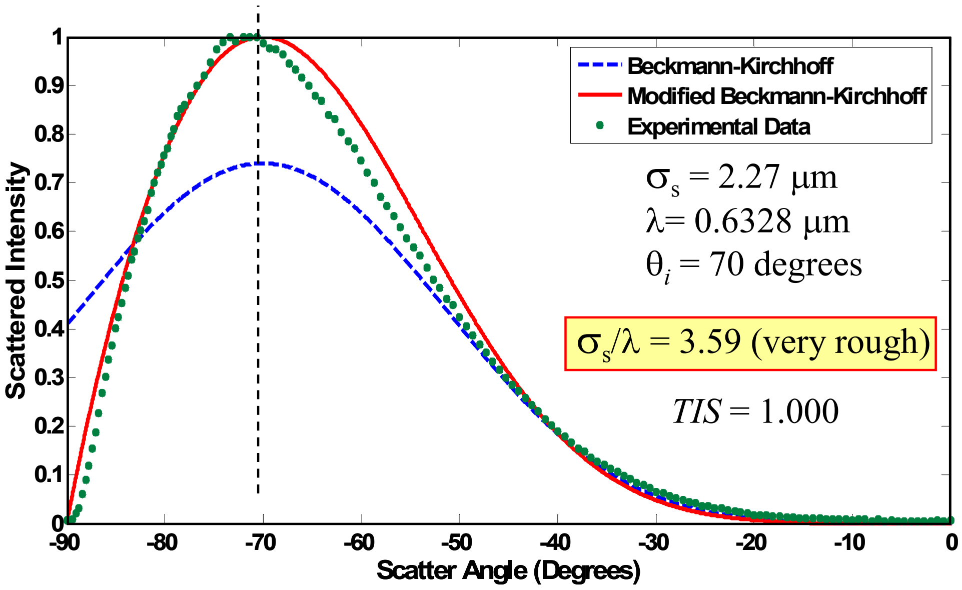
$K =$ Re$-$normalization Factor **(5**

(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

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

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

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

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

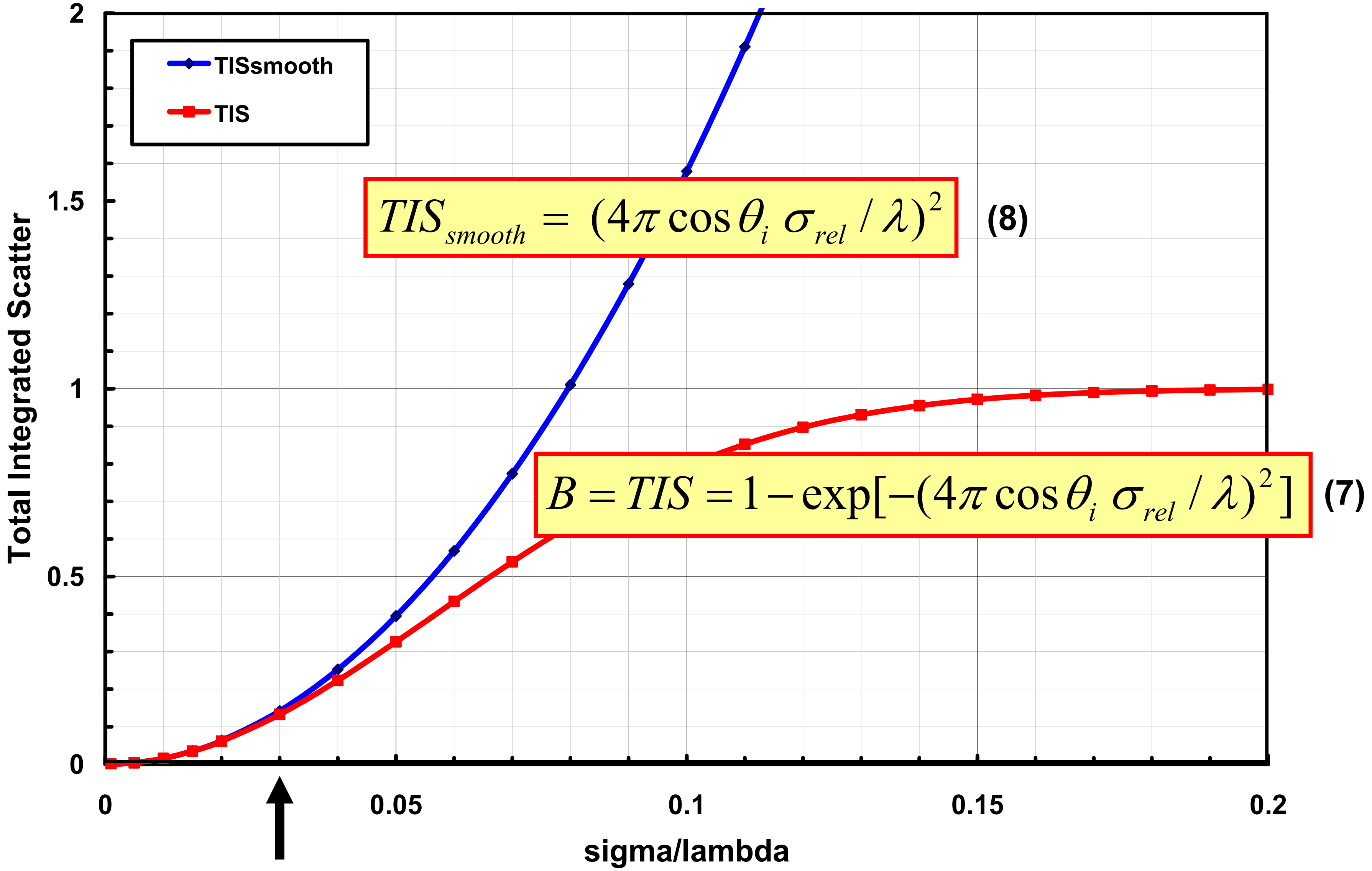
For smooth surfaces ($\sigma \ll \lambda$), the total integrated scatter (TIS_{smooth}) can thus be approximated as

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

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.

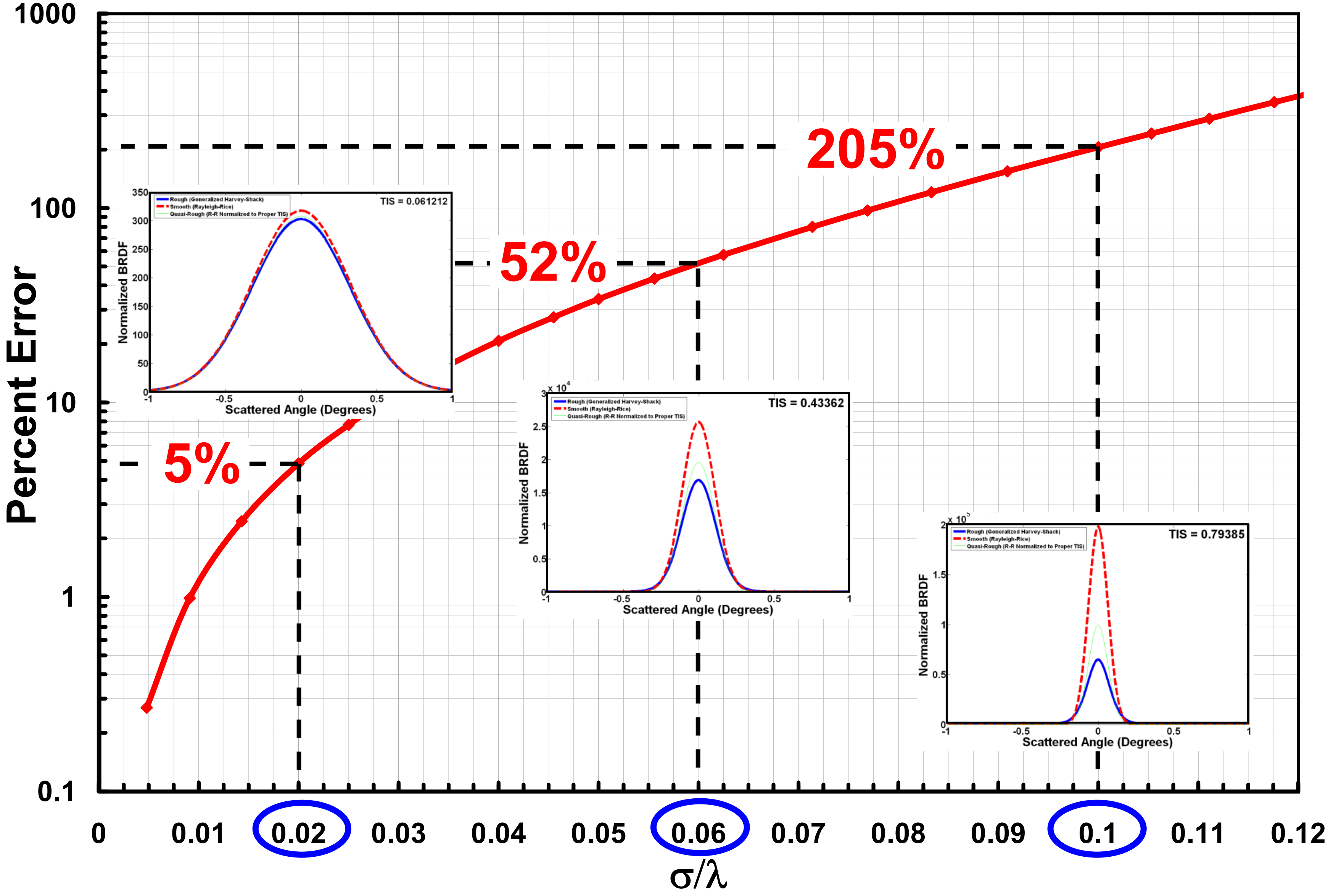


$$TIS_{smooth} = (4\pi \cos\theta_i \, \sigma_{rel} / \lambda)^2 \tag{8}$$

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

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.



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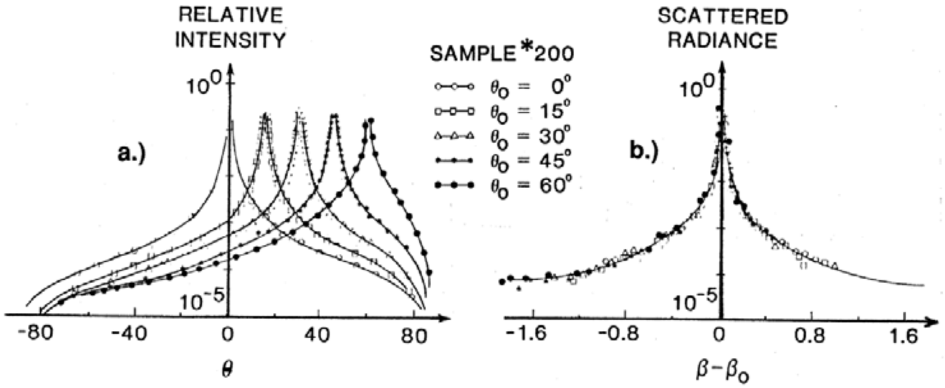
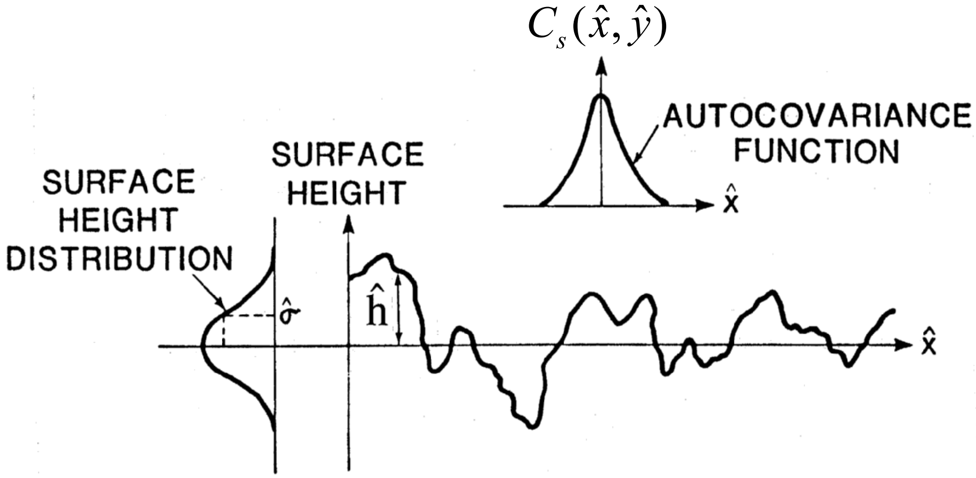
Transfer Function Characterization of Surface Scatter*

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

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

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

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

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

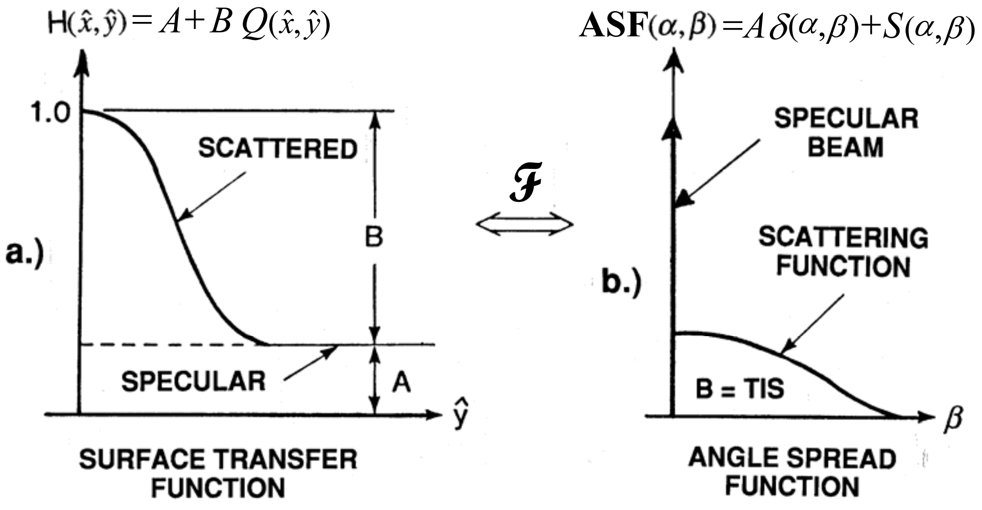
∗ J. E. Harvey, "Light-Scattering Characteristics of Optical surfaces", Ph.D. Dissertation, Univ. of Arizona (1976).

The Associated Angle Spread Function*

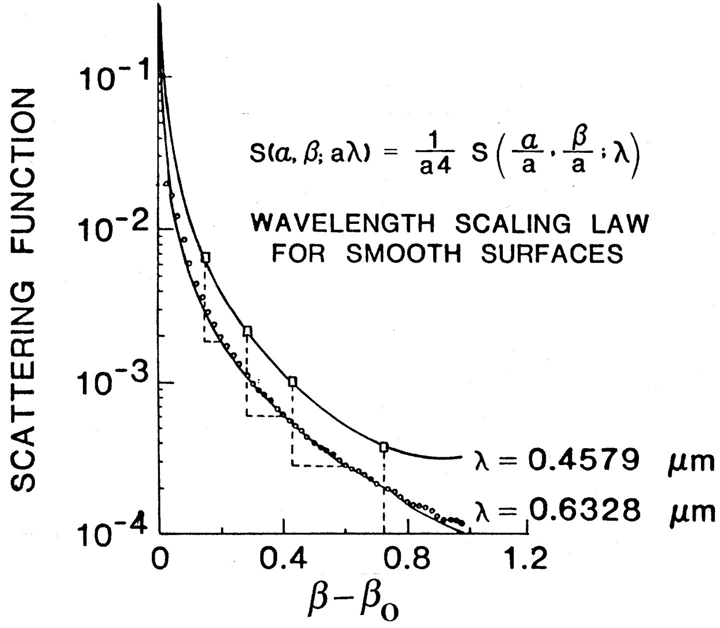
(Scattered Radiance)

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.

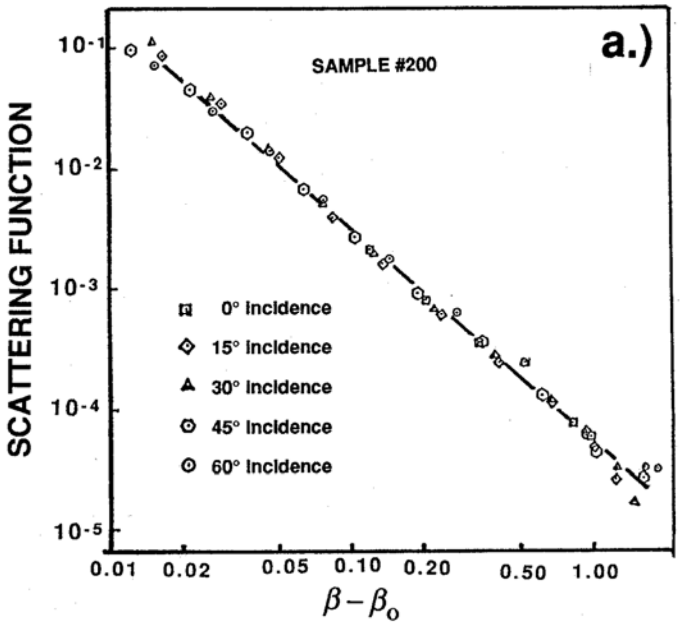
The Associated Angle Spread Function



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 Theory*

ASAP Feature Note
BRO-FN1407(02/00)

Harvey-Shack Overview

Bidirectional Scattering Distribution Function (BSDF)

This ASAP Feature Note briefly discusses the Harvey-Shack model and its use for illumination applications in ASAP™ optical modeling software.

Breault Research Organization, Inc.
Optical Engineering Software and Services

Harvey-Shack BSDF

In his dissertation (J. E. Harvey, "Light-Scattering Properties of Optical Surfaces," Ph.D. Dissertation, U. Arizona, 1976) Harvey found that for many optical surfaces, the BSDF is independent of the direction of incidence if it is expressed as a function of direction cosines instead of angles. Harvey called this property "shift-invariant," as in linear systems theory. Referring to Figure 7.4, β_0 is a projection onto the surface of the unit vector $\mathbf{r}_0$ in the specular direction, β is a projection onto the surface of the unit vector $\mathbf{r}$ in the scattering direction, and the magnitude of their difference, $|\beta-\beta_0|$, is the argument of the BSDF. Note that β and β_0 are not unit vectors. They are projections of unit vectors, so their lengths are less than or equal to one. The Harvey-Shack method gives a good model for the behavior of most optical surfaces, i.e. those for which:

- Scattering is due mainly to surface roughness
- Scattering (and thus surface roughness) is isotropic
- Surface roughness is small compared to the wavelength of light

USER'S MANUAL
RELEASE 3.0

Lambda Research Corporation

ZEMAX
Optical Design Program
User's Guide
Version 9.0

Harvey-Shack (ABg) scattering

The Harvey-Shack or ABg scattering model is a very powerful and widely used Bidirectional Scattering Distribution Function, or BSDF. BSDF is defined as the s incident irradiance, or

$$BSDF(\theta_i, \phi_i, \theta_s, \phi_s) = \frac{dL_s(\theta_s, \phi_s)}{dE_i(\theta_i, \phi_i)}$$

where θ is measured from the normal, and ϕ is the azimuthal angle, and the subscri and scattered directions, respectively. Note BSDF has units of inverse steradians. The general term BSDF can refer to two separate functions, the BRDF and BTDF, fo distributions, respectively. ZEMAX allows separate specification of the BRDF and B following sections.

Harvey-Shack BSDF properties

For many optical surfaces, the BSDF is independent upon incident direction if it is plotte cosines instead of angles. This was first reported by James E. Harvey ("Light-Scatt Surfaces", J. E. Harvey, Ph.D. Dissertation, University of Arizona, 1976; "Scattering Ef Fabrication Errors", J. Harvey and A. Kotha, Proceedings of the SPIE, July, 1999).

The Harvey-Shack representation is to plot BSDF as a function of $|\beta - \beta_0|$, which distance between the scattered and unscattered ray vectors when projected down to the discussion under "Scattering" above).

---

* 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!

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.

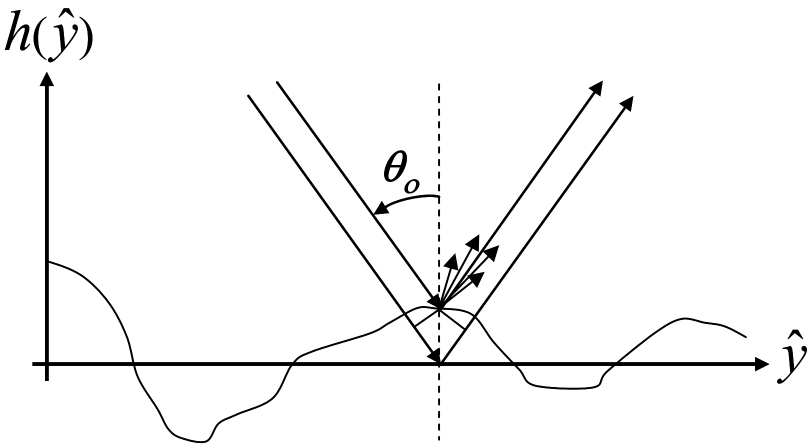
$$\phi(\hat{x},\hat{y}) = (2\pi/\lambda)\, OPD \;=\; (4\pi/\lambda)\, h(\hat{x},\hat{y}) \cos(\theta_o)$$

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 β_o = sin θ_o and γ_o = cos θ_o.

Optical Path Difference (OPD) upon Reflection



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

Modified Surface Transfer Function

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

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

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).

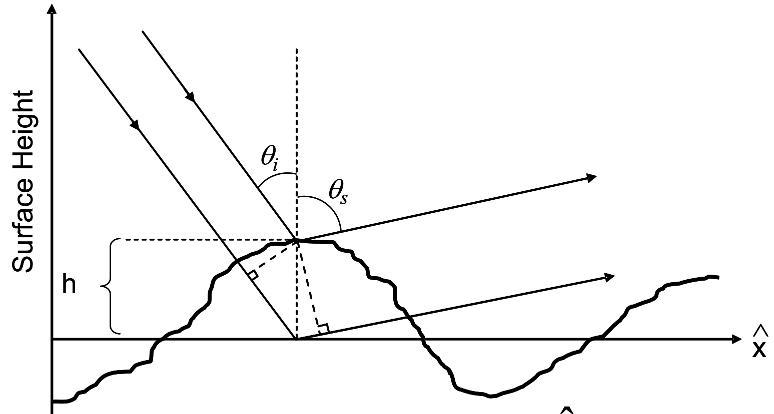
Generalized Harvey-Shack Surface Scatter Theory*

(Arbitrarily Rough Surfaces, Large Incident and Scatter Angles)

Limitations of Original Harvey-Shack Theory

- **Scalar theory (no polarization effects).**
- **Does not account for redistribution of energy from evanescent to propagating waves.**
- **Surface transfer function has a built-in paraxial limitation.**

Phase Variation Depends on Scattering Angle



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

New Surface Transfer Function

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

(11)

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

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

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

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

(12)

New 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 quazi-vectorized by merely substituting the polarization reflectance factor, Q, for the reflectance, R, in the scalar treatment.

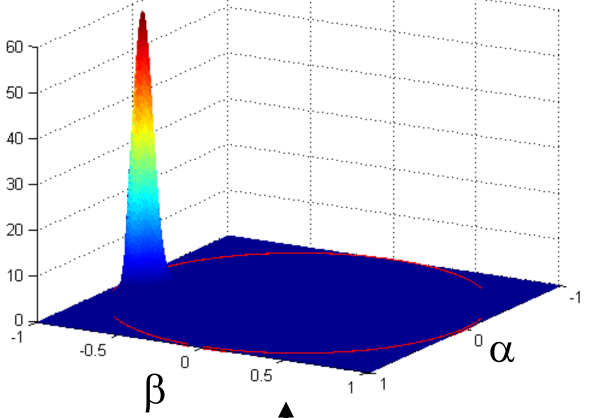
---

* A. Krywonos, *Predicting Surface Scatter using a Linear Systems Formulation of Non-paraxial Scalar diffraction*, PhD Dissertation, UCF (2006).

** A. Krywonos, J. E. Harvey and N, Choi, "A Linear Systems Formulation of Scattering Theory for Rough Surfaces with Large Incident and Scattering Angles", to be submitted to JOSA A (Mar 2010).

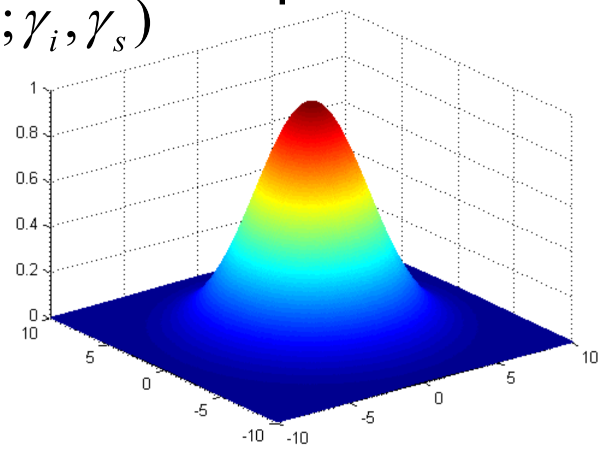
Description of Generalized Harvey-Shack Calculations

$\mathcal{S}(\alpha,\beta)$



$\uparrow \mathcal{F}$

$H(\hat{x},\hat{y};\gamma_i,\gamma_s)$

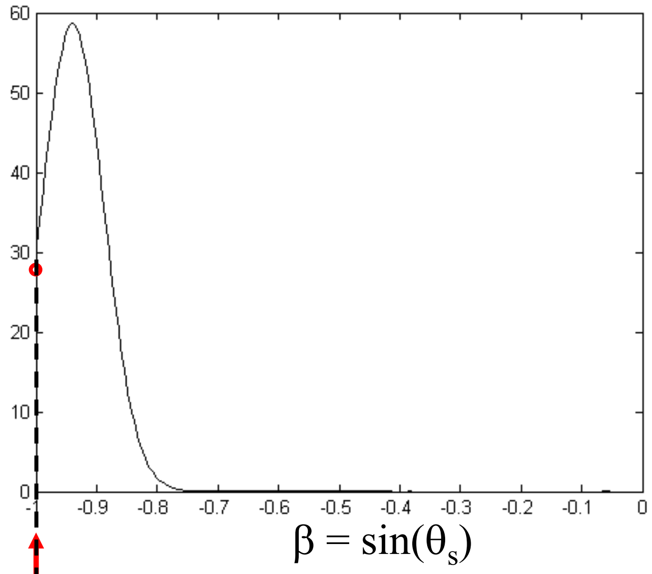


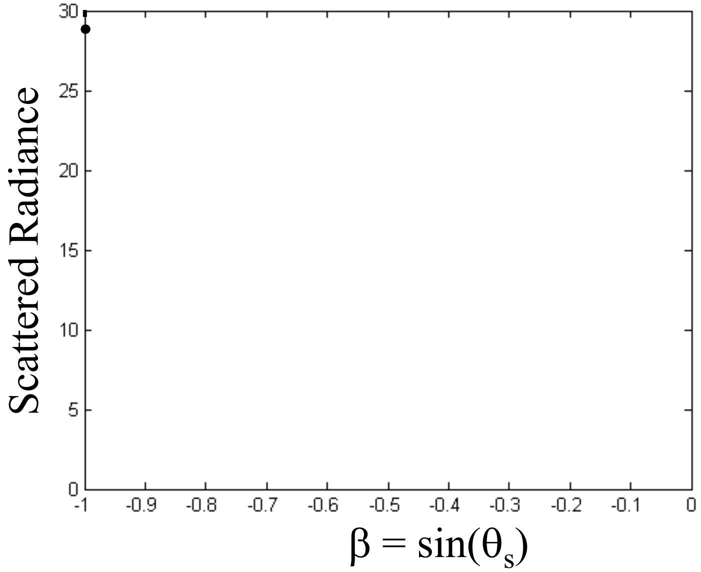
θ_i = 70°

θ_s = - 90°

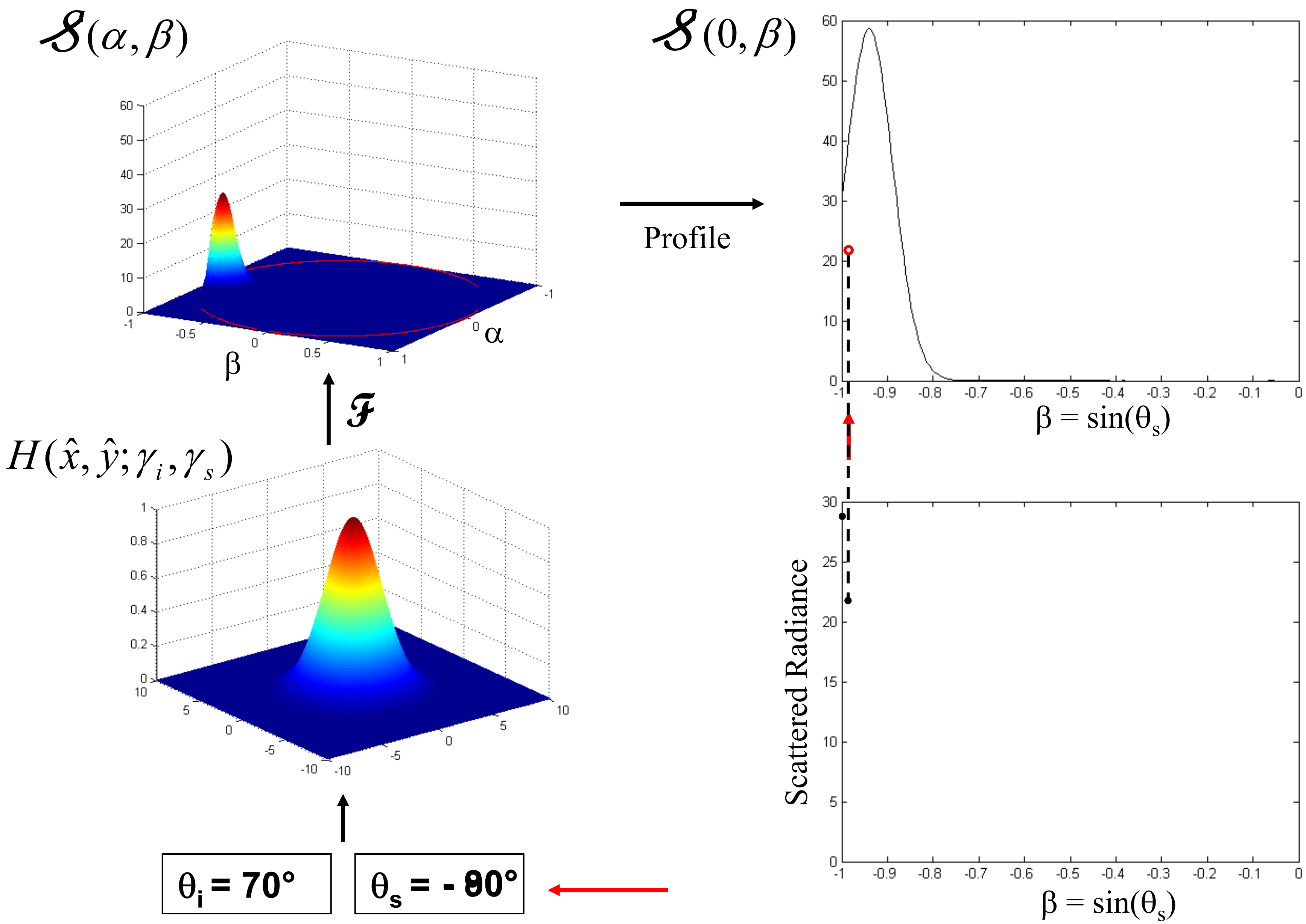
$\mathcal{S}(0,\beta)$

Profile





Description of Generalized Harvey-Shack Calculations



$\mathcal{S}(\alpha,\beta)$

Profile

$\mathcal{S}(0,\beta)$

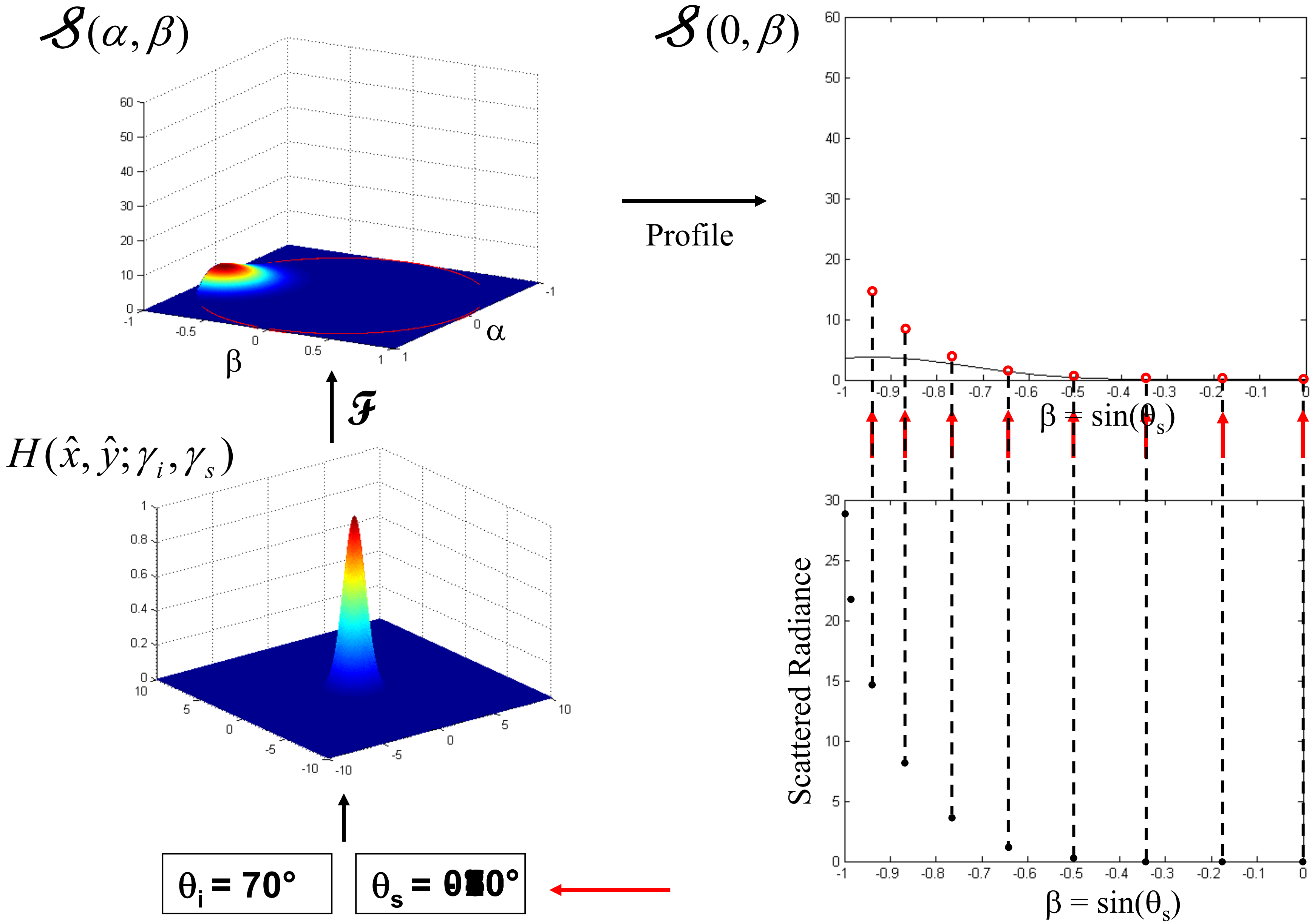
$\mathcal{F}$

$H(\hat{x},\hat{y};\gamma_i,\gamma_s)$

θ_i = 70°

θ_s = - 80°

Description of Generalized Harvey-Shack Calculations



$\mathcal{S}(\alpha,\beta)$

Profile

$\mathcal{S}(0,\beta)$

$\mathcal{F}$

$H(\hat{x},\hat{y};\gamma_i,\gamma_s)$

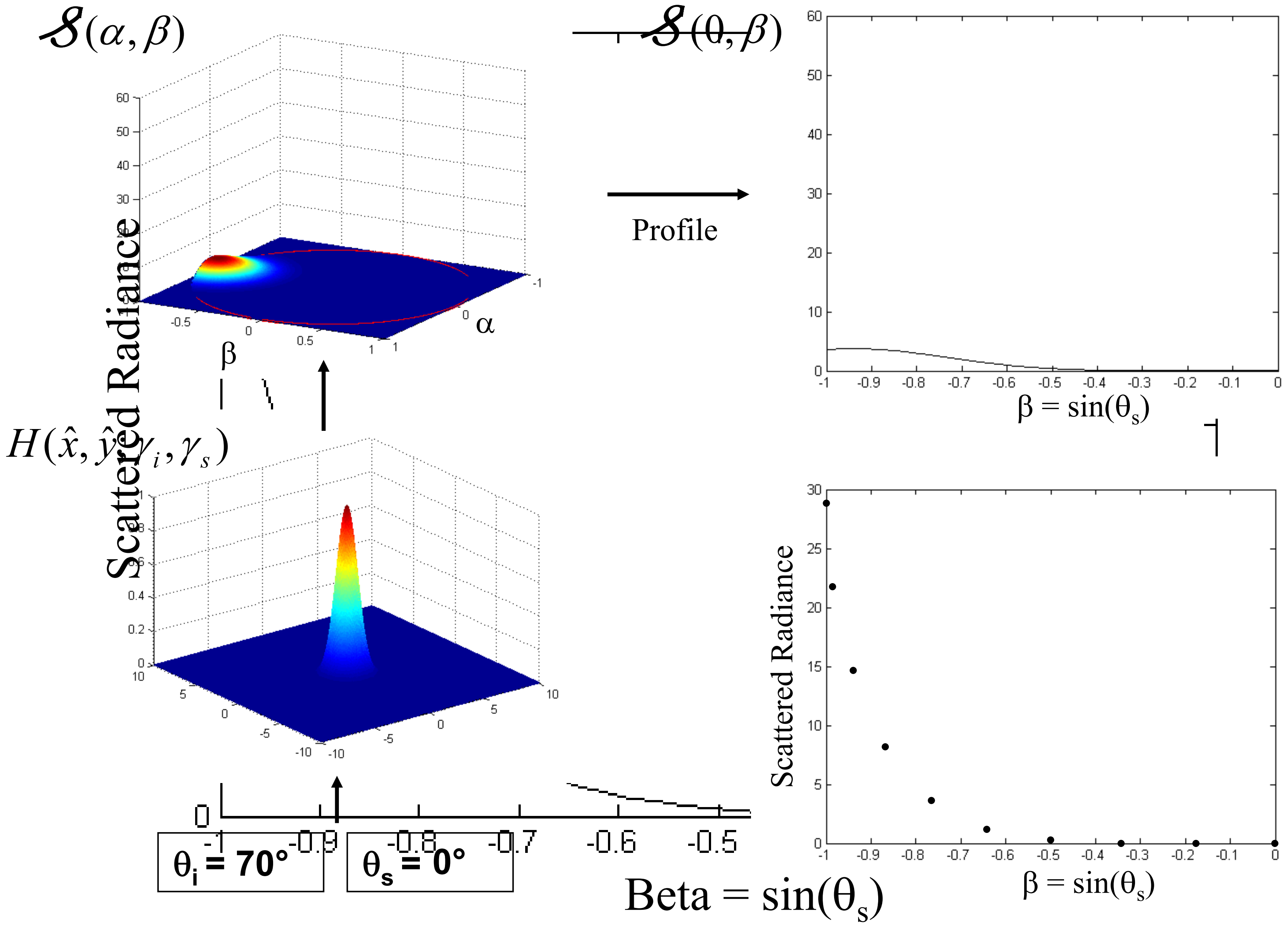
θ_i = 70°

θ_s = 0[illegible]0°

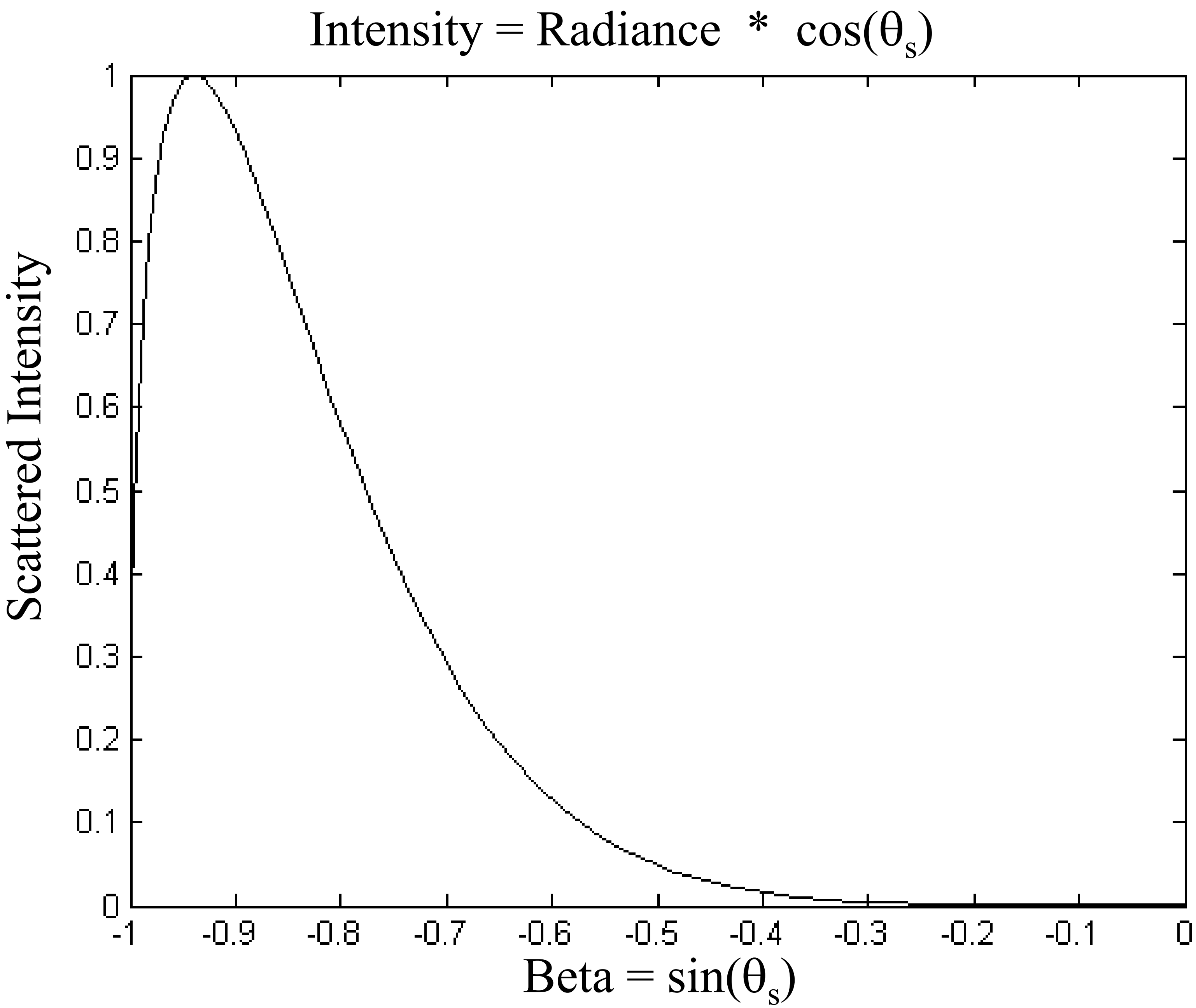
Scattered Radiance

$\beta = \sin(\theta_s)$

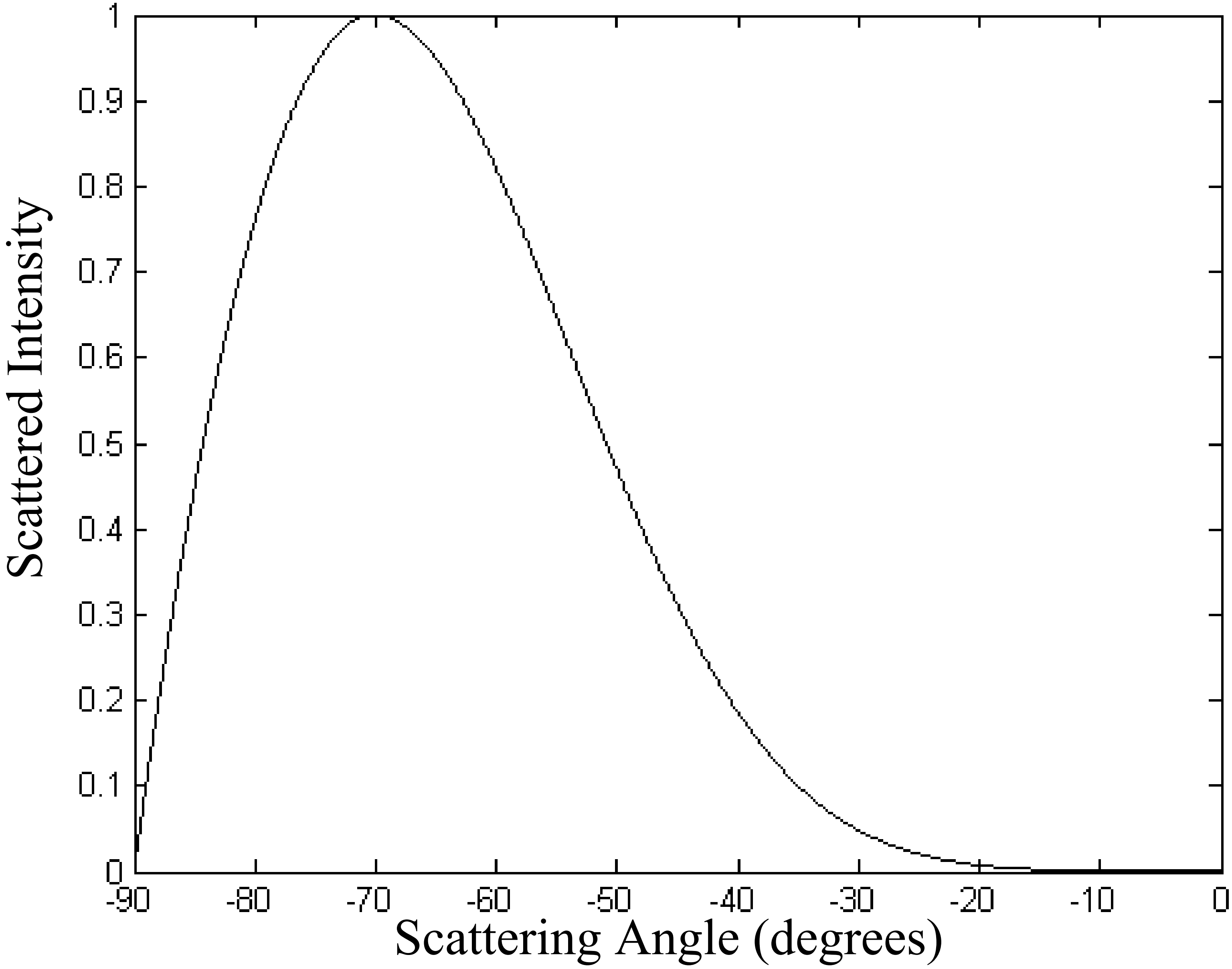
Description of Generalized Harvey-Shack Calculations



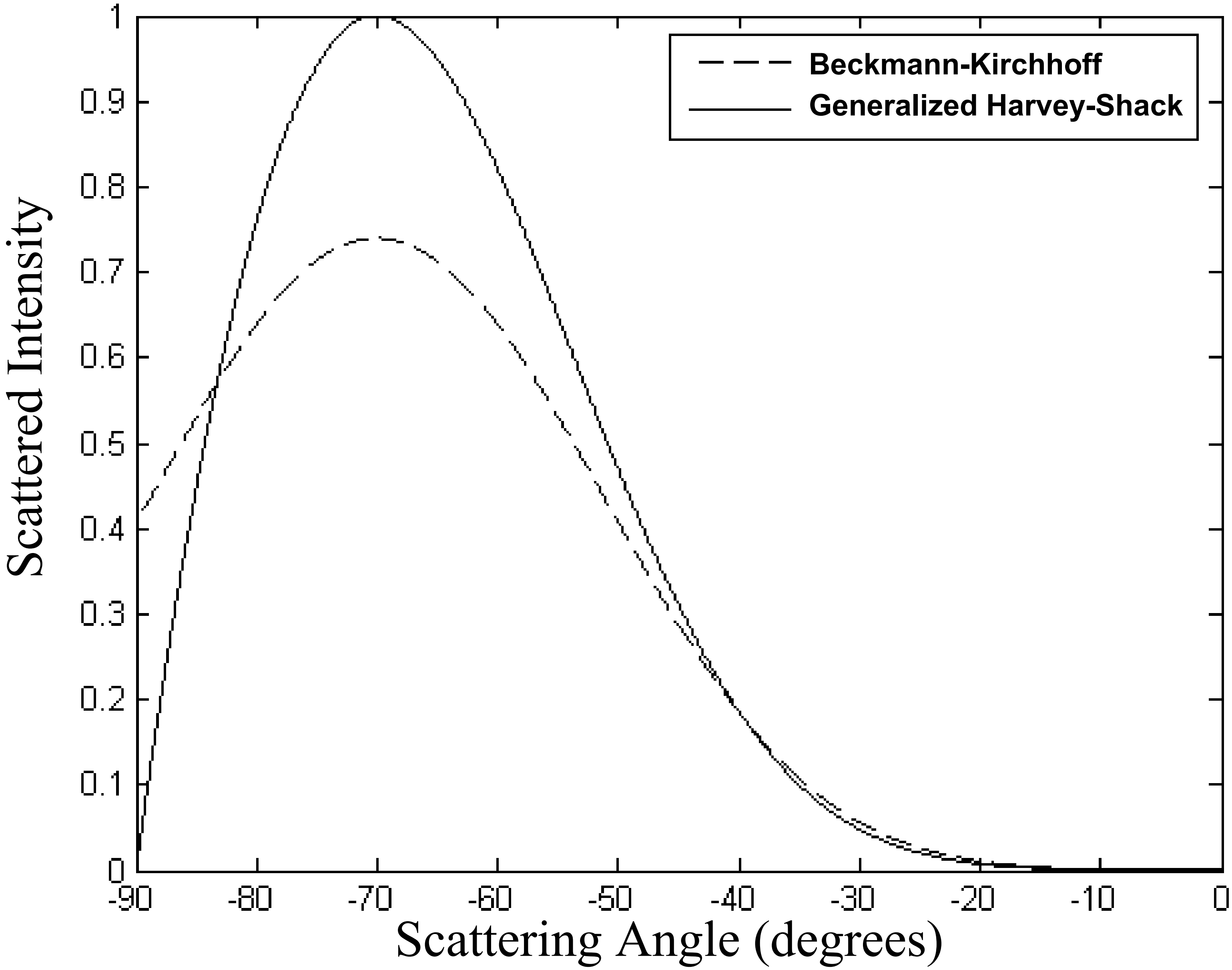
Description of Generalized Harvey-Shack Calculations



Description of Generalized Harvey-Shack Calculations



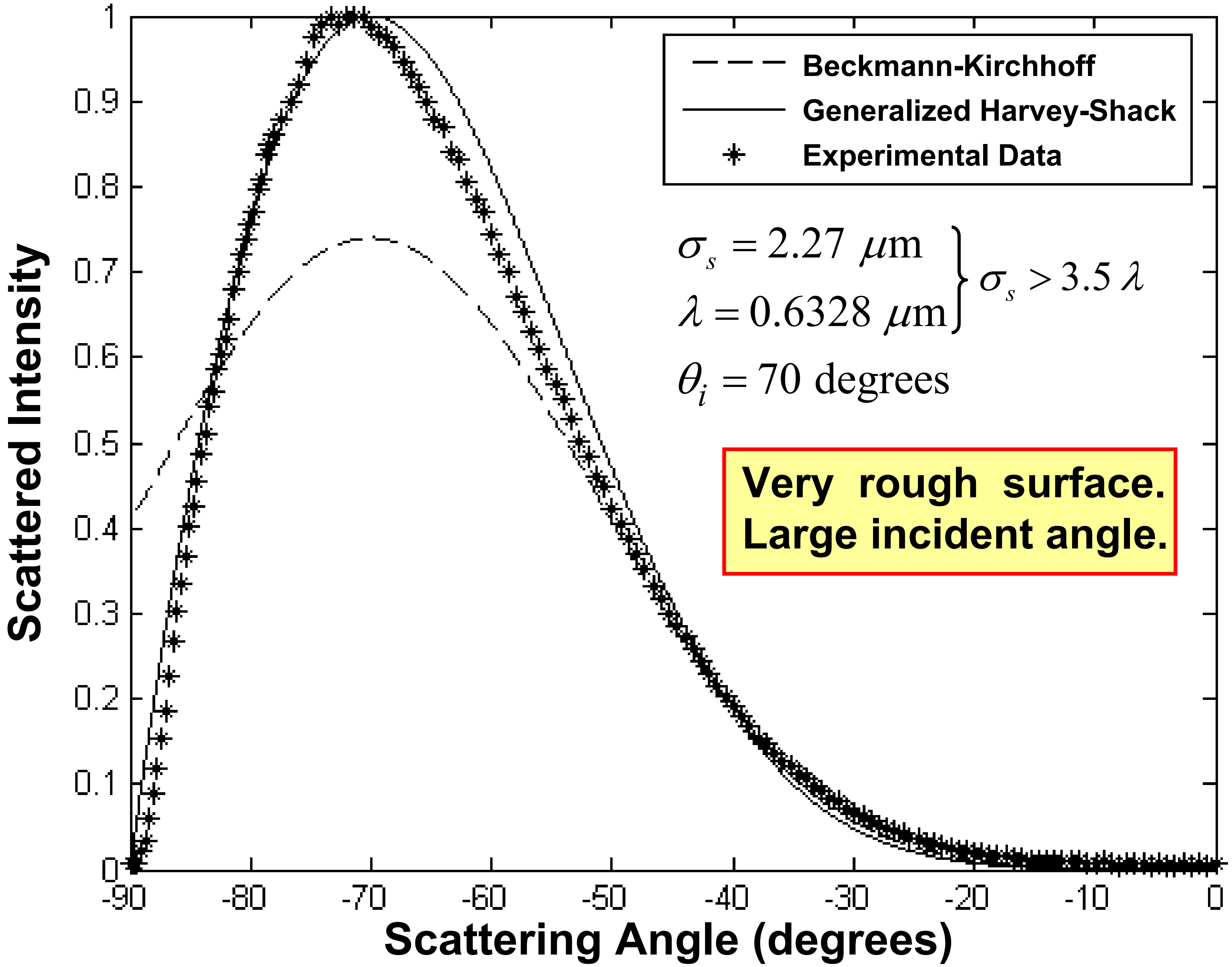
Description of Generalized Harvey-Shack Calculations



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).



$$\left.\begin{aligned}\sigma_s &= 2.27\ \mu\text{m} \\ \lambda &= 0.6328\ \mu\text{m}\end{aligned}\right\}\ \sigma_s > 3.5\,\lambda$$

$$\theta_i = 70 \text{ degrees}$$

Very rough surface.
Large incident angle.

Smooth-surface Approximation to GHS Theory*

(Obliquity Factor Differs from Rayleigh-Rice Theory)

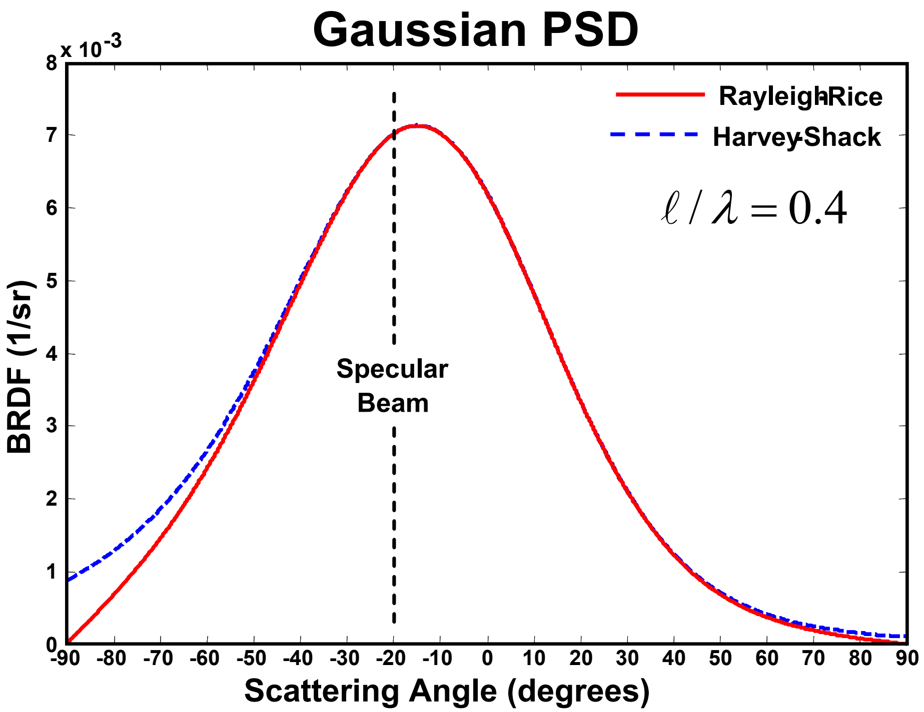
Generalized Harvey-Shack

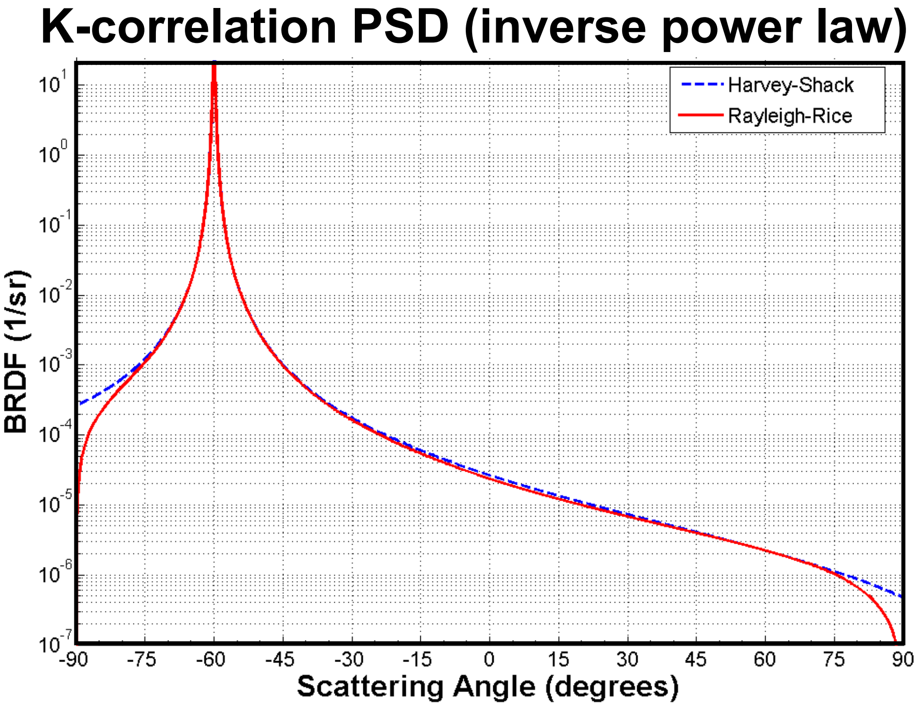
$$BRDF = \frac{4\pi^2}{\lambda^4}(\cos\theta_o + \cos\theta_s)^2 \, Q \, PSD(f_x, f_y) \qquad (13)$$

Rayleigh-Rice

$$BRDF = \frac{16\pi^2}{\lambda^4}\cos\theta_o \cos\theta_s \, Q \, PSD(f_x, f_y) \qquad (14)$$

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.

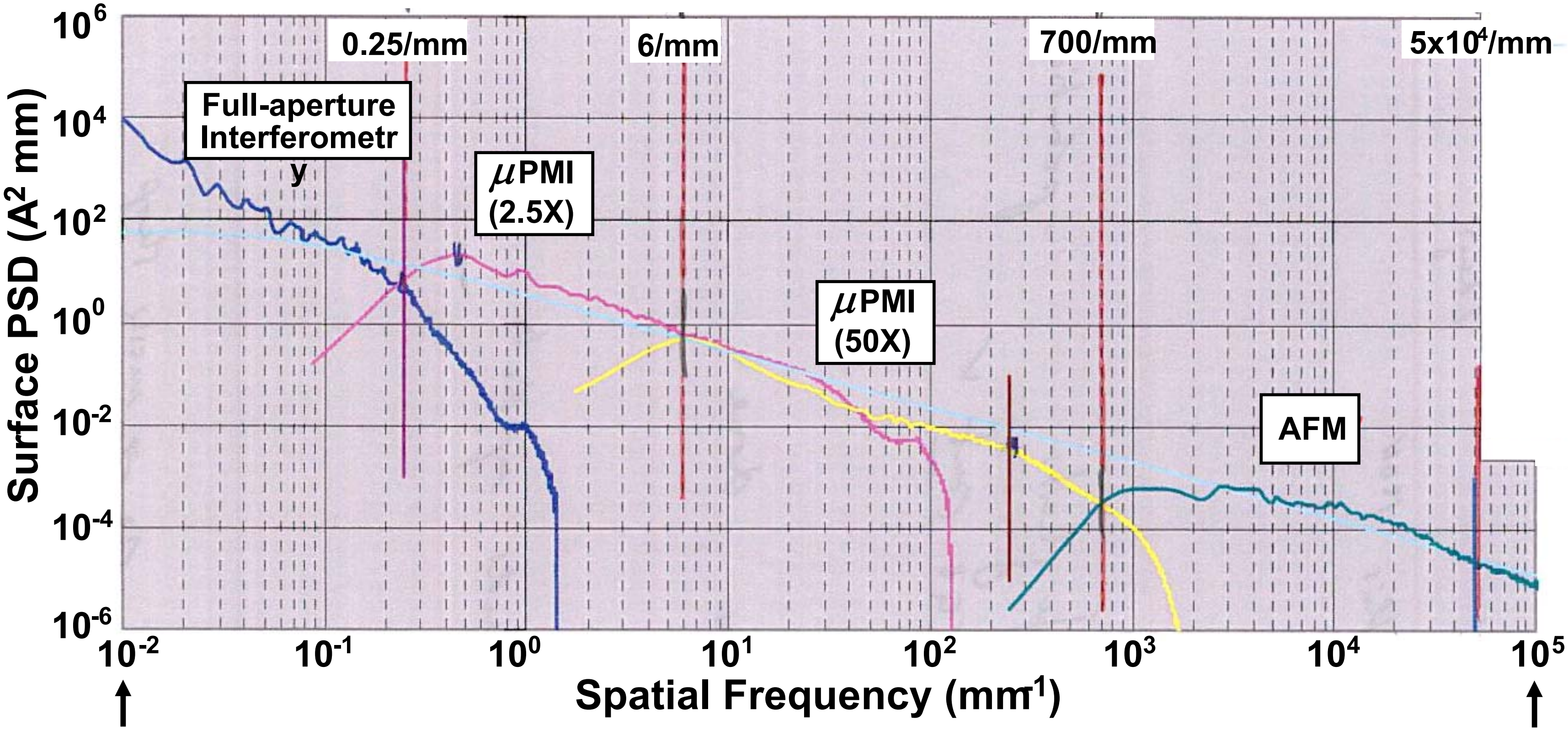
Outline

- **Historical Review of Surface Scatter Theory.**
- **Statement of the EUV Imaging Problem (Summary of Results).**
- **Non-paraxial Scalar Diffraction Theory.**
  - **Scalar Treatment of Sinusoidal Phase Grating,**
  - **Modified Beckmann-Kirchhoff Surface Scatter Model.**
- **Total Integrated Scatter (TIS) for Moderately Rough Surfaces.**
- **Generalized Harvey-Shack (GHS) Scatter Theory.**
  - **Two-parameter Family of Surface Transfer Functions.**
  - **Very Computationally Intense Calculations.**
- **Example of Measured Metrology Data from an EUV Mirror.**
  - **Problem: Large dynamic Range of Relevant Spatial Frequencies.**
  - **Solution: FFTLog Numerical Hankel Transform Algorithm.** → **NEW**
- **BRDFs from Real Metrology Data from Moderately Rough Surfaces. (that violate the smooth surface approximation).**
- **Generalized Peterson Analytical Scattering Model.**
  - **Dealing with the "Scattered-Scattered" Light.**
  - **Numerical Validation with ASAP and ZEMAX.**
- **Results and Conclusions.**

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.



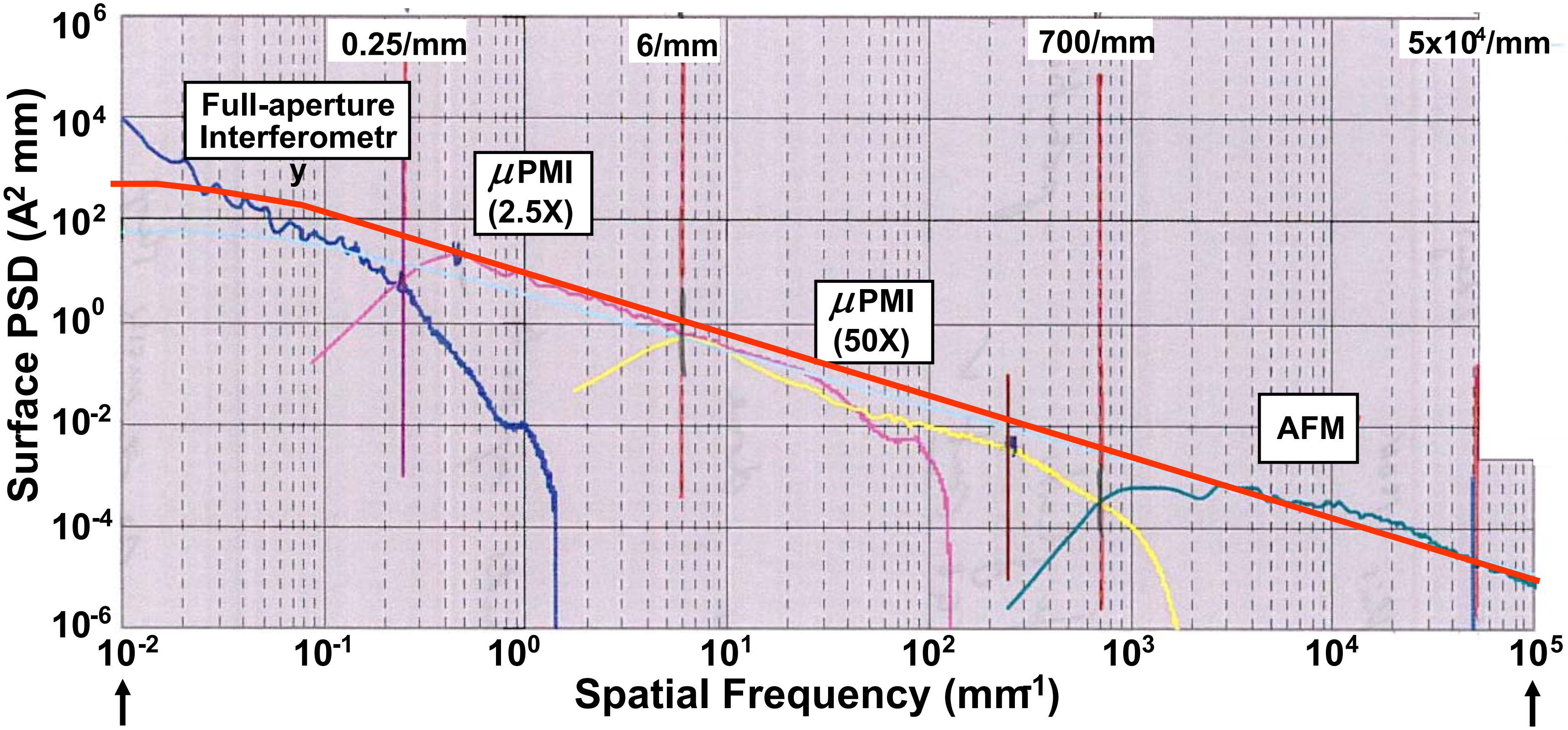
$1/D$ **Seven Decades of Dynamic Range in Spatial Frequency!!!** $1/\lambda$

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.

$$PSD(f_x)_{1-D} = \frac{A}{\left[1+(B\,f_x)^2\right]^{C/2}} \qquad \textbf{(15)}$$



$1/D$ **Seven Decades of Dynamic Range in Spatial Frequency!!!** $1/\lambda$

---

* 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.(12) 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.(13). The total volume under the 2-D surface PSD is given by Eq.(14), and the Fourier transform of the 2-D K-correlation function is given by Eq.(15).

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

3-parameter K-correlation function or ABC function. **(16)**

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

2-D surface PSD. **(17)**

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

$$\sigma_{Total}^2 = \frac{2\pi\,K\,A}{\left(C-1\right)B}$$

Total volume under 2-D surface PSD. **(18)**

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

Surface Autocovariance Function. **(19)**

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).

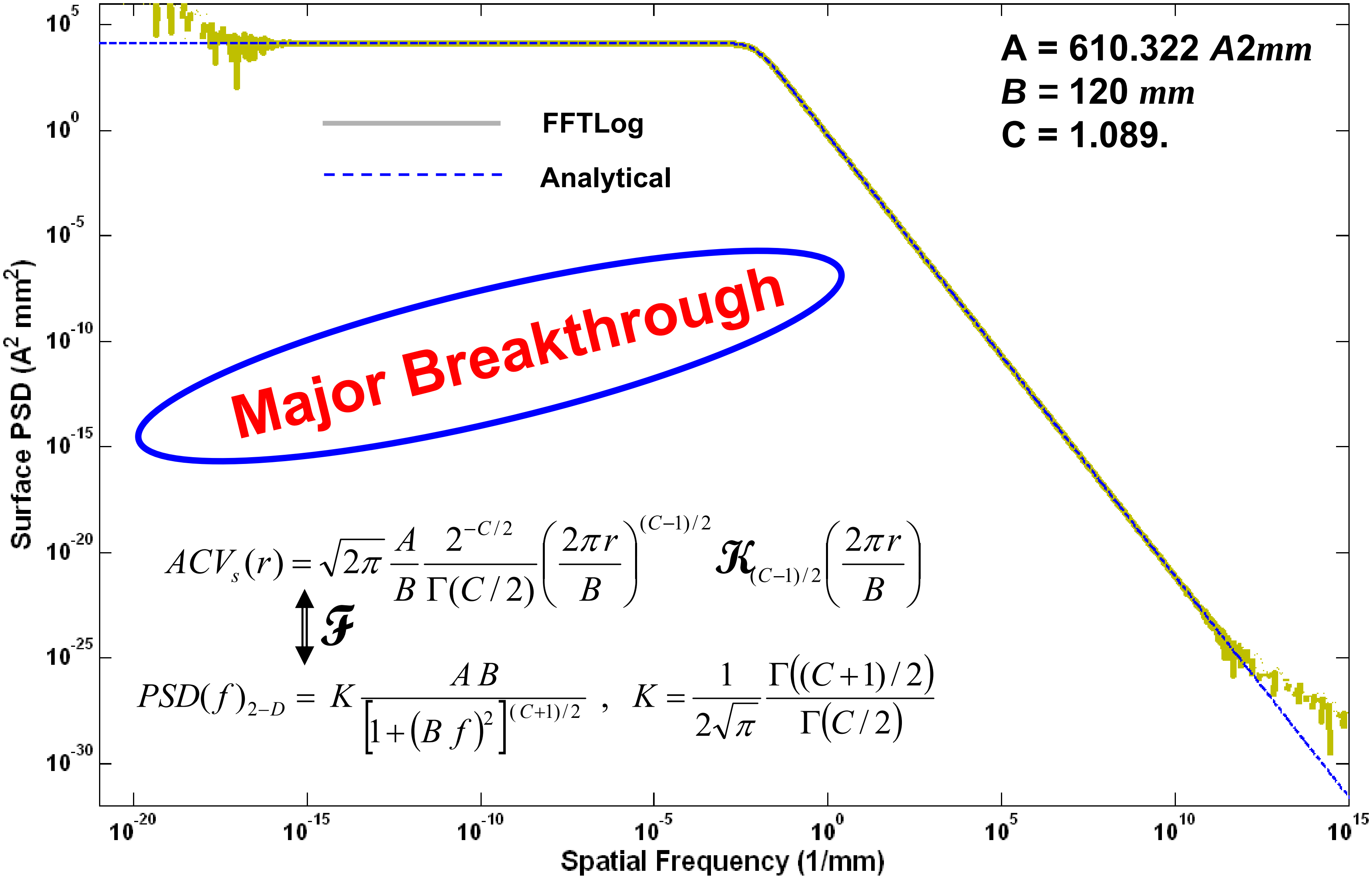
The *FFTLog* Hankel Transform Algorithm*

- ***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 ABC 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).



A = 610.322 *A2mm*
B* = 120 *mm
C = 1.089.

Major Breakthrough

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

$$\Updownarrow\ \mathcal{F}$$

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

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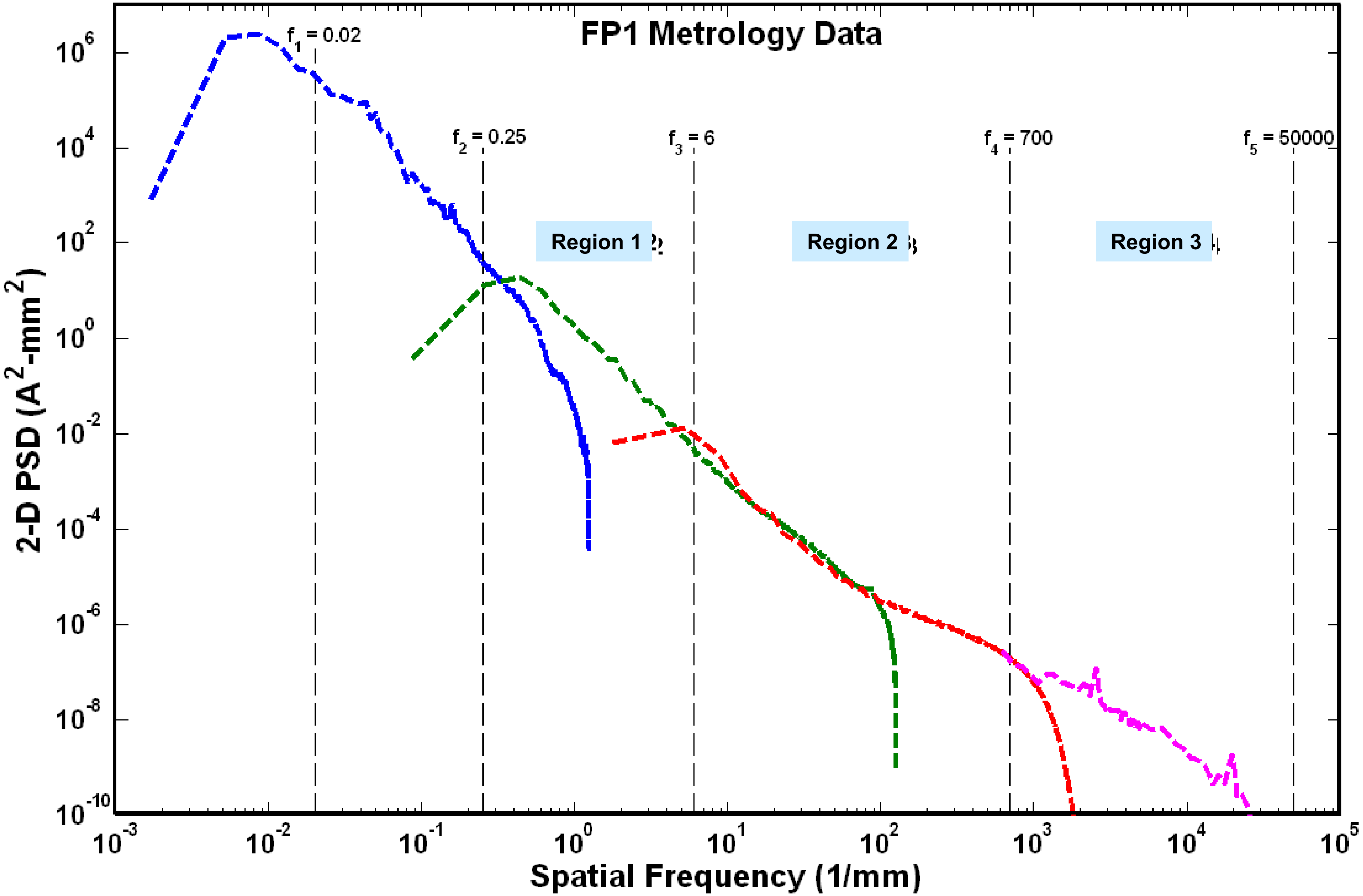
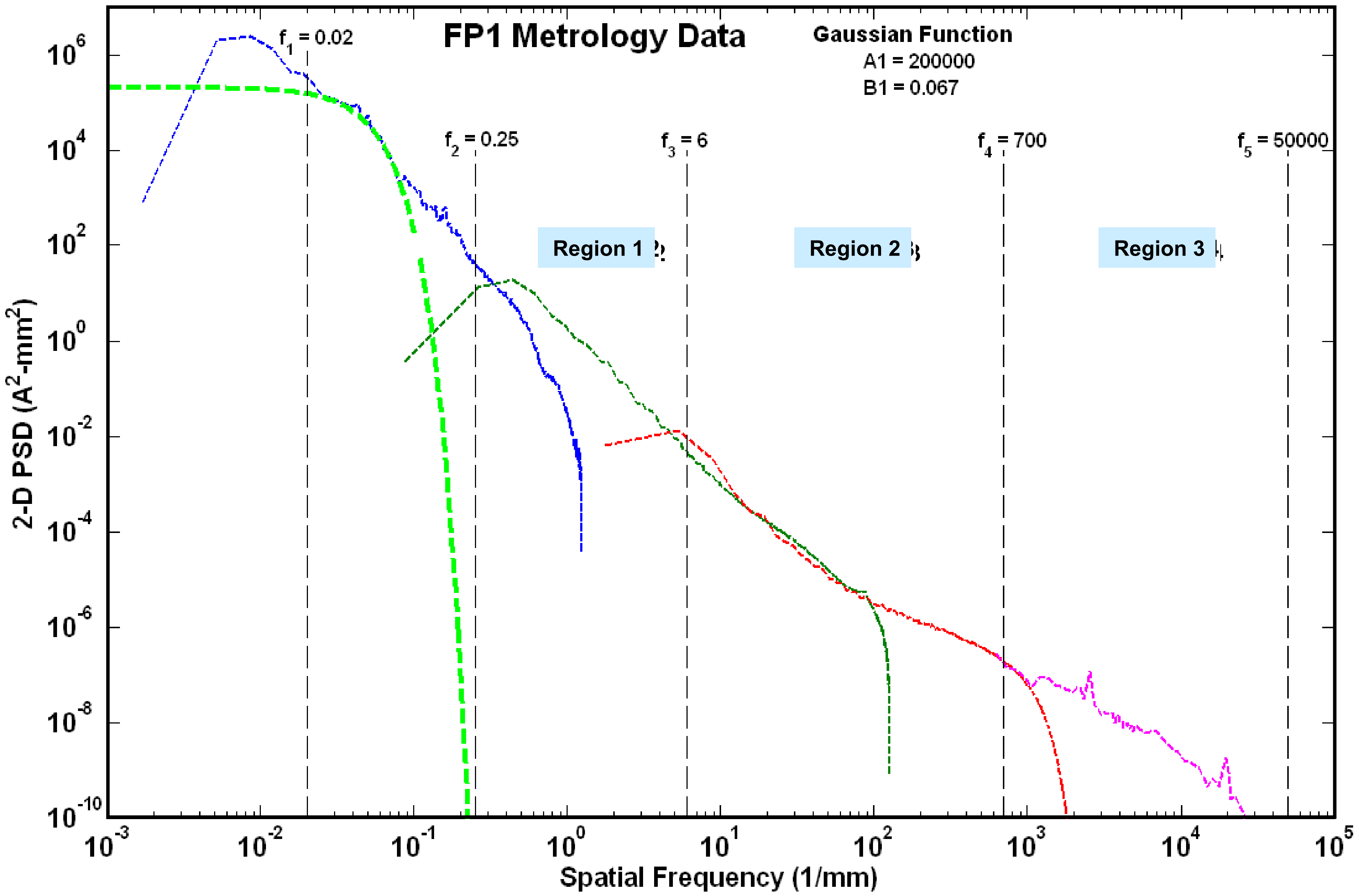
SUVI FP1 Metrology Data

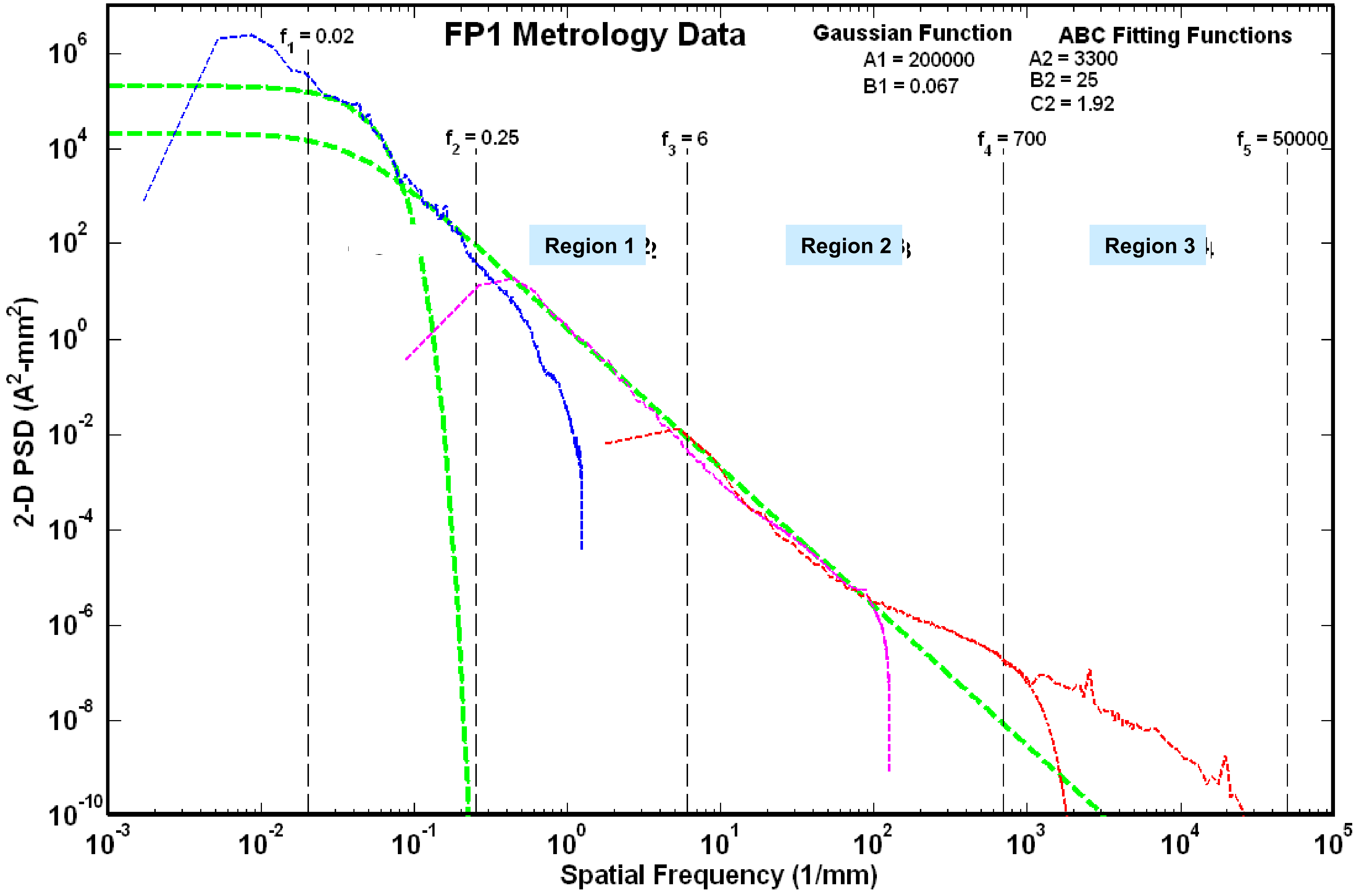
(SUVI Primary Mirror)



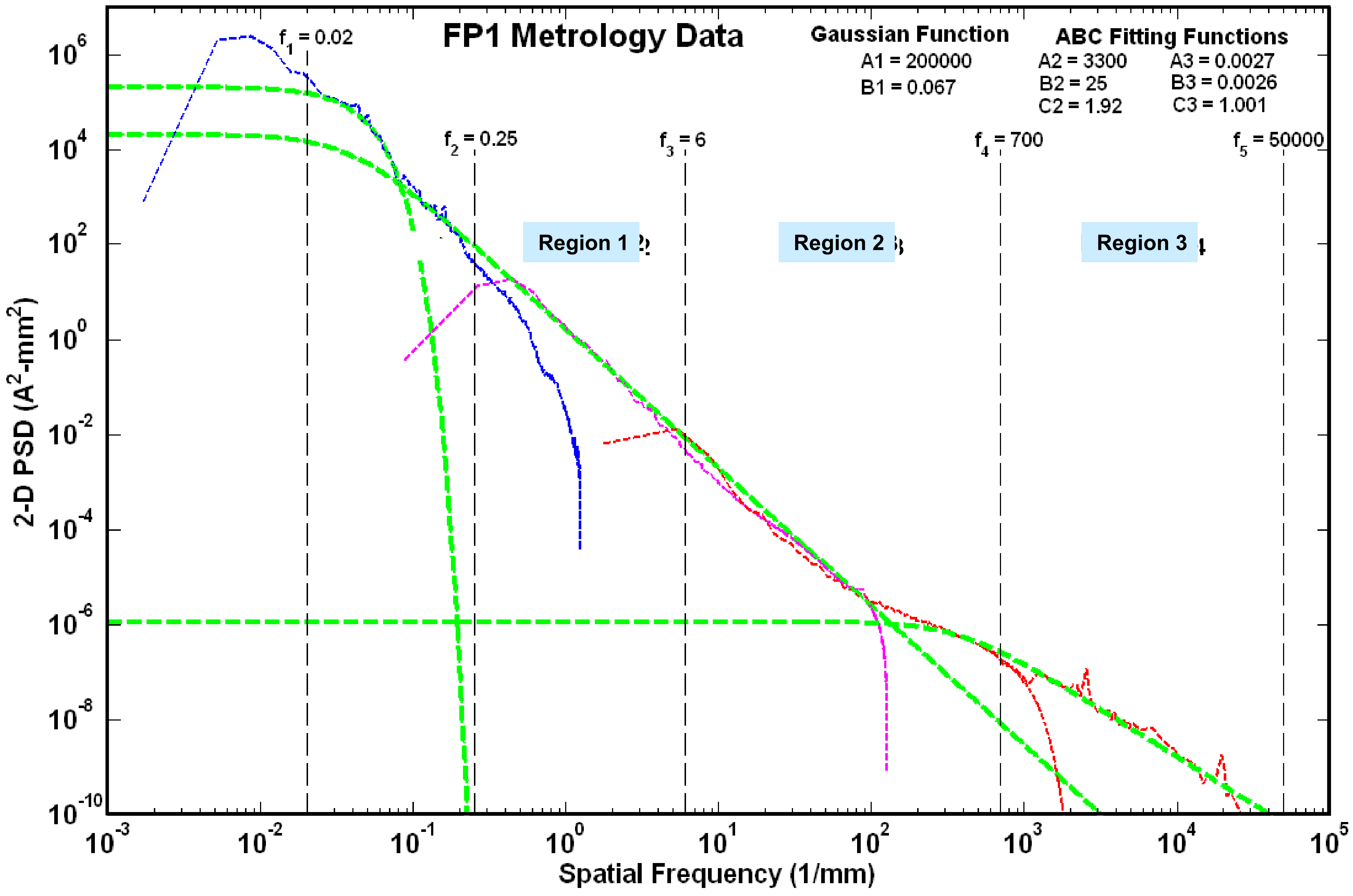
1st Fitting Function to FP1 Metrology Data



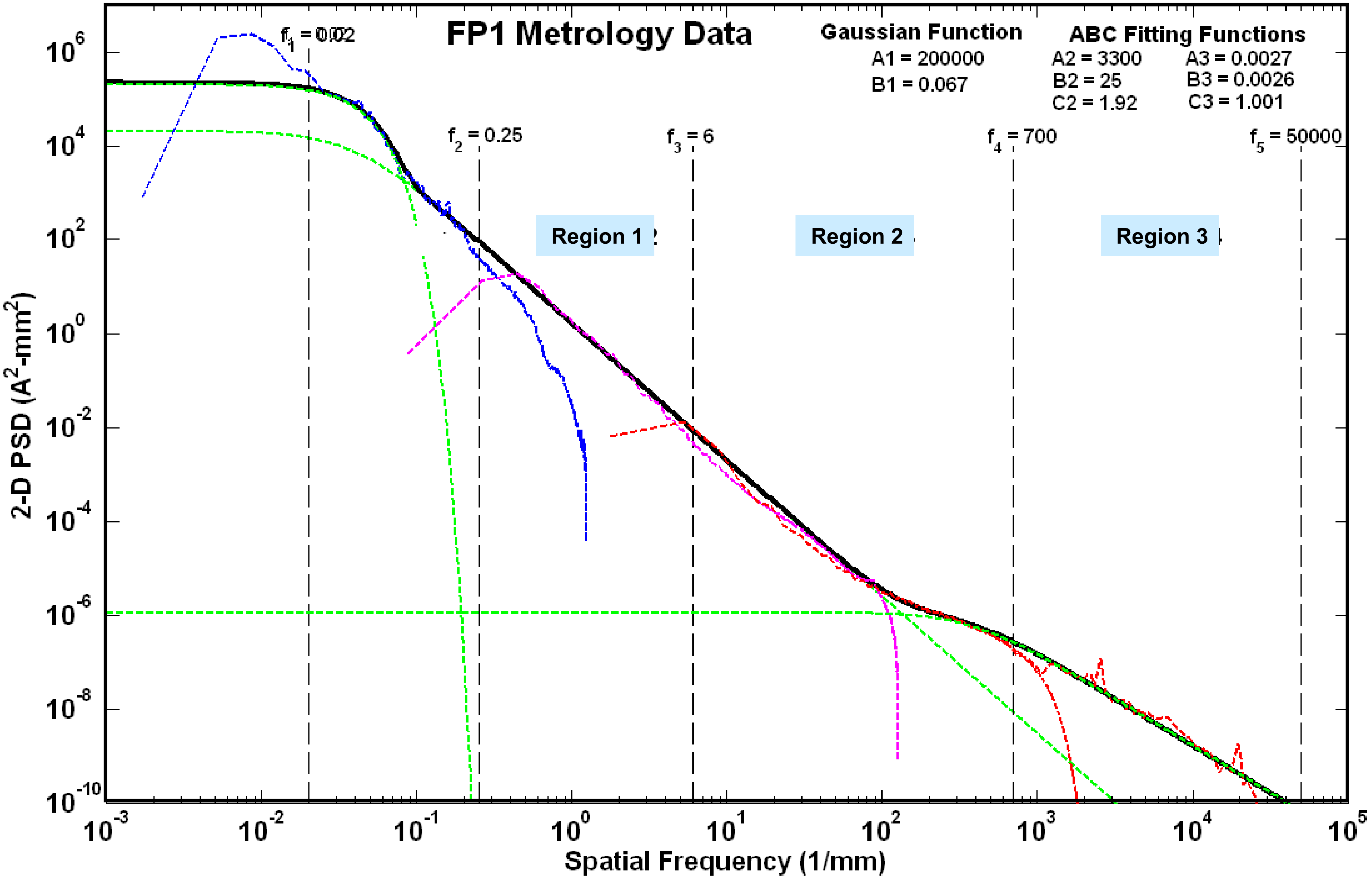
2^{nd} Fitting Function to FP1 Metrology Data



3rd Fitting Function to FP1 Metrology Data



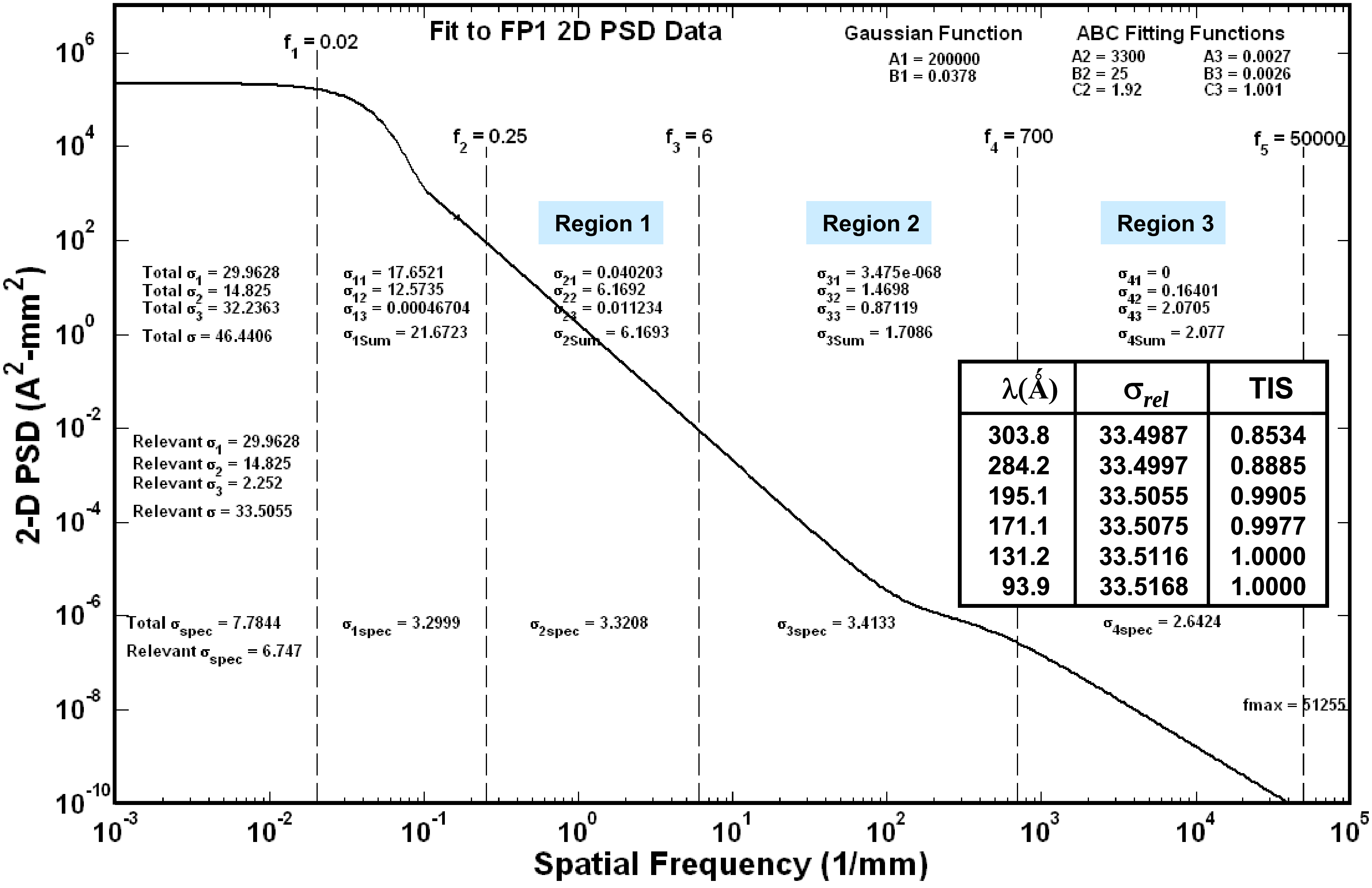
Sum of three Fitting Functions



FP1 2-D PSD Metrology Data

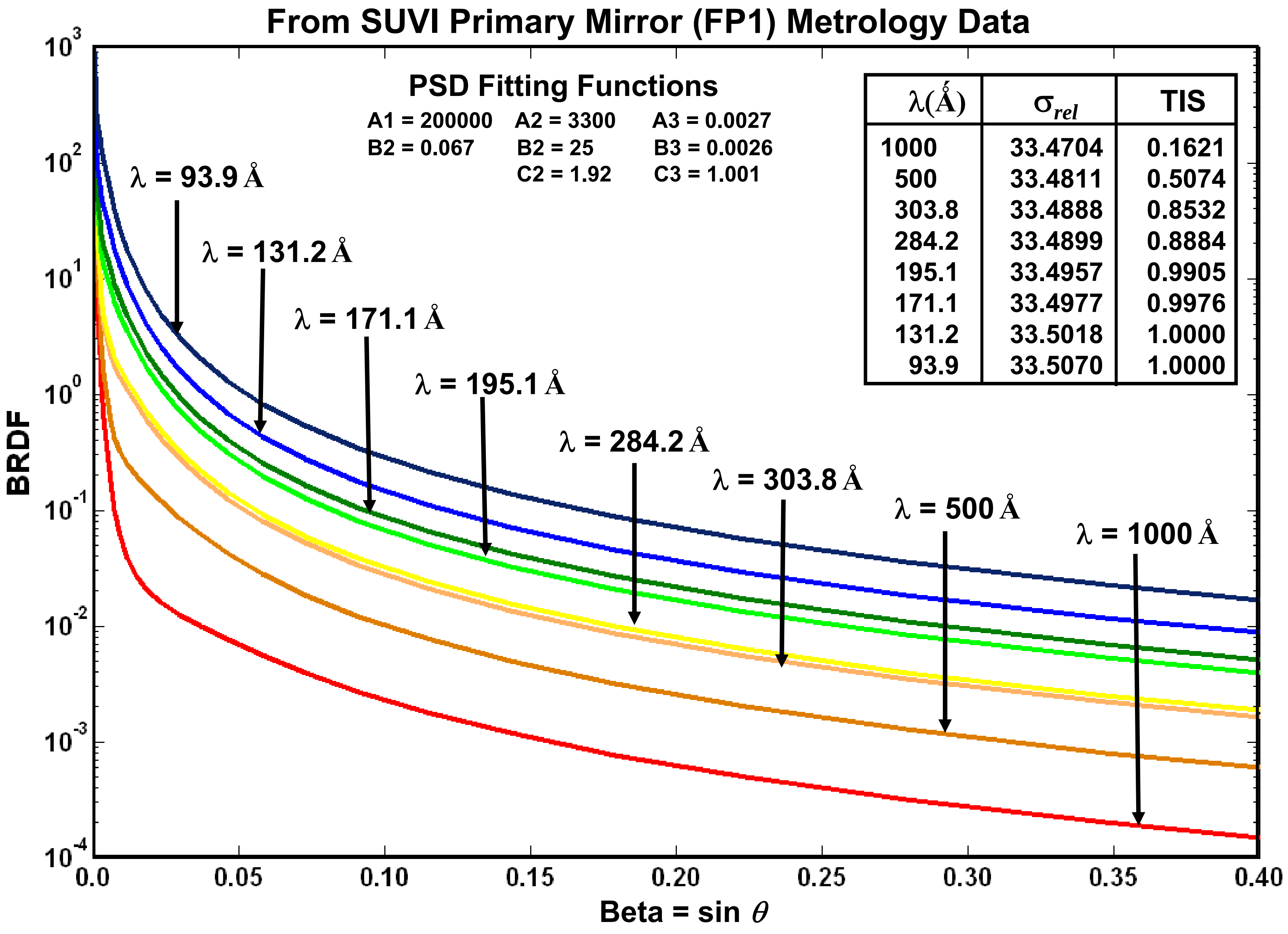
(With Band-limited Roughness Values)

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



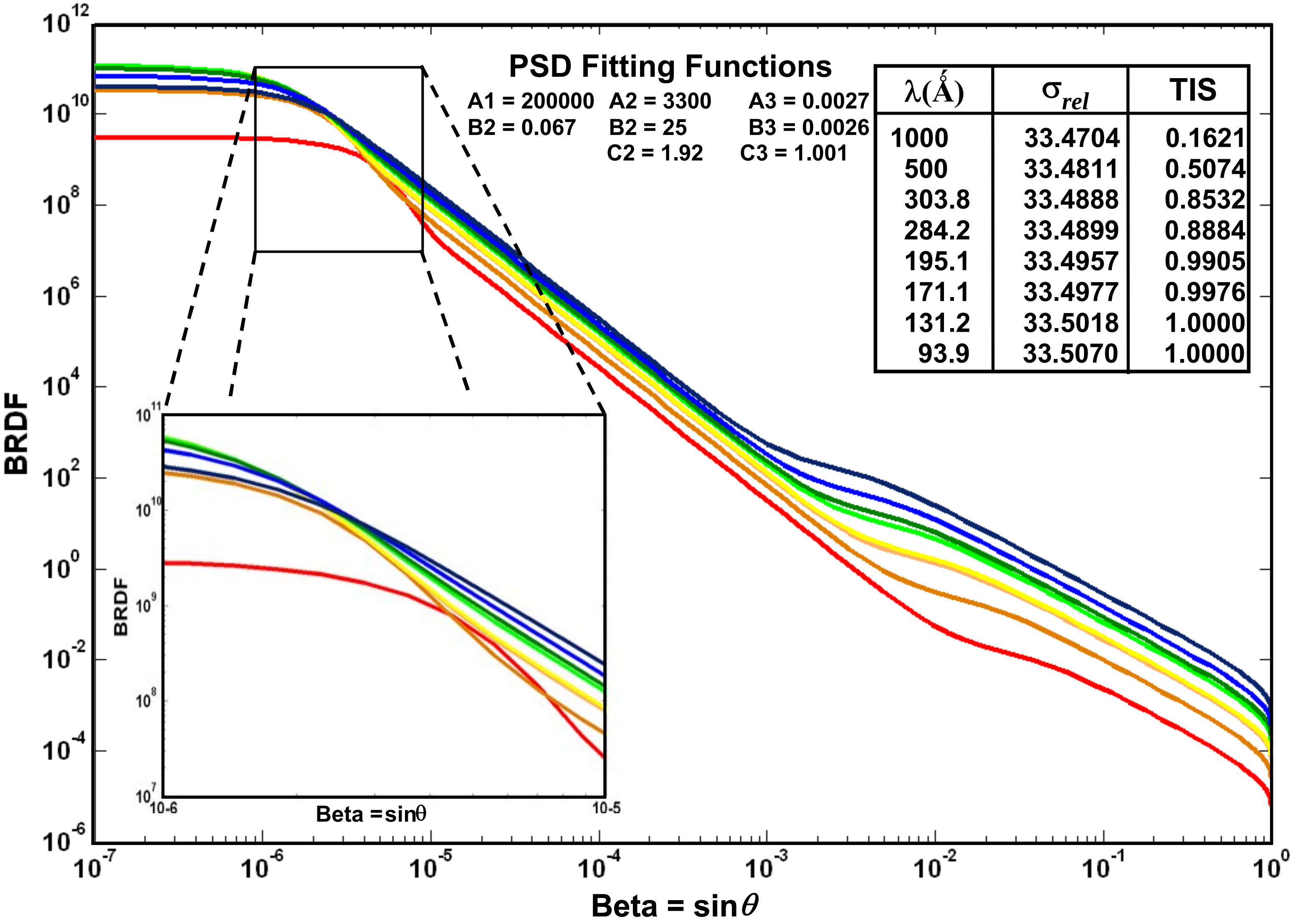
From SUVI Primary Mirror (FP1) Metrology Data

PSD Fitting Functions

A1 = 200000
B2 = 0.067
A2 = 3300
B2 = 25
C2 = 1.92
A3 = 0.0027
B3 = 0.0026
C3 = 1.001

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



PSD Fitting Functions

A1 = 200000 A2 = 3300 A3 = 0.0027
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λ(Å)	σ_{rel}	TIS
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Outline

- **Historical Review of Surface Scatter Theory.**
- **Statement of the EUV Imaging Problem (Summary of Results).**
- **Non-paraxial Scalar Diffraction Theory.**
  - **Scalar Treatment of Sinusoidal Phase Grating,**
  - **Modified Beckmann-Kirchhoff Surface Scatter Model.**
- **Total Integrated Scatter (TIS) for Moderately Rough Surfaces.**
- **Generalized Harvey-Shack (GHS) Scatter Theory.**
  - **Two-parameter Family of Surface Transfer Functions.**
  - **Very Computationally Intense Calculations.**
- **Example of Measured Metrology Data from an EUV Mirror.**
  - **Problem: Large dynamic Range of Relevant Spatial Frequencies.**
  - **Solution: FFTLog Numerical Hankel Transform Algorithm.**
- **BRDFs from Real Metrology Data from Moderately Rough Surfaces.**
  (that violate the smooth surface approximation).
- ➡ **Generalized Peterson Analytical Scattering Model.**
  - **Dealing with the “Scattered-Scattered” Light.**
  - **Numerical Validation with ASAP and ZEMAX.**
- **Results and Conclusions.**

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

$$\boxed{E_{sj}(r) = E_{ent}\,\pi(na)^2\,T\,\frac{s_{ent}^2}{s_j^2}\,BRDF\left((na)\frac{r}{s_j}\right)} \qquad (20)$$

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

$$E_s(r) = E_{ent}\,\pi\,(na)^2\;T\;s_{ent}^2\left[\frac{BRDF_P\big((na)\,r/s_p\big)}{s_p^2} + \frac{BRDF_s\big((na)\,r/s_s\big)}{s_s^2}\right] \qquad (21)$$

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

$$\boxed{\frac{E_s(r)}{P_T} = \left(\frac{1}{f'}\right)^2\left[BRDF_P\big(r/f'\big) + \left(\frac{s_p}{s_s}\right)^2 BRDF_s\big((s_p/s_s)(r/f')\big)\right]} \qquad (22)$$

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

Generalized Peterson Analytical Scattering Model

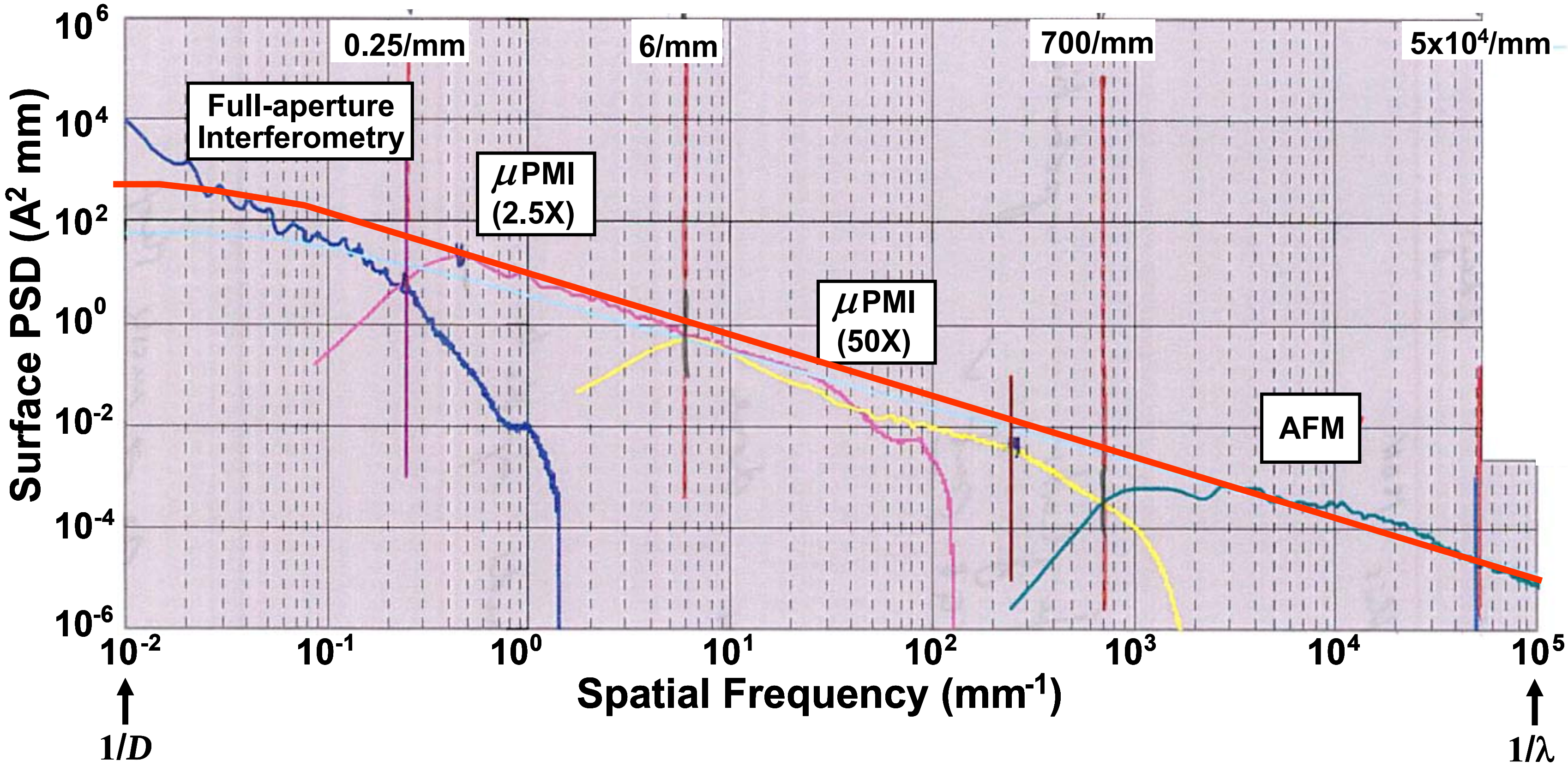
Since Peterson's elegant and insightful treatment is limited by both a *paraxial* and a *smooth-surface* assumption, it must be generalized to include scattering from moderately rough surfaces before applying to the NOAA Solar UV Imager (SUVI) Program. We have thus:

- 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

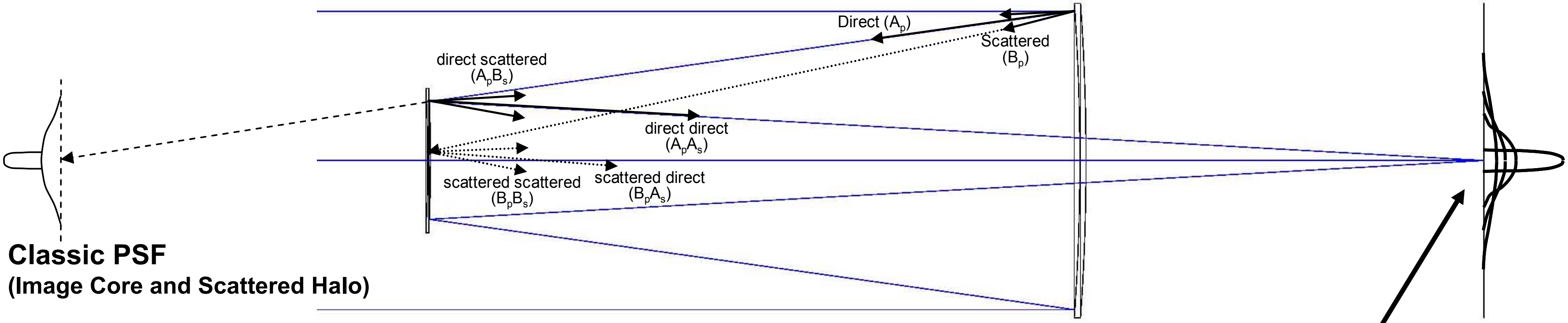
$$PSD(f_x)_{1-D} = \frac{A}{\left[1+(B\ f_x)^2\right]^{C/2}}$$

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.



Classic PSF
(Image Core and Scattered Halo)

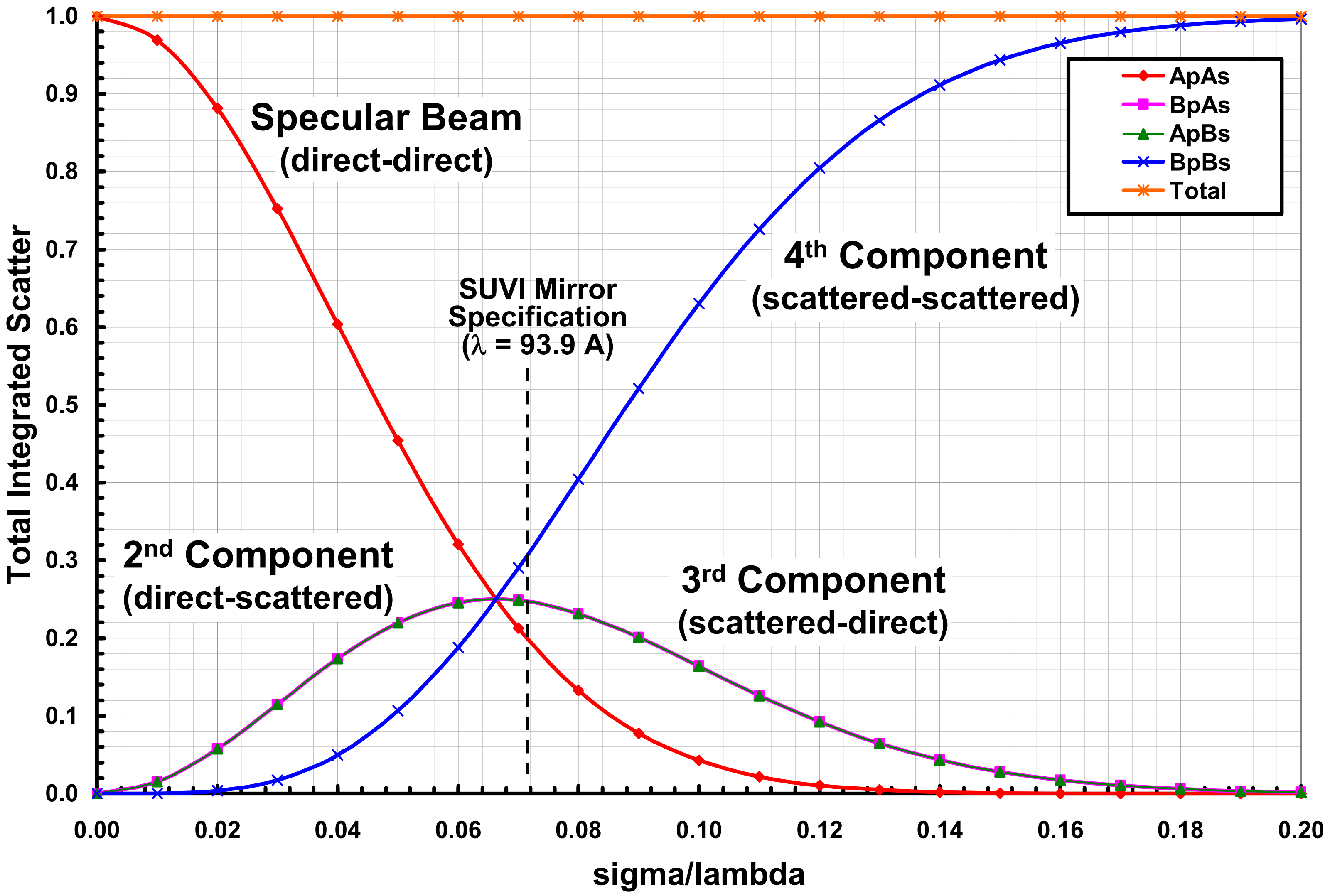
$$A = \exp\left[-(4\pi\sigma_{rel}/\lambda)^2\right] = \text{Fraction of total reflected energy in specular beam.}$$
$$B = TIS = 1 - A = \text{Fraction of total reflected energy in scattered halo.} \qquad (23)$$

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 $\sigma/\lambda > 0.066$, 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.(18) of Peterson's analytic treatment

$$\boxed{PSF = PSF_{dd} + PSF_{sd} + PSF_{ds} + PSF_{ss}} \tag{24}$$

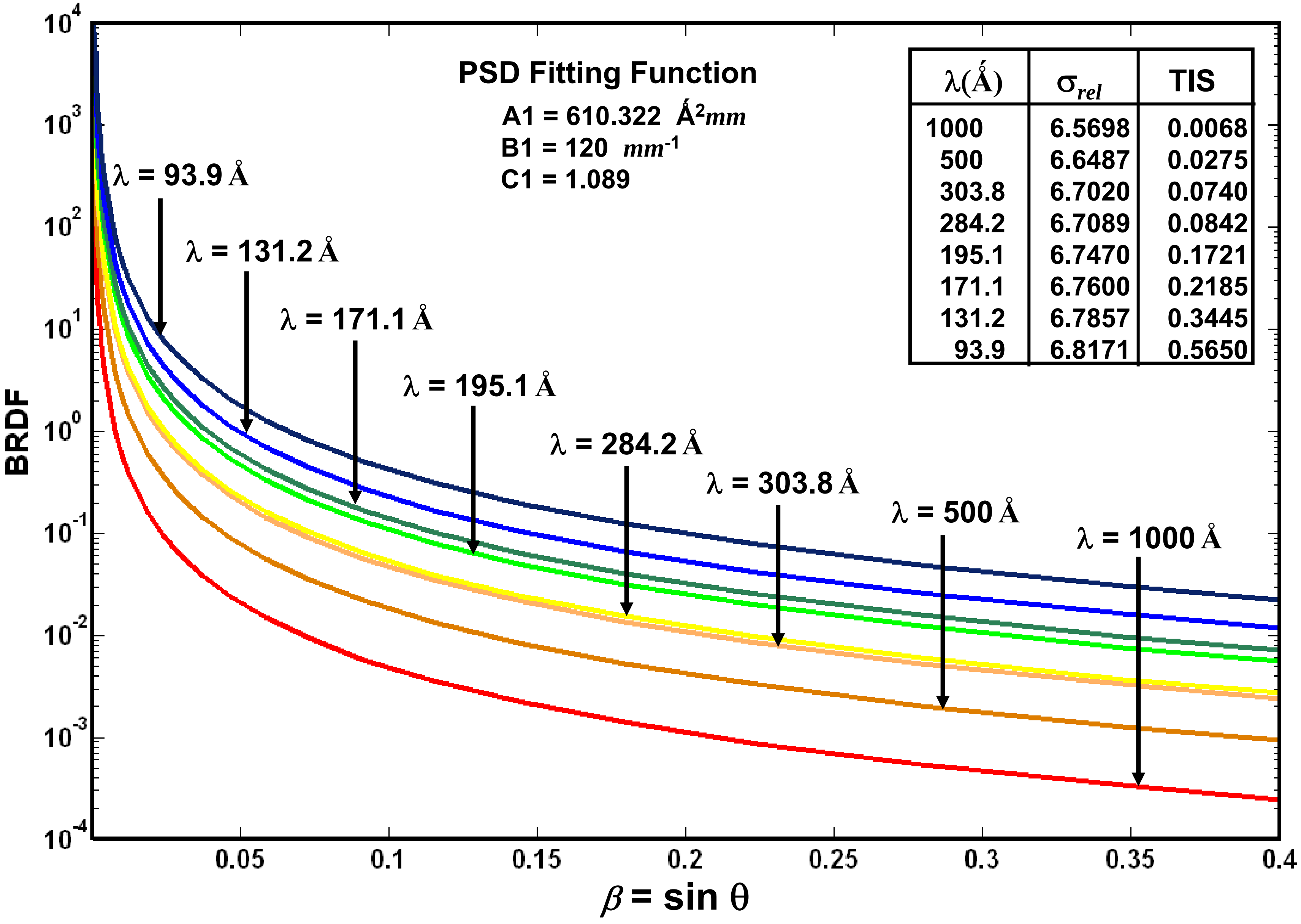
Care is taken to normalize each component such that their respective volumes (fractional total reflected radiant power) will be given by A_pA_s, B_pA_s, A_pB_s, and B_pB_s.

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

$$PSF_{dd}(r) = \frac{1}{\left(1-\varepsilon^2\right)^2}\left[\frac{2J_1(x)}{(x)} - \varepsilon^2\,\frac{2J_1(\varepsilon x)}{\varepsilon x}\right]^2 \quad \textbf{where} \quad x = \frac{\pi r}{\lambda f / D}. \tag{25}$$

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



PSD Fitting Function

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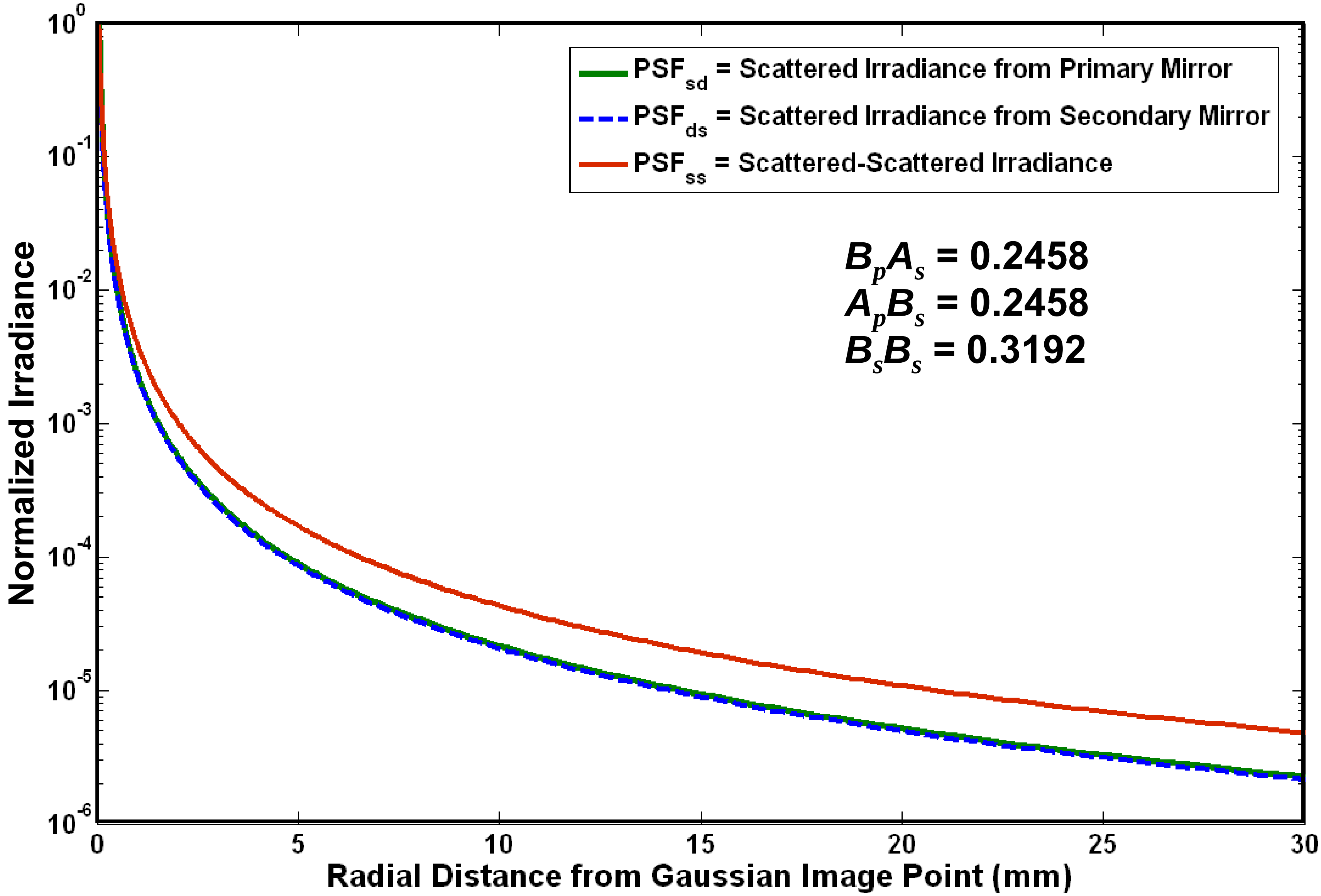
93.9	6.8171	0.5650

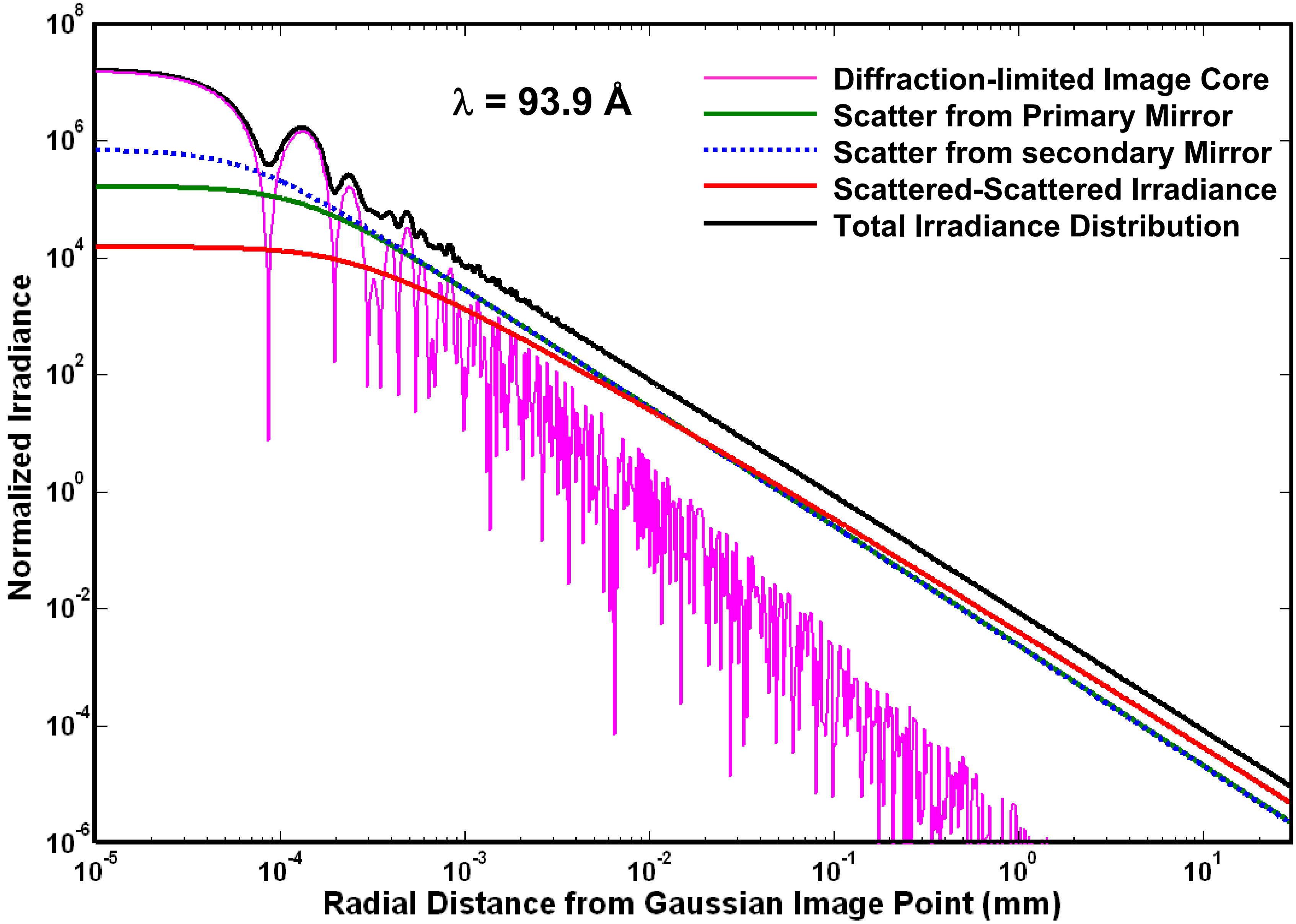
Scattered-Scattered Light Dominates

(λ = 93.9 A)



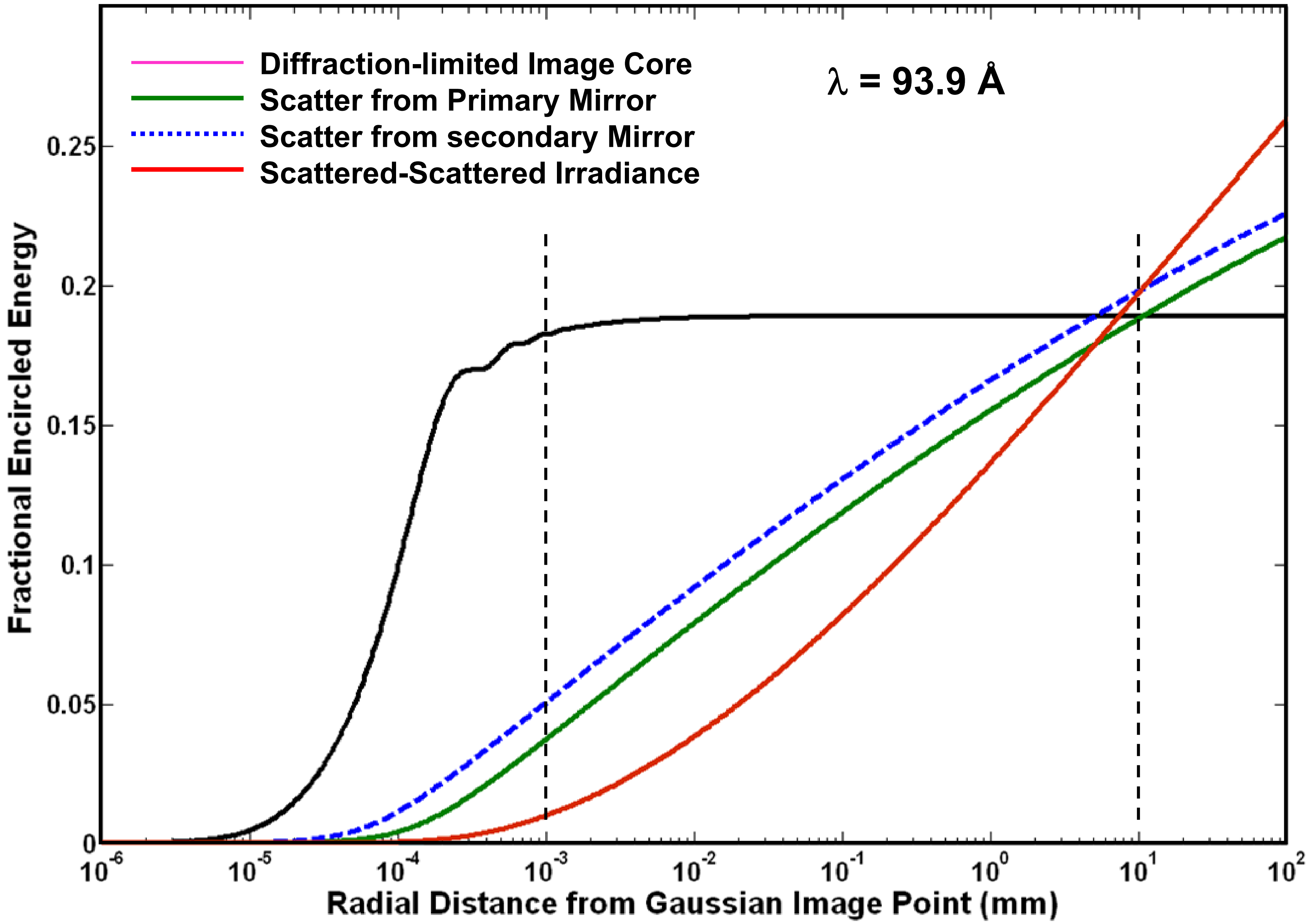
Radial Profiles of Four Components

(λ = 93 A)



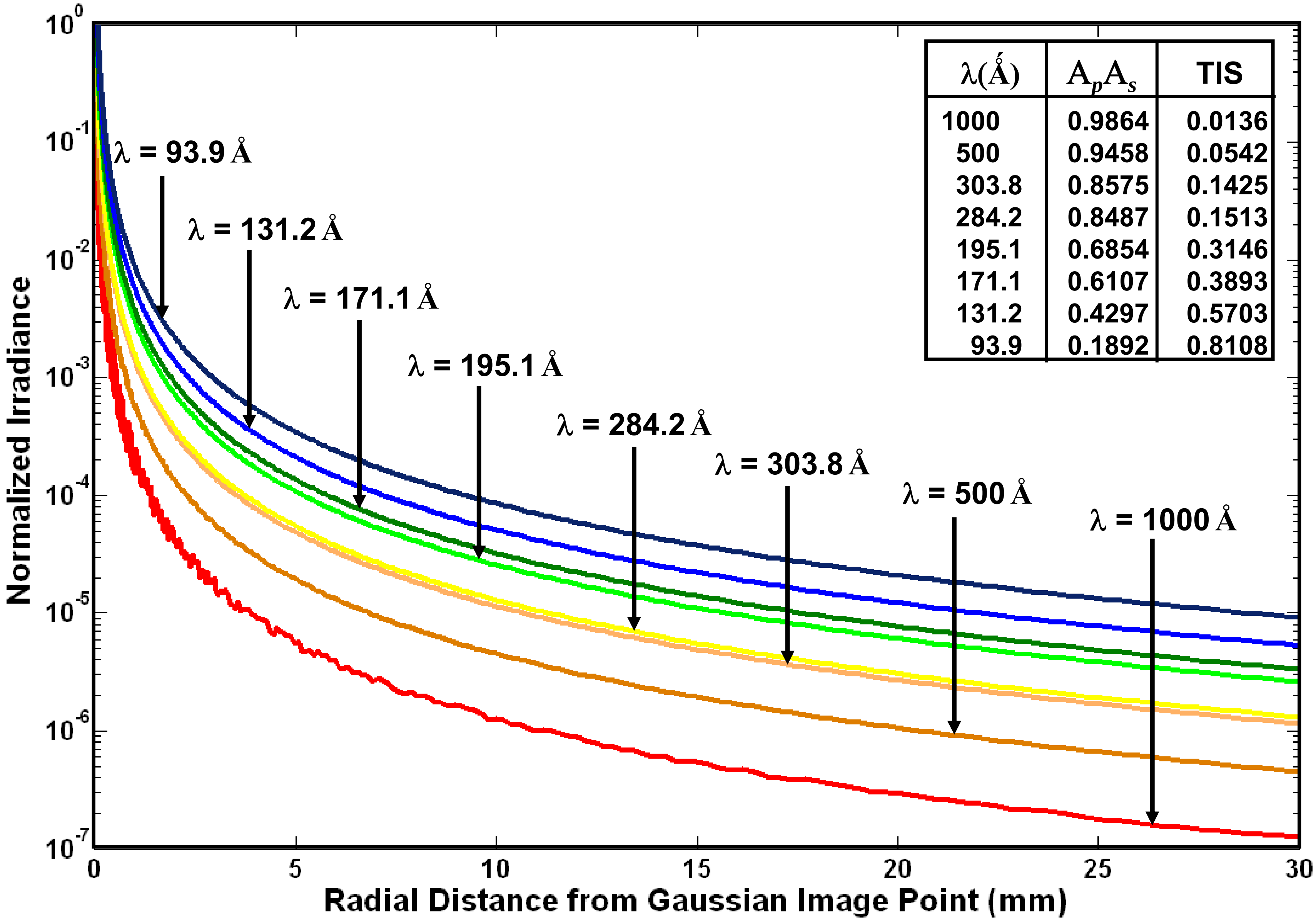
FEE Plots of the 4 Components of PSF

(λ = 93.9 A)



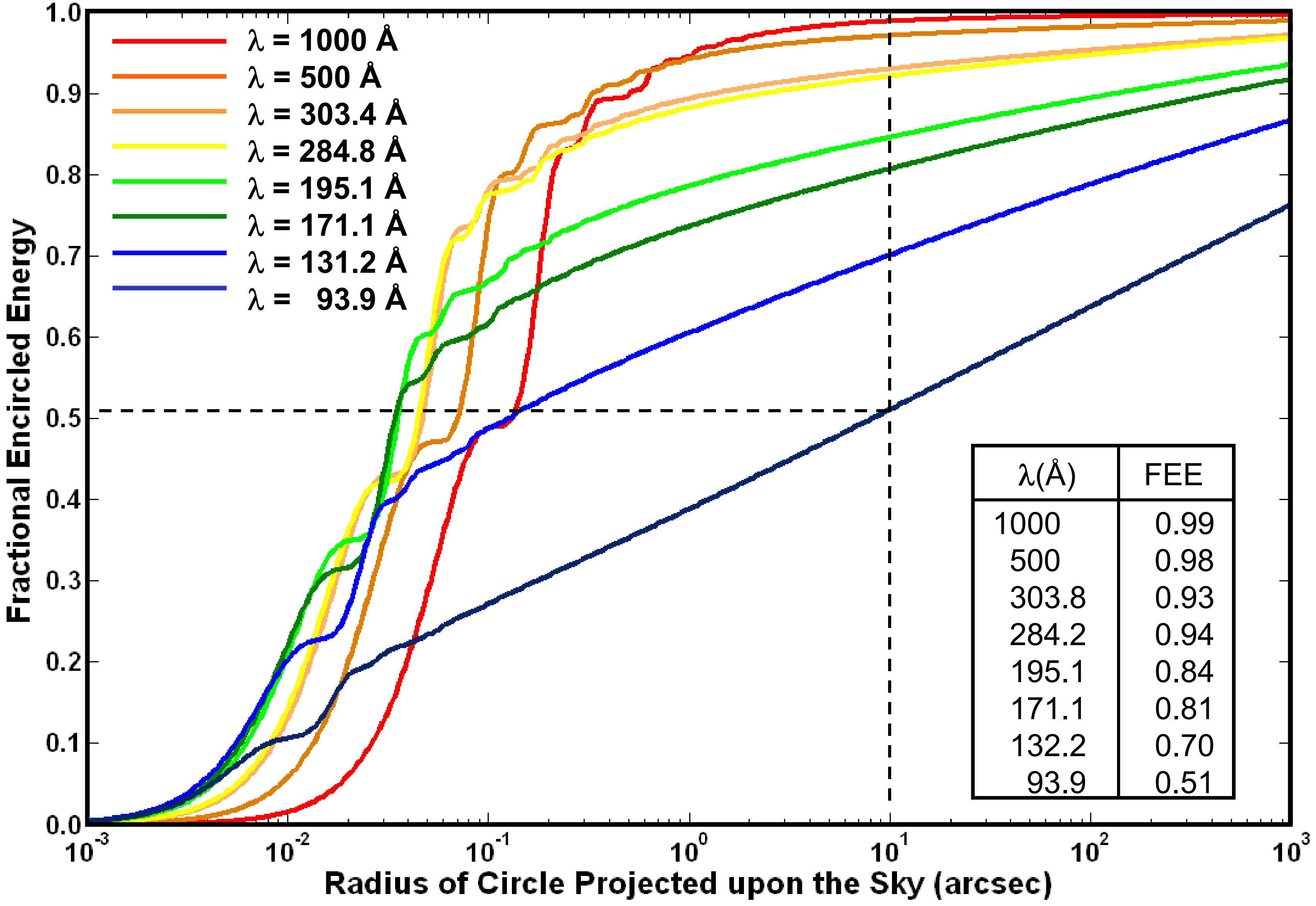
Irradiance Profile in Telescope Focal Plane

(Predicted by Generalized Peterson Model)



λ(Å)	A_pA_s	TIS
1000	0.9864	0.0136
500	0.9458	0.0542
303.8	0.8575	0.1425
284.2	0.8487	0.1513
195.1	0.6854	0.3146
171.1	0.6107	0.3893
131.2	0.4297	0.5703
93.9	0.1892	0.8108

FEE Plots of the Total PSF Projected onto Sky



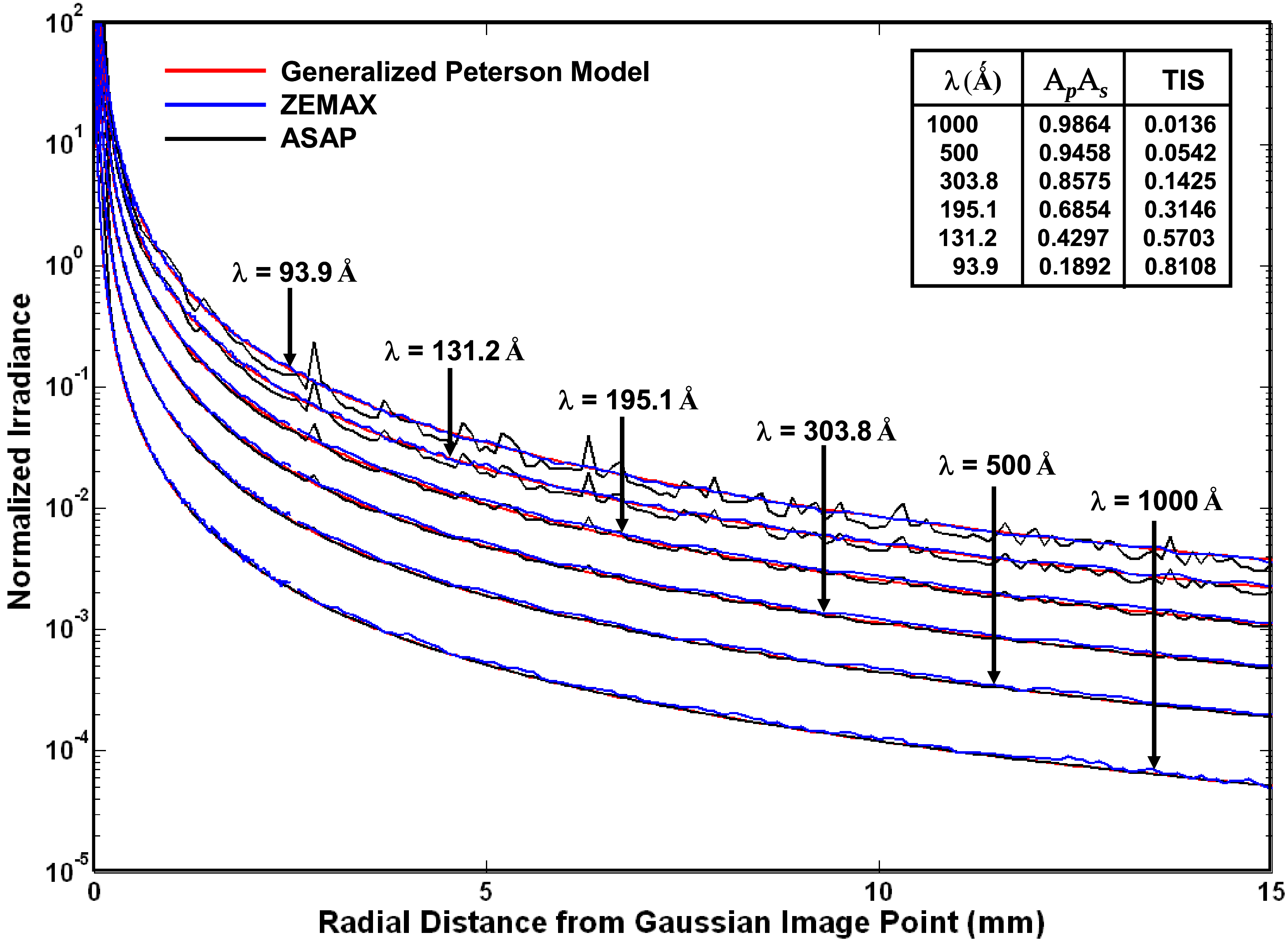
λ(Å)	FEE
1000	0.99
500	0.98
303.8	0.93
284.2	0.94
195.1	0.84
171.1	0.81
132.2	0.70
93.9	0.51

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*



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* 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)

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.