X-RAY SCATTERING FROM OPTICAL SURFACES

- Diffraction from an imperfect surface
- The general scattering equation
- The Debye-Waller-factor treatment
- Conventional versus fractal surfaces
- Specifications and performance estimates
- Effect of errors on the image
  - Strehl factor
  - Image width factor
- Natural breakdown into “figure” and “finish”
- Practical example

DIFFRACTION FROM AN IMPERFECT SURFACE

Fraunhofer diffraction integral:

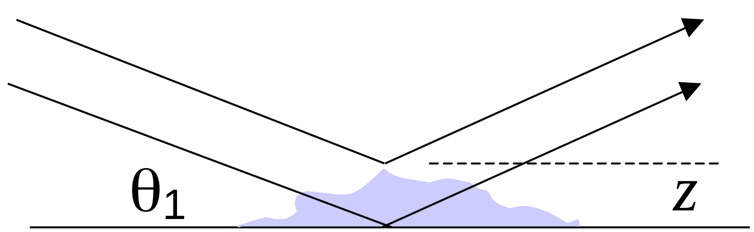
S. Sinha, 1988; E. L. Church, various publications

$$U_1 = \frac{U_0 r(\theta_1)\sin(\theta_1)}{\lambda z} \int_{\text{surface}} e^{i\Delta\phi(\mathbf{x})} A(\mathbf{x})\, e^{2\pi i \mathbf{x}.\mathbf{f}}\, d\mathbf{x}$$

Surface shape

Aperture illumination

$$\frac{1}{I_0}\frac{dI}{d\Omega} = \frac{R(\theta_1)\sin(\theta_1)}{\lambda^2}\left|\int_{-\infty}^{+\infty} \Omega(\mathbf{x})\, e^{2\pi i \mathbf{x}.\mathbf{f}}\, d\mathbf{x}\right|^2$$



$$\Delta\phi(\mathbf{x}) = \frac{2\pi}{\lambda} 2z \sin\theta_1$$
$$= 2\pi f_z z(\mathbf{x})$$

INTERPRETATION OF THE INTEGRAL

$$\frac{1}{I_0}\frac{dI}{d\Omega} = \frac{R(\theta_1)\sin(\theta_1)}{\lambda^2}\left|\int_{-\infty}^{+\infty}\Omega(\mathbf{x})\, e^{2\pi i\mathbf{x}.\mathbf{f}}\; d\mathbf{x}\right|^2$$

$$= \frac{R(\theta_1)\sin(\theta_1)}{\lambda^2}\iint e^{2\pi i\mathbf{f}.(\mathbf{x}_1-\mathbf{x}_2)}\,\Omega(\mathbf{x}_1)\,\Omega(\mathbf{x}_2)\,d\mathbf{x}_1 d\mathbf{x}_2$$

$$= \frac{R(\theta_1)\sin(\theta_1)}{\lambda^2}\int e^{2\pi i\mathbf{f}.\tau}\,[\Omega \quad \Omega]_\tau\, d\tau$$

τ means the “lag” distance, means correlation

MEANING OF THE AUTOCORRELATION OF Ω

$$\Omega(\mathbf{x}) = A(\mathbf{x})\ e^{2\pi i f_z z(\mathbf{x})}$$

$$[\Omega \quad \Omega]_\tau = \int A(\mathbf{x}+\tau) A(\mathbf{x})\ e^{2\pi i f_z \{z(\mathbf{x}+\tau) - z(\mathbf{x})\}}\ d\mathbf{x}$$

$$\langle [\Omega \quad \Omega]_\tau \rangle = \int A(\mathbf{x}+\tau) A(\mathbf{x}) d\mathbf{x}\ \left\langle e^{2\pi i f_z \{z(\mathbf{x}+\tau) - z(\mathbf{x})\}} \right\rangle$$

$$= AA(\tau)\ .\ \chi_2\left(2\pi f_x, -2\pi f_x ; \tau\right)$$

- Autocorrelation of A
- System OTF

- Joint characteristic function of $z(\mathbf{x}+\tau)$ and $z(\mathbf{x})$
- Roughness OTF

DIGRESSION ON THE CHACTERISTIC FUNCTION

For a probability distribution p, the characteristic function is

$$\chi_1(\omega) = \left\langle e^{i\omega z} \right\rangle = \int_{-\infty}^{+\infty} p(z)\, e^{i\omega z} dz$$

$$\chi_2(\omega_1,\omega_2) = \left\langle e^{i(\omega_1 z_1 + \omega_2 z_2)} \right\rangle = \int_{-\infty}^{+\infty} p(z_1, z_2)\, e^{i(\omega_1 z_1 + \omega_2 z_2)} dz_1 dz_2$$

We want $\left\langle \left(e^{i\omega z_1}\right)\left(e^{i\omega z_2}\right) \right\rangle = \chi_2(\omega, -\omega)$ for the Gaussian bivariate distribution

$$p(Z_1, Z_2) = \frac{1}{2\pi\sigma^2\sqrt{1-\rho^2}} \exp\left\{ -\frac{Z_1^2 - 2\rho Z_1 Z_2 + Z_2^2}{2\left(1-\rho^2\right)} \right\}$$

where $Z_1 \equiv \dfrac{z_1}{\sigma}$ etc

and $\rho \equiv \langle Z_1 Z_2 \rangle$

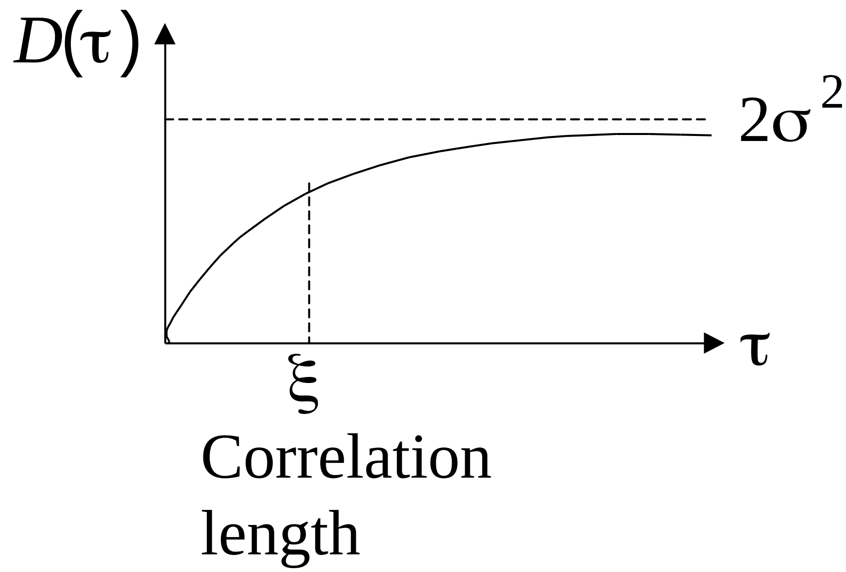
$$\left[\chi_2(\omega, -\omega)\right]_{GB} = e^{-\frac{1}{2}\omega^2 D(\tau)}$$

Structure function

STRUCTURE FUNCTION

The structure function $D(\tau)$ appears naturally in scattering theory

$$D(\tau) = \left\langle (z_1 - z_2)^2 \right\rangle$$
$$= \left\langle z_1^2 - 2z_1 z_2 + z_1^2 \right\rangle$$



In one or two dimensions:

$$D(\tau) = \mathrm{FT}\{S_1(f_x)\} \quad \text{or} \quad \mathrm{FT}\{S_2(\mathbf{f})\}$$

where S_1 and S_2 are the 1D and 2D power spectra of the roughness

THE BASIC SURFACE-SCATTERING EQUATION

$$\left\langle \frac{1}{I_0}\frac{dI}{d\Omega} \right\rangle = \frac{\sin(\theta_1)}{\lambda^2} R(\theta_1) \int AA(\tau)\ \exp\left\{ -\frac{1}{2}\left(2\pi f_z\right)^2 D(\tau) \right\} e^{2\pi i \mathbf{f}.\tau} d\tau$$

- System OTF
- Coherence width W, where $1/W$ is a critical spatial wavelength
- WL's > W diffract into the system image
- WL's < W diffract outside the system image

- Joint characteristic function of $z(\mathbf{x}+\tau)$ and $z(\mathbf{x})$
- Roughness OTF

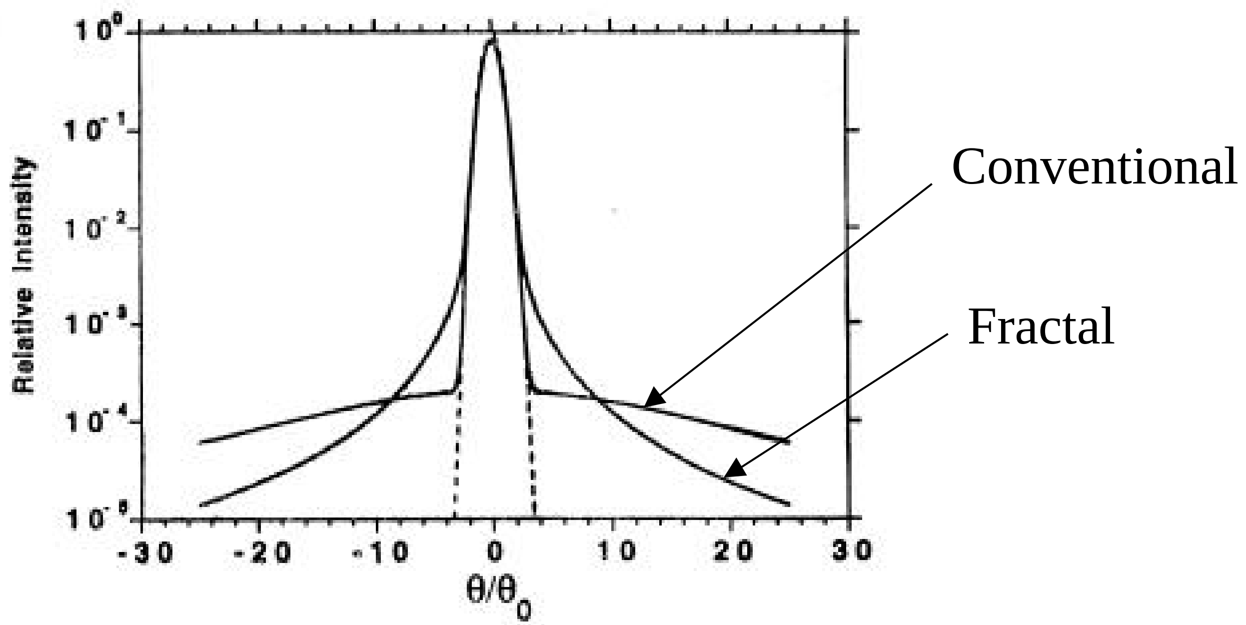
DEBYE-WALLER FACTOR TREATMENT

$$\left\langle \frac{1}{I_0}\frac{dI}{d\Omega} \right\rangle = \frac{\sin(\theta_1)}{\lambda^2} R(\theta_1) \int AA(\tau)\ \exp\left\{ -\frac{1}{2}\left(2\pi f_z\right)^2 D(\tau) \right\} e^{2\pi i \mathbf{f}.\tau} d\tau$$

- $AA(\tau)$ limits the range of τ to a width W
- $D(\tau)$ has a correlation length ξ
- If $\xi << W$ then most of the included roughness is uncorrelated: “conventional” surface
- In such case $D(\tau) = 2\sigma_z^2$ and the roughness OTF goes outside the integral

$$\left\langle \frac{1}{I_0}\frac{dI}{d\Omega} \right\rangle = \left\{ \frac{1}{I_0}\frac{dI}{d\Omega} \right\}_{\text{perfect mirror}} e^{-\left(2\pi f_z \sigma_z\right)^2}$$

CONVENTIONAL VS REAL OPTICAL SURFACES



- For a good optical surface made on a large lap, the roughness correlations are often long range so x-ray mirrors normally have fractal rather than conventional surfaces
- Fractal surfaces have large ξ and PSD's of the form $S_1 = K_n / f^n$
- In the smooth surface limit the Gaussian can be approximated by its first two terms (valid for non-Gaussian surfaces as well)

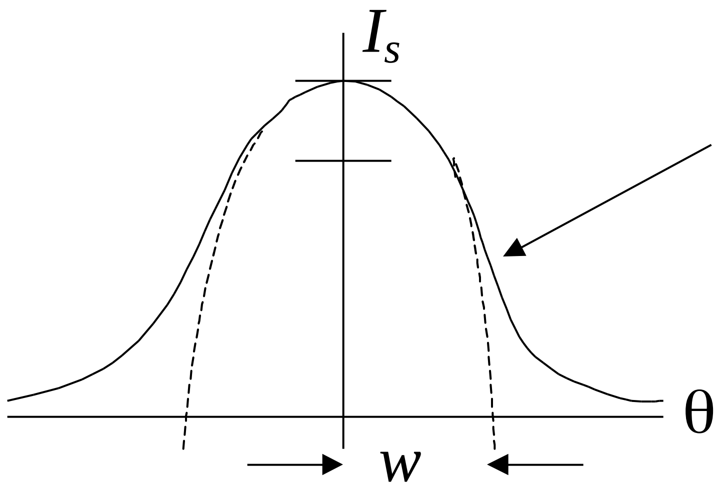
SPECIFICATIONS AND PERFORMANCE ESTIMATES

$$\frac{I(\theta)}{I_S(0)} = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \cos(st)\, e^{-\frac{t^2}{8}} \left\{ 1 - \frac{1}{2} f_z^2 D\left(\frac{2t}{f\Theta_z} \right) \right\} dt$$

- Simplified 1D form for a mirror length L and magnification M
- $s = \dfrac{\theta}{\Theta}$
- $t = f_z \Theta \tau / 2$
- $D(\tau) = 4 \int_0^{\infty} S_1(f_x) \sin^2(\pi f_x \tau)\, df_x$
- $I_s(\theta) = I_s(0) \exp\left\{ -2 \left(\dfrac{\theta}{\Theta} \right)^2 \right\}$

where $\Theta^2 = \left(\dfrac{\lambda}{L \sin(\theta_1)} \right)^2 + (M\theta_{\text{source}})^2 + (\theta_{\text{detector}})^2$ and $W = \dfrac{\sqrt{2}\lambda}{\Theta \sin(\theta_1)}$

EFFECT OF ERRORS ON THE IMAGE



$$I_s(\theta) = I_s(0)\left[1 - a\theta^2 + \ldots\right]$$

(without errors)

- For a real mirror (with errors) there will be a similar curve with reduced height and increased width
- Define two measures of error:
- Strehl factor: (Born and Wolf para 9.3) equals $I(0)/I_s(0)$
- Image width factor:

$$\frac{w_i}{w_{si}} = \left\{ \frac{d^2}{d\theta^2}\left(\frac{I(\theta)}{I(0)}\right)_0 \right\}^{-1/2} \Bigg/ \left\{ \frac{d^2}{d\theta^2}\left(\frac{I_s(\theta)}{I_s(0)}\right)_0 \right\}^{-1/2}$$

STREHL FACTOR

(Marechal 1947)

$$\frac{I(0)}{I_s(0)} = 1 - \left(\frac{4\pi \sin\theta_i}{\lambda}\right)^2 \sigma_{eff}^2 \quad \text{where} \quad \sigma_{eff}^2 = \int_0^\infty S_1(f_x)\left\{1 - \exp\left(-W^2 f_x^2\right)\right\} df_x$$

$$\boxed{\frac{I(0)}{I_s(0)} = 1 - \frac{8\mu_1^2}{\Theta^2} - \left(\frac{4\pi \sin\theta_i}{\lambda}\right)^2 \sigma_1^2}$$

$$\mu_1^2 = (2\pi)^2 \int_{1/L}^{1/W} S_1(f_x)\, f_x^2\, df_x \quad \text{and} \quad \sigma_1^2 = \int_{1/W}^{1/\lambda} S_1(f_x)\, df_x$$

RMS slope error (figure) | RMS height error (finish)

Acceptable value? traditionally 80%, say 10% figure error, 10% finish error

IMAGE-WIDTH FACTOR

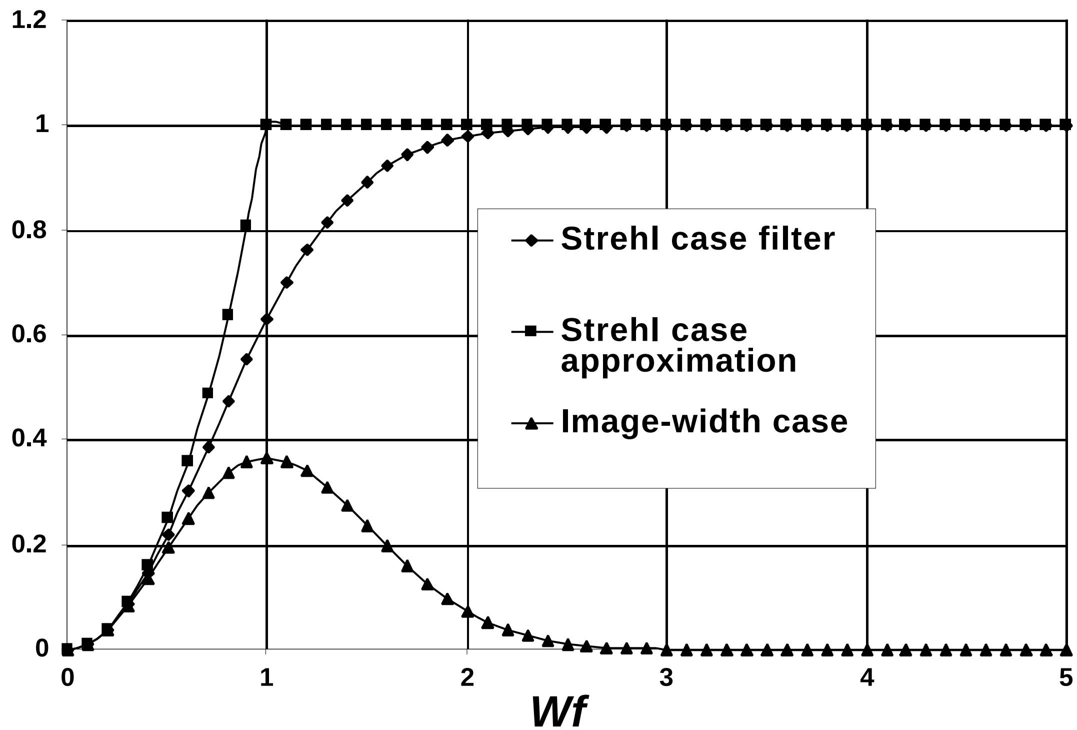
$$\frac{w_i}{w_{si}} = 1 + \left(\frac{4\pi \sin\theta_i}{\lambda} \right)^2 \sigma_{iw}^2$$

where

$$\sigma_{iw}^2 = \int_0^\infty S_1(f_x) \left\{ W^2 f_x^2 \exp\left(-W^2 f_x^2\right) \right\} df_x$$

Acceptable value? let’s say 120%

SPATIAL-FREQUENCY FILTER FUNCTIONS



$$1 - \exp\left(-W^2 f_x^2\right)$$

(Strehl factor)

$$W^2 f_x^2 \exp\left(-W^2 f_x^2\right)$$

(Image-width factor)

Approximation:

$$1 - \exp\left[-\left(W f_x\right)^2\right] \quad \left(W f_x\right)^2 \ \text{ when } \ 0 \le f_x \le 1/W \ \text{ (figure)}$$

$$1 \ \text{ otherwise } \ \text{(finish)}$$

FRACTAL POWER SPECTRA

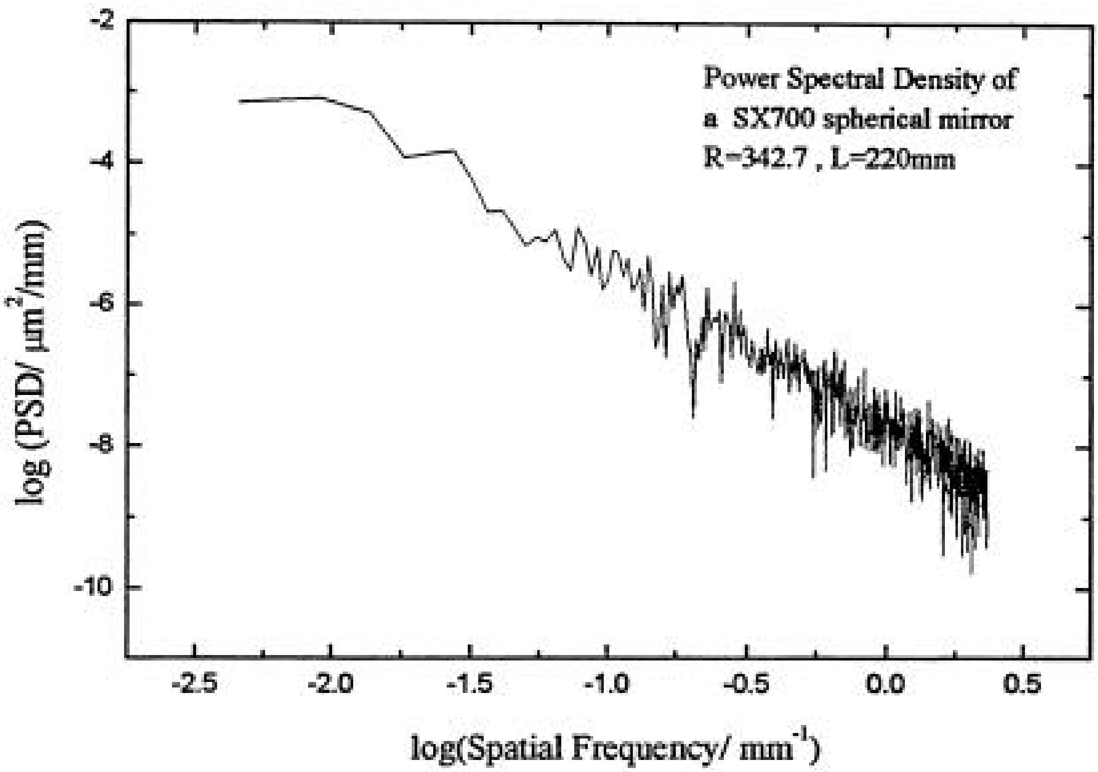
$$S_1(f_x) = \frac{K_n}{f_x^n}$$

$$\mu_1^2 = \frac{(2\pi)^2 K_n}{3-n}\left[\left(\frac{1}{W}\right)^{3-n} - \left(\frac{1}{L}\right)^{3-n}\right]$$

$$\sigma_1^2 = \frac{K_n}{1-n}\left[\left(\frac{1}{\lambda}\right)^{1-n} - \left(\frac{1}{W}\right)^{1-n}\right]$$

$$\sigma_{iw}^2 = \frac{K_n}{2}\,\Gamma\left(\frac{3-n}{2}\right)W^{n-1}$$

REAL MIRROR EXAMPLE



- Zeiss-made BESSY mirror measuerd by Zeiss
- Fractal power spectrum
- $S_1 = 2.4\times10^{-12}/f^{2.3}$
- Finish PSD not available
- Zeiss bench mark for mirror quality - this is their best routine production - anything better requires new tools to be made

SPECIFICATION AND PERFORMANCE SPREADSHEET

Scattering statistics

		Mirror------->	Church paper Opt Eng Feb 95	Zeiss Proc SPIE 3152
		Application-->	Church paper (test case)	SX700
Input data	**Unit**	**Name**		
Mirror length	m	L	1	0.22
Wavelength	nm	lam	0.15	2
Grazing angle	mr	alph	3	50
Fractal PSD:				
Kn	µm^(3-n)	kn	6.64E-09	2.40E-12
n	none	n	1.61	2.3
Acceptable Strehl decr	none		0.1	0.1
Acceptable image growth	none		0.2	0.2
Source size	µm	s	60	100
Source distance	m	sd	400	30
System magnification	none	m	0.25	0.2
Detector width	µm	dw	100	1
Calculated data				
Focal distance	m	F	100	6
System image width	µr	theta	1.012	3.342
Church's P	nm^-2	P	3.16E-02	4.93E-02
System coherence width (Constrained<0.95L)	mm	W	69.843	16.931
Strehl:				
Strehl factor	none		0.115	0.854
Roughness decrement	none		0.620	0.057
Figure decrement	none		0.265	0.089
Strehl % decrement	none		88.503	14.582
mu1 Strehl want	µr		0.113	0.374
mu1 Strehl get	µr		0.184	0.352
Sig1 Strehl want	nm		1.258	1.007
Sig1 Strehl get	nm		3.132	0.762
Image:				
Image growth factor	none		1.247	1.095
Image % increment	none		24.688	9.469
sigeff image want	nm		1.779	1.424
sigeff image get	nm		1.977	0.980