# Surface Roughness Scattering in Grazing-incidence X-ray Telescopes

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# Reflecting Surface: Smooth or Rough?

## 1 Rayleigh criterion (1877) for "smooth" surface

Reflected wavefront phase shift: $\Delta\phi < \pi/2$

$$\sigma < \frac{\lambda}{8\ sin\alpha} \tag{1}$$

$\sigma$ scale of the surface roughness
$\lambda$ wavelength
$\alpha$ grazing angle

## 2 Some examples of "smooth" surface

| Surface | $\lambda$ | $\alpha$ | $\sigma$ (Å) |
|---|---|---|---|
| Airport radar dish (∼3GHz) | ∼10 cm | ∼80° | < 1.3 cm |
| Satellite TV dish (∼10GHz) | ∼3 cm | ∼60° | < 4.3 mm |
| Mirror in your bath room | 5500Å | 90° | < 690Å |
| Chandra X-ray Observatory (0.1–10keV) | 1.24Å–124Å | 27.1′–51.3′ | < 10Å |

## 3 Chandra mirrors (HRMA) is polished according to this criterion

- HRMA surface: $\sigma_{Middle} \sim 1.95 - 3.58$Å — about the size of one Ir atom (r=1.35Å)!
- However, a scattering free mirror requires: $\Delta\phi < 0.1 \quad \rightarrow \quad \sigma << \frac{\lambda}{8\ sin\alpha}$
- Scattering from HRMA surface is not negligible.

# Random Rough Surface and Power Spectral Density

## 1 Random Rough Surface

## 2 Power Spectral Density

**Power Spectral Density of a 1-dimensional surface:**

$$PSD(f) \equiv 2W_1(f) = \frac{2}{L}\left|\int_{-L/2}^{L/2} e^{\imath 2\pi x f} h(x)dx\right|^2 \quad (2)$$

| | |
|---|---|
| $f$ | **surface spatial frequency** |
| $L$ | **surface length** |
| $x$ | **coordinate along the surface** |
| $z = h(x)$ | **surface height (i.e. deviation from a perfectly flat surface)** |

## 3 Surface Roughness Amplitude RMS

$$\sigma^2_{f_1-f_2} = \int_{f_1}^{f_2} 2W_1(f)df \quad (3)$$

## 4 Total Power $\sigma^2$

$$\sigma^2 = \int_0^{\infty} 2W_1(f)df \quad (4)$$

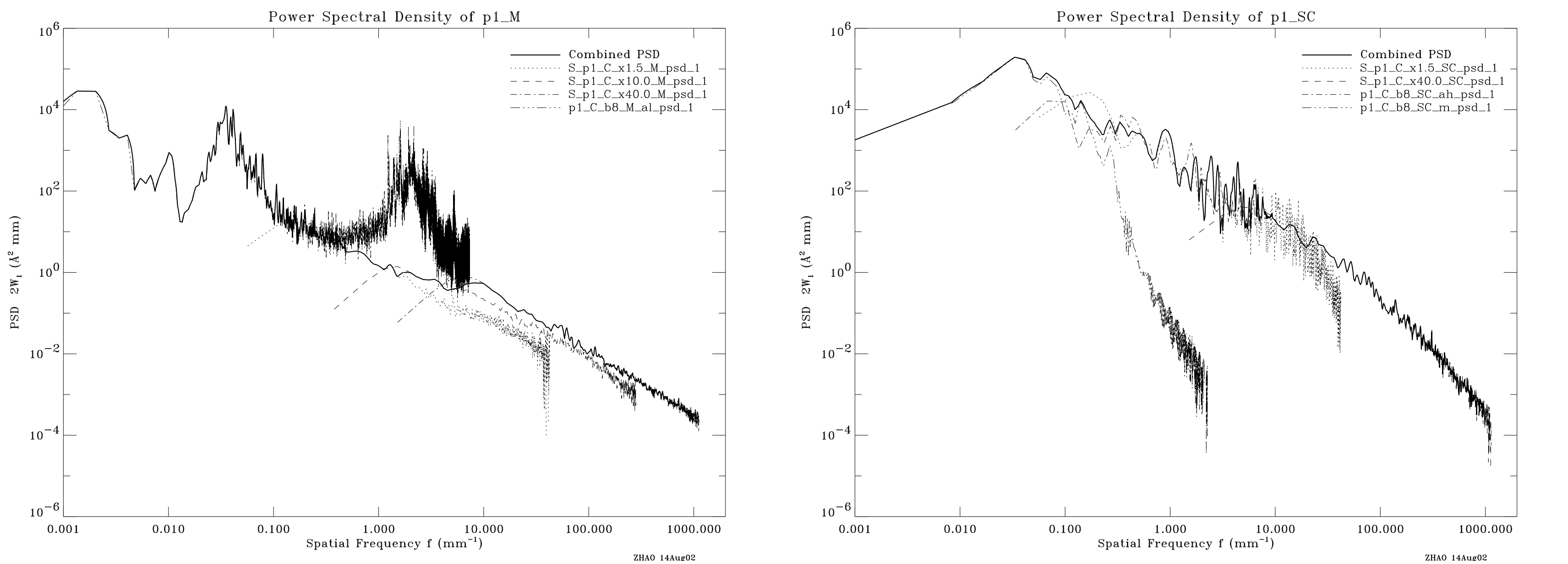
# Chandra X-ray optics – HRMA

- The HRMA surface roughness is based on the HDOS metrology measurements with the instruments of: Circularity and Inner Diameter Station (CIDS), Precision Metrology Station (PMS), and the Micro Phase Measuring Interferometer (MPMI, aka WYKO).
- The mirror surface roughness has little variation with azimuth, but tends to become worse near the mirror ends. So each mirror was divided into several axial sections based on the roughness. This resulted in a total of 61 sections as listed below.
- Surface PSD was derived for each section using the Fourier transform.

## HRMA Mirror Sections and Their Surface Roughness

| HRMA Mirror | Sections<br>Surface Roughness Amplitude RMS $\sigma_{1-1000/\mathrm{mm}}$ (Å) | | | | | | | | | | | Num of Sections |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| P1 | | LC | LB | LA | M (88%) | SA | SB | SC | | | | 7 |
| | | 50.3 | 8.49 | 4.51 | 3.58 | 4.91 | 5.94 | 53.9 | | | | |
| P3 | | | LB | LA | M (92%) | SA | SB | | | | | 5 |
| | | | 5.37 | 5.26 | 1.96 | 2.38 | 4.83 | | | | | |
| P4 | | | LB | LA | M (93%) | SA | SB | | | | | 5 |
| | | | 6.41 | 3.15 | 2.57 | 3.21 | 6.81 | | | | | |
| P6 | | | LB | LA | M (94%) | SA | SB | | | | | 5 |
| | | | 37.1 | 5.23 | 3.34 | 5.65 | 20.9 | | | | | |
| H1 | LD | LC | LB | LA | M (88%) | SA | SB | SC | SD | SE | SF | 11 |
| | 26.9 | 5.34 | 3.64 | 3.34 | 3.32 | 3.32 | 3.32 | 3.32 | 3.53 | 7.30 | 60.3 | |
| H3 | | LC | LB | LA | M (92%) | SA | SB | SC | SD | | | 8 |
| | | 4.87 | 2.90 | 2.23 | 2.08 | 2.08 | 2.10 | 3.95 | 5.56 | | | |
| H4 | LD | LC | LB | LA | M (93%) | SA | SB | SC | SD | SE | | 10 |
| | 7.18 | 3.83 | 2.61 | 2.57 | 2.36 | 2.36 | 2.74 | 2.68 | 4.01 | 29.4 | | |
| H6 | LD | LC | LB | LA | M (94%) | SA | SB | SC | SD | SE | | 10 |
| | 19.0 | 4.92 | 2.51 | 2.23 | 1.95 | 1.95 | 1.95 | 2.07 | 2.96 | 15.9 | | |
| Total | | | | | | | | | | | | 61 |

# PSD of Chandra X-ray optics




**Surface PSD of Chandra mirror P1-M, the middle section of mirror P1 (left); and P1-SC, the small end section of mirror P1 (right). P1 and H1 were the first polished mirror pair and are slightly "rougher" than other pairs (see Table). The dash and dotted lines show the data from four different measurements. The solid line is the combined PSD from all four frequency ranges. The SC section obviously is much rougher than the M section, with higher PSD value for given frequency band.**

# Construction of Model Surfaces

**For a given PSD, a model surface can be constructed as $N$ consecutive surface height values $h_i = h(x_i)$ with a fixed interval $\Delta x$ to cover the surface (i.e. $N\Delta x = L$), and its surface tangent values $h'_i = h'(x_i)$, using the discrete Fourier transforms:**

$$h_i = \frac{1}{N} \sum_{j=-(N/2-1)}^{N/2} H_j \, e^{-\imath \frac{2\pi ij}{N}} \tag{5}$$

$$h'_i = \frac{-\imath 2\pi}{N} \sum_{j=-(N/2-1)}^{N/2} f_j \, H_j \, e^{-\imath \frac{2\pi ij}{N}} \tag{6}$$

**where**

$$H_j = N \sqrt{\frac{PSD(f_j)\ \Delta f}{2}} \; e^{\imath \varphi_j} \tag{7}$$

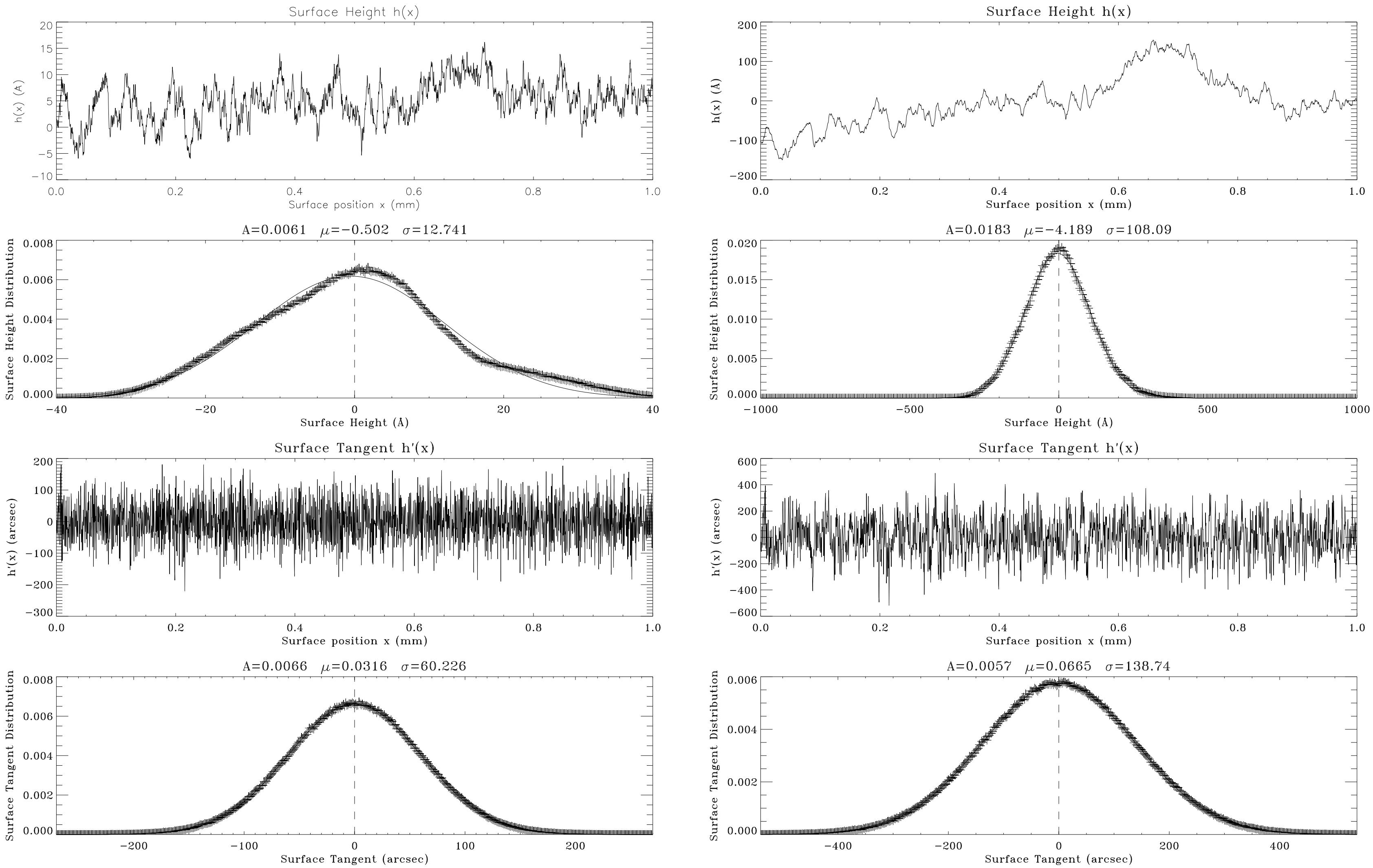
$\Delta f = 1/N\Delta x$**; and** $\varphi_j$ **is a random phase factor.**

**Both** $h_i$ **and** $h'_i$ **are real, this requires** $H_{-j} = H_j^*$**, i.e.** $PSD(f_{-j}) = PSD(f_j)$ **and** $\varphi_{-j} = -\varphi_j$**.**

**To construct the model surfaces of HRMA, we choose:**

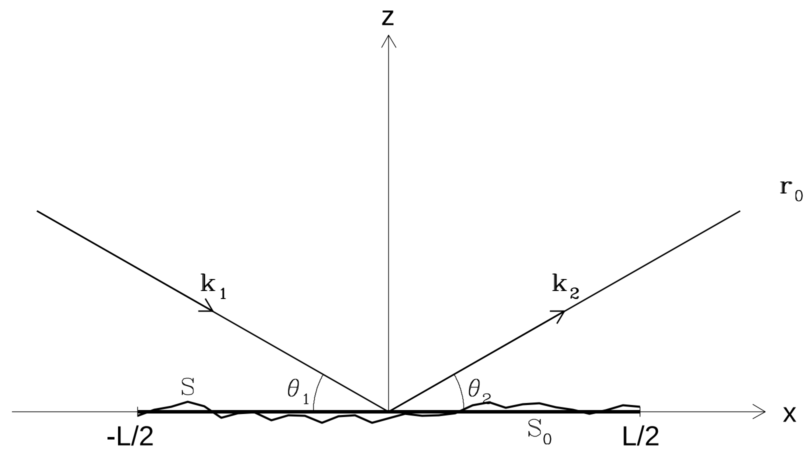
$N = 2^{21}$
$\Delta x = 0.0004$ **mm**
$L = N\Delta x = 838.86$ **mm**
$\Delta f = 1/N\Delta x = 0.001192$ **mm**$^{-1}$

# Constructed Model Surface Height and Surface Tangent




**Model surfaces of Chandra mirror section P1-M (left) and P1-SC (right).**

## Kirchhoff Integral of Scattering




# 1 Definition:

- $S_0$ — **2-dimensional flat surface at** $z = 0$.
- $S$ — **2-dimensional rough surface at** $z = h(x, y)$.
- $\mathbf{E}_1 e^{\imath \mathbf{k_1} \cdot \mathbf{r}} \;=\; \mathbf{E}_1 e^{\imath (k_1 x + k_3 z)}$ — **incident plane wave.**
- $\mathbf{E}_2 e^{\imath \mathbf{k_2} \cdot \mathbf{r}} \;=\; \mathbf{E}_2 e^{\imath (k_x x + k_y y + k_z z)}$ — **reflected or scattered wave.**
- $\theta_1$, $\theta_2$ — **incident and reflecting grazing angles.**

# 2 Kirchhoff Integral:

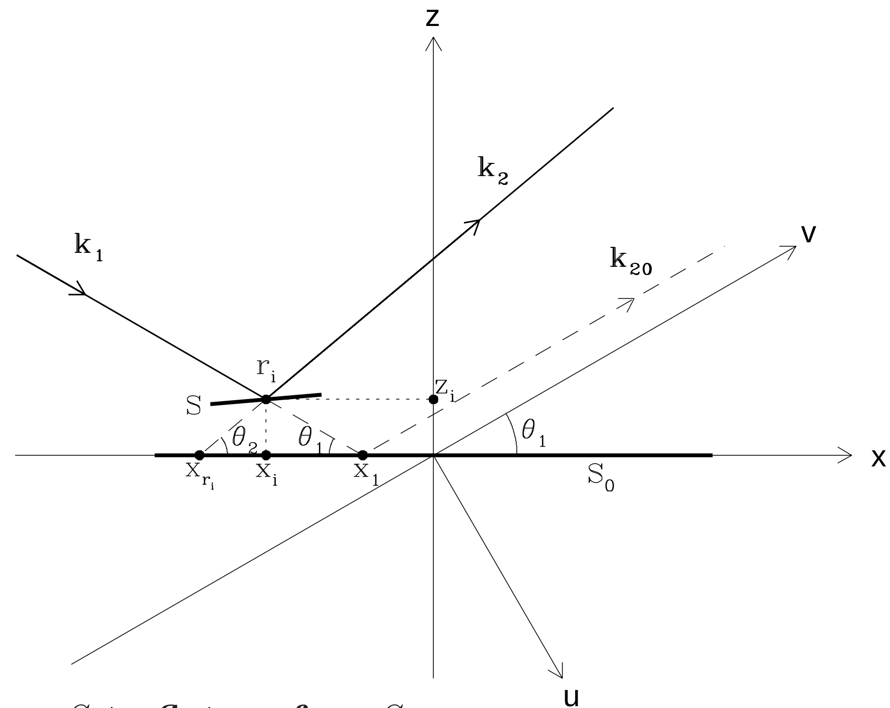
$$\mathbf{E}(\mathbf{r}_0) \;=\; \frac{1}{\imath\lambda} \int_S \int ds\, \mathbf{E}(s) e^{\imath(k_1 x + k_3 z)} \frac{e^{\imath k r}}{r^2} \left(\hat{\mathbf{n}} \cdot \mathbf{r}\right) \tag{8}$$

# 3 Far-field Approximation ($x << x_0$, $y << y_0$, $z << z_0$)

$$\mathbf{E}(\mathbf{r}_0) \;\approx\; \frac{\imath e^{\imath k r_0}}{2\pi r_0} \iint dxdy\, \mathbf{E}(s) e^{\imath[(k_1 - k_x)x - k_y y + (k_3 - k_z) h(x,y)]} \left[ k_x \frac{\partial h(x,y)}{\partial x} + k_y \frac{\partial h(x,y)}{\partial y} - k_z \right] \tag{9}$$

# Scattering from 1-D Surface

**For grazing incidence, in-plane (of incident) scattering dominates. So let's first consider the Kirchhoff solution in a 1-D surface, i.e. $h(x, y) = h(x)$ and $k_y = 0$. Out-of-plane scattering is reduced by a factor of $sin\,\theta_1$, which we will consider later.**




**Transfer the integral from the rough surface $S$ to flat surface $S_0$:**

$$\mathbf{E}(\mathbf{r}_0) = -\frac{\imath k_z e^{\imath k r_0}}{2\pi} \int dx\, \mathbf{E}(x)\; e^{\imath(k_1-k_x)x} = -\frac{\imath e^{\imath k r_0} sin(\theta_1-\theta)}{\lambda} \int dx\, \mathbf{E}(x)\, e^{\imath 2\pi\xi x} = \mathbf{E}(\xi(\theta)) \quad (10)$$

**where $\theta$ $(= \theta_1 - \theta_2)$ is the scattering angle, and define a new variable $\xi$ as a function of $\theta$:**

$$\xi \equiv \frac{k_1-k_x}{2\pi} = \frac{k\,cos\,\theta_1 - k\,cos\,(\theta_1-\theta)}{2\pi} = -\frac{k}{\pi}\; sin(\theta_1-\frac{\theta}{2})\; sin\,\frac{\theta}{2} \quad (11)$$

$$\theta = \theta_1 - cos^{-1}\left(cos\,\theta_1 - \frac{2\pi\xi}{k}\right) = \theta_1 - cos^{-1}\,(cos\,\theta_1 - \xi\lambda) \quad (12)$$

**Field $\mathbf{E}(x)$ on non-uniform grid $(x_{r_i})$ on surface $S_0$:**

$$\mathbf{E}(x_{r_i}) = \mathbf{E}(r_i)\, e^{\imath\,\phi_i} \quad ; \quad x_{r_i} = x_i - \frac{h_i}{tan\,\theta_2} \quad ; \quad \phi_i = -2\,k\,h_i\,\frac{sin^2\frac{\theta_1+\theta_2}{2}}{sin\,\theta_2} \quad (13)$$

## Scattering Formulae

# 1 Exact solution of the 1-D scattering equation

$$\mathbf{E}(\mathbf{r}_0) \;=\; \mathbf{E}(\xi(\theta)) \;=\; -\frac{\imath e^{\imath k r_0} sin(\theta_1-\theta)}{\lambda}\int dx\,\mathbf{E}(x)\,e^{\imath 2\pi\xi x} \tag{14}$$

# 2 Redistribute field $\mathbf{E}(x_{r_i})$ onto uniform grid $x_i$

$$\mathbf{E}_i \;\equiv\; \mathbf{E}(x_i) \;=\; A_i\,B_i\,\mathbf{E}(x_{r_i}) \;=\; A_i\,B_i\,\mathbf{E}(r_i)\,e^{\imath\phi_i} \;=\; A_i\,B_i\,\mathbf{E}_1\,R(\theta_1+tan^{-1}(h_i'))\,e^{\imath\phi_i} \tag{15}$$

**where:** $A_i$ **is the beam uniform mapping factor for the incident wave density;**

$B_i$ **is the beam uniform maping factor for the outgoing wave density;**

$R(\theta_1+tan^{-1}(h_i'))$ **is the reflection coefficient with the local grazing angle at** $r_i$**;**

$\phi_i$ **is the phase delay between** $x_{r_i}$ **and** $r_i$**.**

# 3 Fourier mapping into $\xi$ space (let $\Delta x\Delta\xi = 1/N$)

$$\mathbf{E}_j \;\equiv\; \frac{\mathbf{E}(\xi_j)}{\Delta x} \;=\; -\frac{\imath e^{\imath k r_0} sin(\theta_1-\theta_j)}{\lambda}\sum_{i=-(N/2-1)}^{N/2}\mathbf{E}_i\;e^{\imath\frac{2\pi ij}{N}} \tag{16}$$

# 4 Scattering intensity

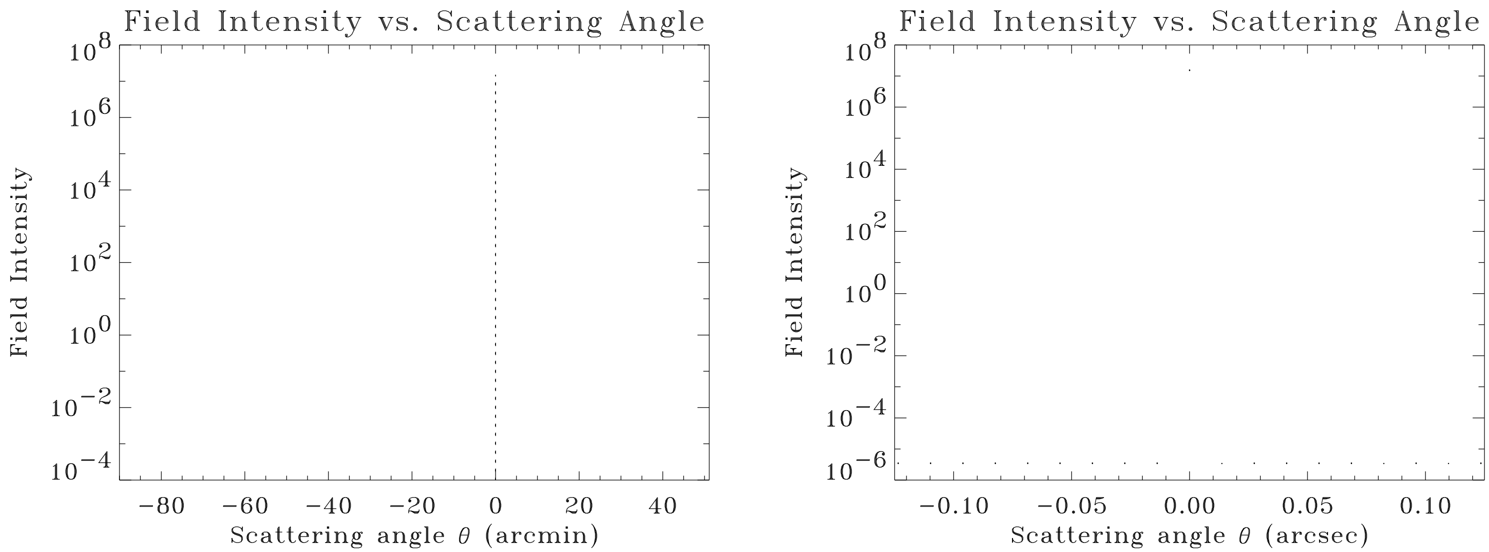
$$I(\theta_j) \;=\; I(\xi(\theta_j)) \equiv \mathcal{A}\,\mathbf{E}(\xi_j)\mathbf{E}^*(\xi_j) \;=\; \mathcal{A}\left(\frac{\Delta x\,sin(\theta_1-\theta_j)}{\lambda}\right)^2\left|\sum_{i=-(N/2-1)}^{N/2}\mathbf{E}_i\;e^{\imath\frac{2\pi ij}{N}}\right|^2 \tag{17}$$

**where** $\mathcal{A}$ **is a normalization factor.**

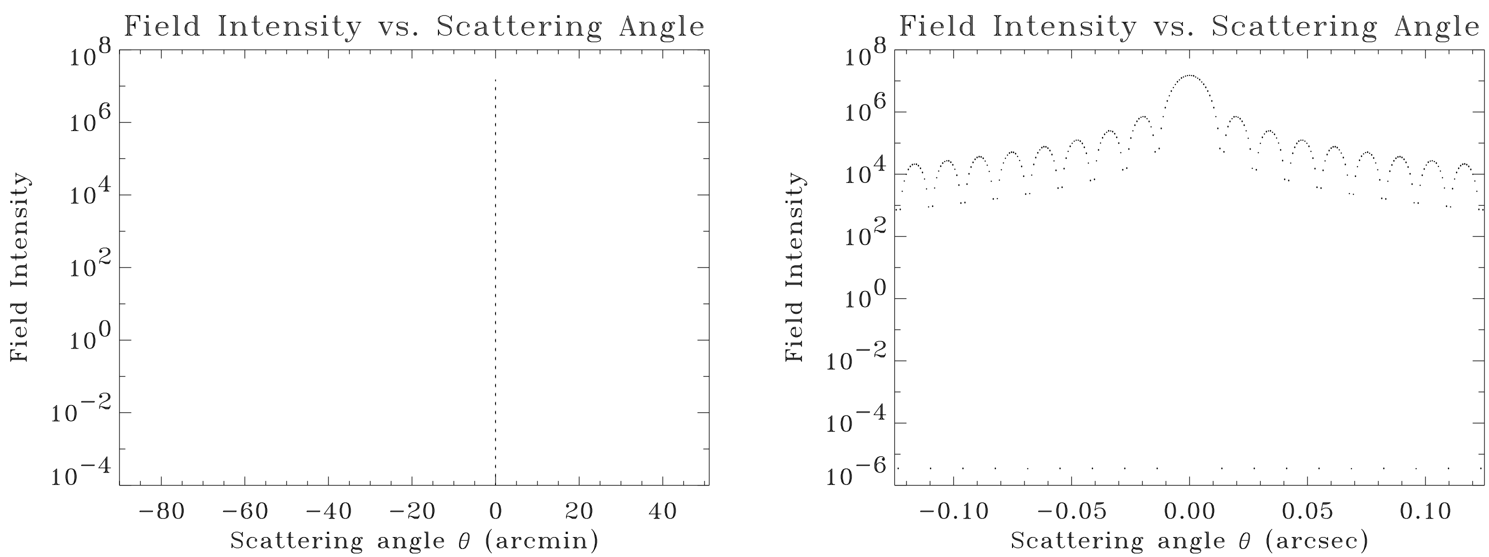
**Now we are finally done! Just plug everything into the above equation to get your beautiful scattering profile from the rough surface. Right?**

**Well, not quite ... WHY?**

# Scattering from Flat Surface




**The scattering of 1.49 keV X-rays at 51.26′ grazing incident angle from a perfectly flat surface, using Eq. (17). All the points except the central peak ($\theta_j = 0$) are calculated in the valleys of the Fraunhofer diffraction pattern.**




**The scattering of 1.49 keV X-rays at 51.26′ grazing incident angle from a perfectly flat surface, using Eq. (18) with $p = 16$. The scattering model produces the Fraunhofer diffraction pattern due to the finite mirror length.**

# Scattering Formulae (continue)

## 5 Scattering formula

To obtain the diffraction patterns at angles between $\theta_j$ and $\theta_{j+1}$, we divide $\theta_{j+1} - \theta_j$ into $p$ equal spaces. The diffraction pattern at $\theta_{j+q/p}(q < p)$ can be calculated as:

$$I(\theta_{j+q/p}) \;=\; \mathcal{A} \left( \frac{\Delta x \, sin(\theta_1 - \theta_{j+q/p})}{\lambda} \right)^2 \left| \sum_{i=-(N/2-1)}^{N/2} \left( \mathbf{E}_i e^{\imath \frac{2\pi i q/p}{N}} \right) \; e^{\imath \frac{2\pi i j}{N}} \right|^2 \tag{18}$$

where $q = 0, 1, 2, \ldots, p-1$. So we need to perform $p$ Fourier transforms instead one.

## 6 Normalization

Let $\varepsilon$ be the energy carried by each of the $N$ incident rays of the plane wave $\mathbf{E}_1$.

$$\textbf{Total incident energy}: \; \mathcal{E}_i \;=\; N\varepsilon \tag{19}$$

$$\textbf{Total reflected energy on } S_0: \; \mathcal{E}_r \;=\; \sum_{i=-(N/2-1)}^{N/2} |\mathbf{E}_i|^2 = \varepsilon \sum_{i=-(N/2-1)}^{N/2} A_i^2 \, B_i^2 \, \left| R(\theta_1 + tan^{-1}(h_i')) \right|^2 \tag{20}$$

$$\textbf{Total scattered energy from } S_0: \; \mathcal{E}_s \;=\; \int d\theta \, I(\theta) \;=\; \mathcal{A} \int d\xi \, |\mathbf{E}(\xi)|^2 \tag{21}$$

$$\textbf{Rough surface reflectivity}: \; \mathcal{R} \;\equiv\; \frac{\mathcal{E}_r}{\mathcal{E}_i} \;=\; \frac{1}{N} \sum_{i=-(N/2-1)}^{N/2} A_i^2 \, B_i^2 \, \left| R(\theta_1 + tan^{-1}(h_i')) \right|^2 \tag{22}$$

Let $\mathcal{E}_r = \mathcal{E}_s$. We obtain the normalization factor:

$$\mathcal{A} \;=\; \frac{\varepsilon \sum_{i=-(N/2-1)}^{N/2} A_i^2 \, B_i^2 \, \left| R(\theta_1 + tan^{-1}(h_i')) \right|^2}{\int d\xi \, |\mathbf{E}(\xi)|^2} \;=\; \frac{\varepsilon N \mathcal{R}}{\int d\xi \, |\mathbf{E}(\xi)|^2} \;=\; \frac{\mathcal{E}_i \mathcal{R}}{\int d\xi \, |\mathbf{E}(\xi)|^2} \tag{23}$$

# Scattering Formulae (continue)

## 7 Encircled Energies

$$\textbf{Forward scattering:} \quad EE_+(\vartheta) \equiv \frac{1}{\mathcal{E}_s}\int_0^{\vartheta} I(\theta)\,d\theta = \frac{1}{\mathcal{R}\,\mathcal{E}_i}\int_0^{\vartheta} I(\theta)\,d\theta \tag{24}$$

$$\textbf{Backward scattering:} \quad EE_-(\vartheta) \equiv \frac{1}{\mathcal{E}_s}\int_{-\vartheta}^{0} I(\theta)\,d\theta = \frac{1}{\mathcal{R}\,\mathcal{E}_i}\int_{-\vartheta}^{0} I(\theta)\,d\theta \tag{25}$$

$$\textbf{Total scattering:} \quad EE(\vartheta) \equiv \frac{1}{\mathcal{E}_s}\int_{-\vartheta}^{\vartheta} I(\theta)\,d\theta = \frac{1}{\mathcal{R}\,\mathcal{E}_i}\int_{-\vartheta}^{\vartheta} I(\theta)\,d\theta \tag{26}$$

## 8 Scattering function

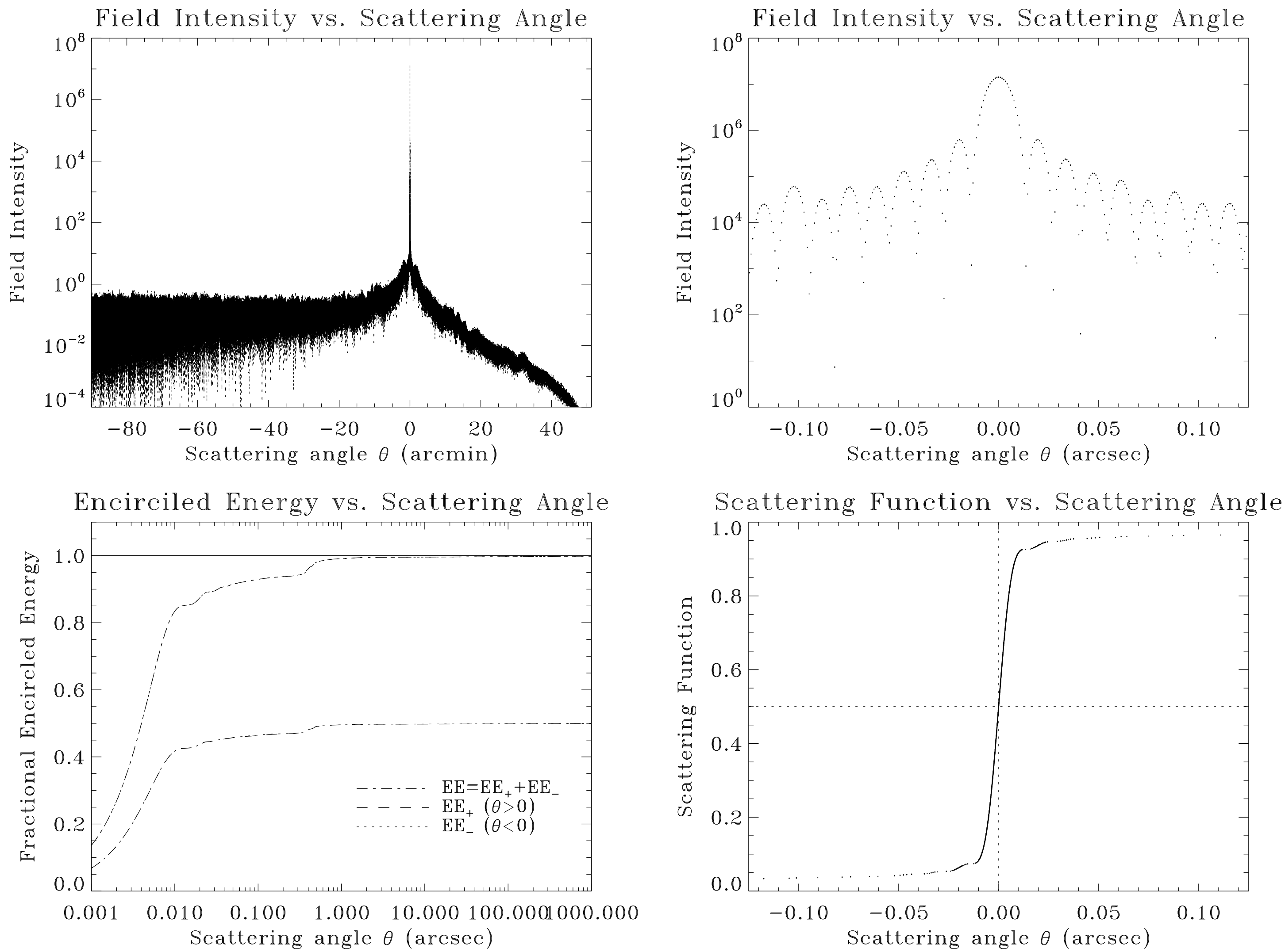
$$\mathcal{S}(\vartheta) \equiv \frac{1}{\mathcal{E}_s}\int_{-\infty}^{\vartheta} I(\theta)\,d\theta = \frac{1}{\mathcal{R}\,\mathcal{E}_i}\int_{-\infty}^{\vartheta} I(\theta)\,d\theta \qquad (0 \le S(\vartheta) \le 1) \tag{27}$$

**A scattering table can be generated using the scattering function and to be used for raytrace simulation.**

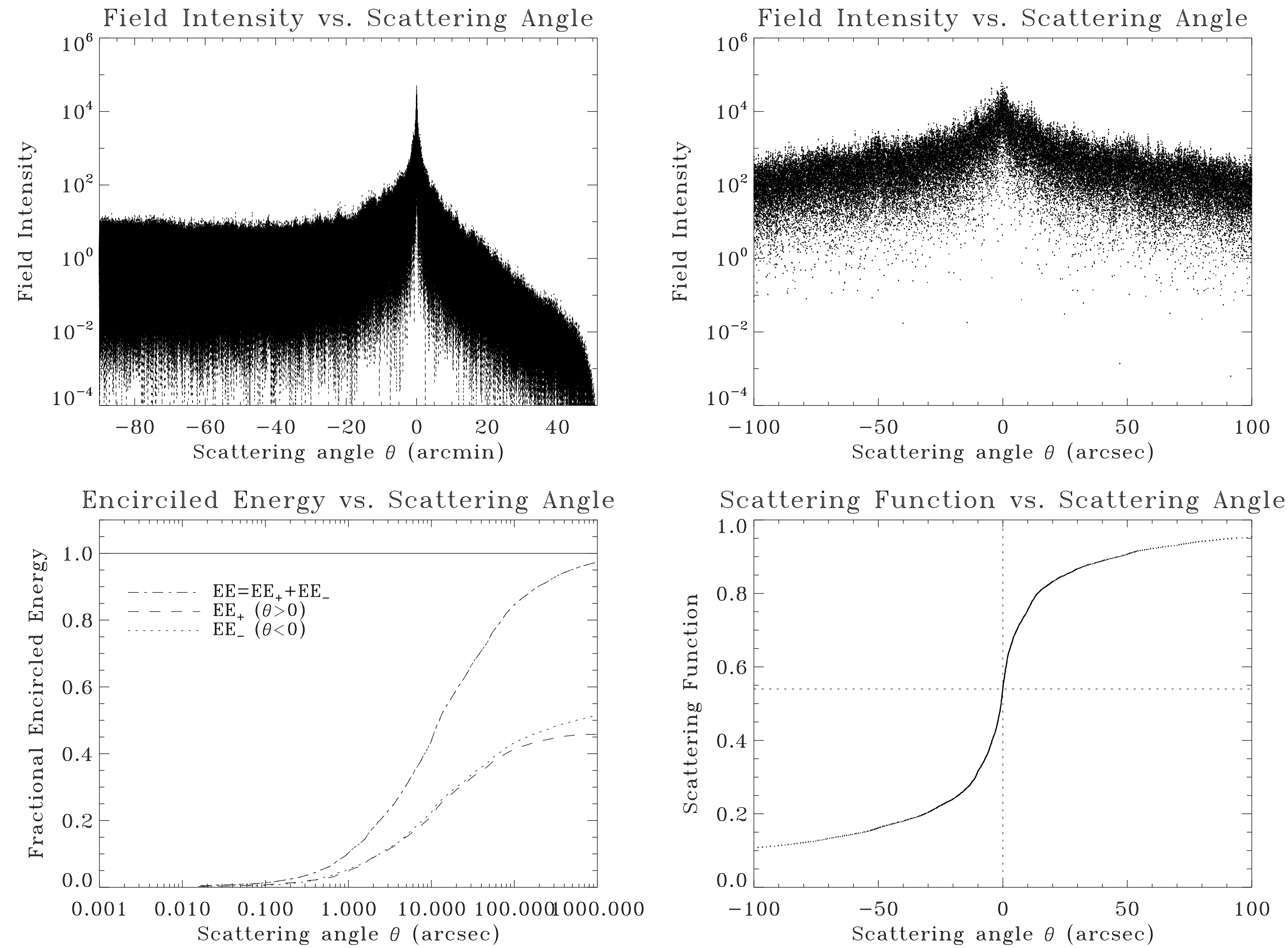
$$\vartheta = \vartheta(P) \qquad where \quad P \in [0,1] \tag{28}$$

## 9 Out-of-plane Scattering

$$\varphi = \sin\theta_1 \frac{|\vartheta(P')| + |\vartheta(1-P')|}{2} \qquad where \quad P' \in [0,1] \tag{29}$$




**The scattering of 1.49 keV X-rays at 51.26′ grazing incident angle from the model surface P1-M. The top-left panel shows the scattering field intensity verses the scattering angle. The very sharp peak is at the specular reflection direction $\theta = 0$. The asymmetric nature of the scattering is clearly shown. The top-right panel is the same plot but zoomed into the core of the peak; it shows the Fraunhofer diffraction pattern due to the finite mirror length. The bottom-left panel shows the fractional Encircled Energy (EE) verses the scattering angle, for both sides of the specular direction, and also their sum. The bottom-right panel shows the scattering function $\mathcal{S}$ verses the scattering angle in the same range as the top-right panel.**




**Scattering from model surface P1-SC. It has much broader scattering peak than P1-M. Notice the asymmetry of of the scattering around the specular reflection direction. The scattering function at zero scattering angle is more than 0.5. This means there are more total backward scattering ($\theta < 0$) than the total forward scattering ($\theta > 0$).**

## 10 Steps Towards Perfect Scattering!

1. Construct a model rough surface $S$ from PSD.
2. Calculate $\mathbf{E}(r_i)$ on the surface $S$.
3. Transfer $\mathbf{E}(r_i)$ to $\mathbf{E}(x_{r_i})$ on non-uniform grid on flat surface $S_0$.
4. Redistribute $\mathbf{E}(x_{r_i})$ into $\mathbf{E}(x_i)$ on uniform grid.
5. Fourier mapping $\mathbf{E}(x_i)$ into $\xi$ space.
6. Perform $p$ equally spaced Fourier transforms to obtain the Fraunhofer diffraction pattern.
7. Normalization.
8. Derive the scattering intensity as a function of scattering angle.
9. Calculate scattering function and generate scattering table.
10. Give a random number in [0,1], look up in the table to get your scattering angle!

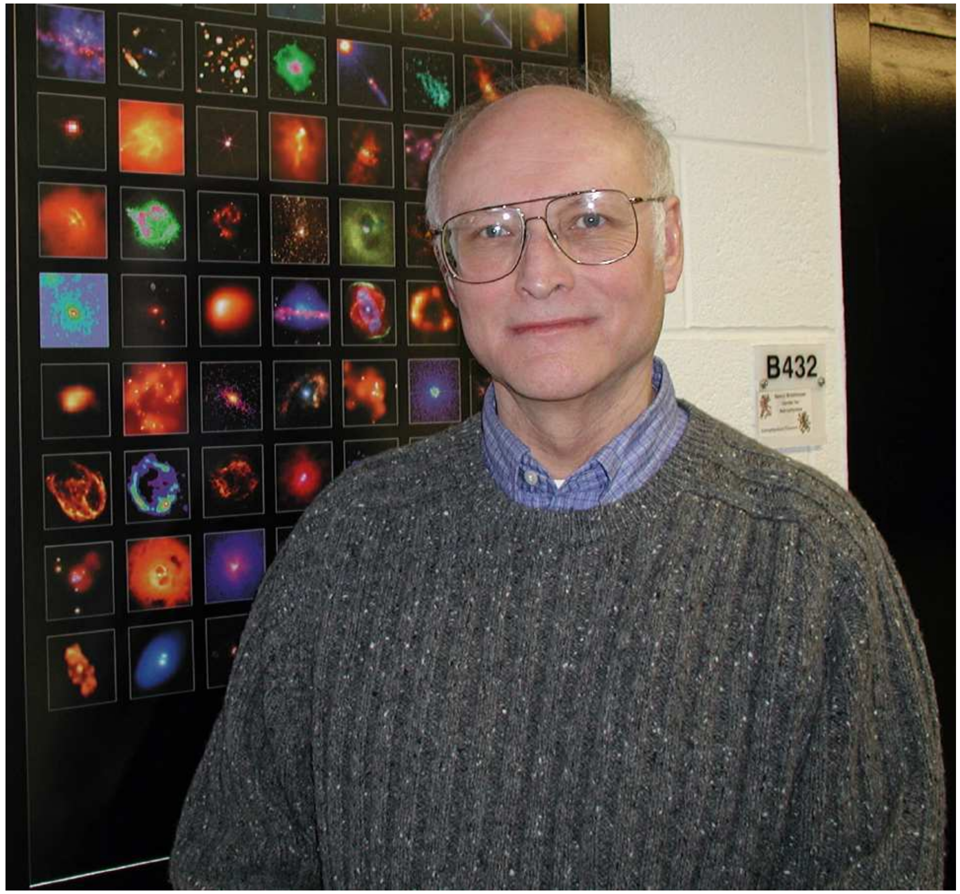
## Comparing The New Method with the Traditional Method

| Compare | Traditional | New |
|---|---|---|
| Scattering angle | $<<$ grazing angle | no restriction |
| | symmetric wrt specular direction | asymmetric |
| Scattered rays | only some rays are scattered | every ray is scattered |
| Scattering and reflection | treated separately | treated together |

## Summary and Future Work

- We have developed a new method to model the wave scattering from random rough surfaces.
- This method is applicable in general and is especially useful for X-ray scattering at grazing angles.
- This method is based on the general Kirchhoff equation but without small angle approximations.
- This method treats the reflection and scattering together and provides the dependence of the reflectivity on the surface roughness.
- This method has been applied to the mirrors of the Chandra X-ray Observatory and the results show that the calculated scattering profile is as expected, including the asymmetrical scattering profile for grazing incidence and the Fraunhofer scattering patterns due to the finite length of the surface.
- Scattering tables are generated based on this new method for all the Chandra mirror sections.
- This new scattering method is implemented in the raytrace to simulated the CXO performance. (This is finally working just last week!)
- The preliminary raytrace runs show the new scattering method produces results in better agreement with the XRCF calibration data. SO, IF YOU CARE, STAY TUNED!
- This new scattering method should be useful for other X-ray telescope missions as well.

Refenrece:
Ping Zhao and Leon P. Van Speybroeck, "A new method to model X-ray scattering from random rough surfaces" 2002, *SPIE Proceedings 4851-11*




This talk is dedicated to

**Dr. Leon P. Van Speybroeck**

**(1935 – 2002)**

**Chandra X-ray Observatory Telescope Scientist**

**The world's foremost designer of X-ray telescopes and a true math genius**

**The spectacular achievement of Chandra is not possible without him!**