EFFECTS OF PARTIALLY COHERENT INCIDENT ILLUMINATION ON IN-LINE IMAGING

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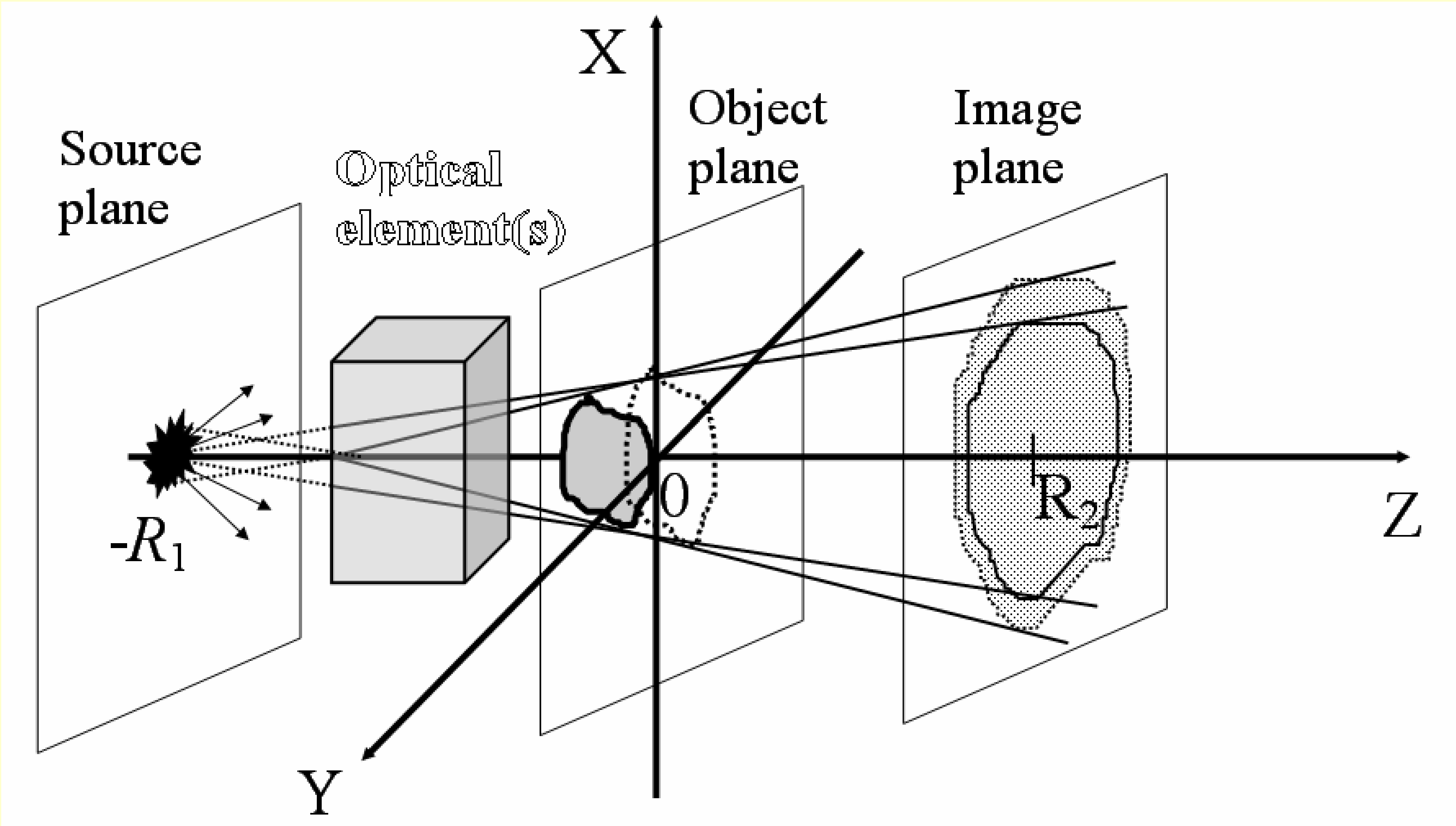
OUTLINE OF TALK

1. Introduction. Formulation of the problems.
2. Schell-model-type partially-coherent illumination - extend to include treatment of coherent aberrations.
3. Spectral density and intensity distribution of projection images - including key instrumental factors.
4. TIE+Born linear approximation – hybrid theory in order to treat much wider class of objects (not just weak objects).
5. Phase retrieval from partially coherent images – quest for linear theories.
6. Contrast transfer function for homogeneous objects – a useful special case.
7. Optimal defocus distance and "automatic phase retrieval" – Scherzer defocus.
8. Some numerical and experimental examples – direct phase retrieval without computation!
9. Conclusions

IMAGING GEOMETRY

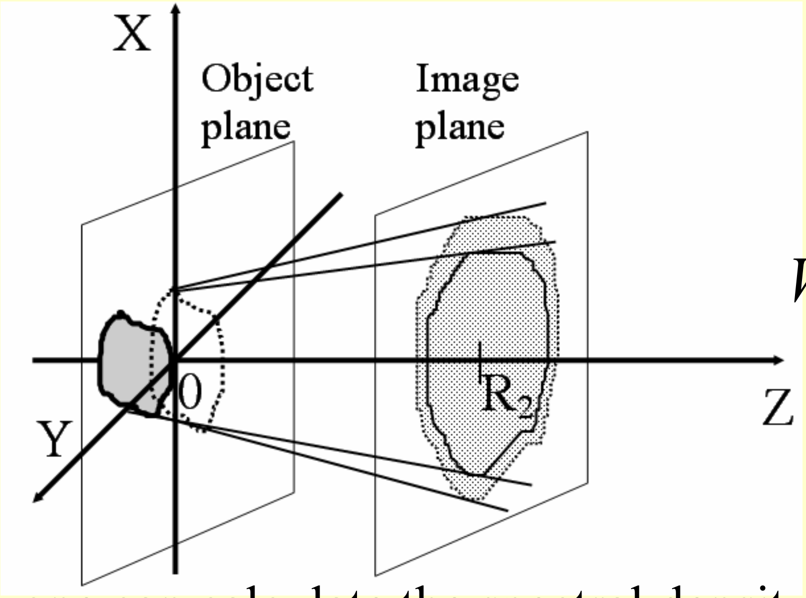


"Incident" problem: determine incident cross-spectral density distribution

Inverse problem: retrieve transmitted phase and intensity distributions

Direct problem: find the spectral density and time-averaged intensity distribution of projection images

GENERAL FORMULA FOR SPECTRAL DENSITY OF PROJECTION IMAGES



Given an incident *cross-spectral density distribution* at the object plane z=0:

$$W^{\text{in}}(\mathbf{r},\mathbf{r}',\nu)=\widetilde{W}^{\text{in}}(\mathbf{r},\mathbf{r}',\nu)e^{ik(r'^2-r^2)/2R_1}$$

and the object transmission function:

$$Q(\mathbf{r},\nu)=q(\mathbf{r},\nu)e^{ik\psi(\mathbf{r},\nu)}$$

one can calculate the spectral density in the image plane $z=R_2$ as:

$$S(\mathbf{r},R_2,\nu)=\iint\iint e^{\frac{ik}{R_2}\left[\frac{M}{2}(r''^2-r'^2)+\mathbf{r}\cdot(\mathbf{r}'-\mathbf{r}'')\right]}\widetilde{W}^{\text{in}}(\mathbf{r}',\mathbf{r}'',\nu)Q^*(\mathbf{r}',\nu)Q(\mathbf{r}'',\nu)\frac{\mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{r}''}{\lambda^2R_2^2}$$

[Based on a similar expression in Mandel & Wolf]

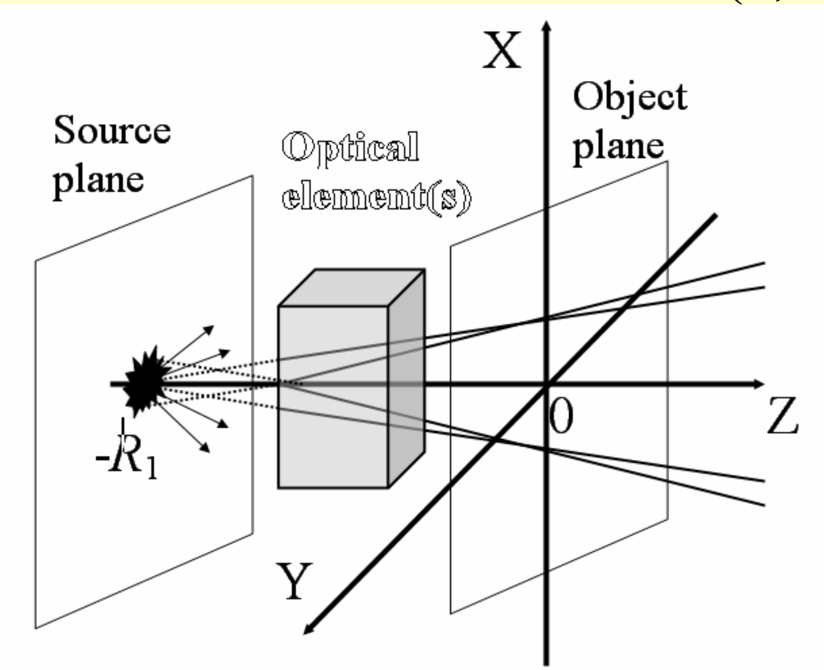
where $M=(R_1+R_2)/R_1$; or after Fourier transformation with respect to $\mathbf{r}$:

$$\hat{S}(\mathbf{u}/M,R_2,\nu)=\iint e^{-i2\pi\,\mathbf{r}\cdot\mathbf{u}}\,\widetilde{W}^{\text{in}}(\mathbf{r}+\alpha\mathbf{u},\mathbf{r}-\alpha\mathbf{u},\nu)Q^*(\mathbf{r}+\alpha\mathbf{u},\nu)Q(\mathbf{r}-\alpha\mathbf{u},\nu)\mathrm{d}\mathbf{r}$$

where $\alpha=\lambda R'/2,\;R'=R_1R_2/(R_1+R_2)$ [cf. J-P.Guigay, Opt.Comm., 1978]

SCHELL-MODEL-TYPE PARTIALLY COHERENT ILLUMINATION

$$W^{\text{in}}(\mathbf{r},\mathbf{r}',\nu) = [S^{\text{in}}(\mathbf{r},\nu)]^{1/2}[S^{\text{in}}(\mathbf{r}',\nu)]^{1/2} g(\mathbf{r}',\mathbf{r},\nu)$$



- incident *cross-spectral density:*

Here $S^{\text{in}}(\mathbf{r},\nu)$ is the incident spectral density,

$g(\mathbf{r}',\mathbf{r},\nu)$ is the incident *spectral degree of coherence*

Consider the following model for the incident spectral degree of coherence which represents an extension of the Schell model illumination:

$g(0, \nu) = 1$ =>

$$g(\mathbf{r},\mathbf{r}',\nu) = \tilde{g}(\mathbf{r}'-\mathbf{r},\nu) e^{ik[\psi^{\text{in}}(\mathbf{r}',\nu)-\psi^{\text{in}}(\mathbf{r},\nu)]} e^{ik(r'^2-r^2)/(2R_1)},$$

$$\tilde{g}(0,\nu) \equiv 1$$

Note: $|\mathbf{g}(\mathbf{r}-\mathbf{r}_{o,}\ \nu)|$ depends only on $\mathbf{r}$-$\mathbf{r}_o$ but coherent aberrations can be included

Some special cases:

When ψ^{in}=0 and R_1=∞, this describes a Schell-model illumination

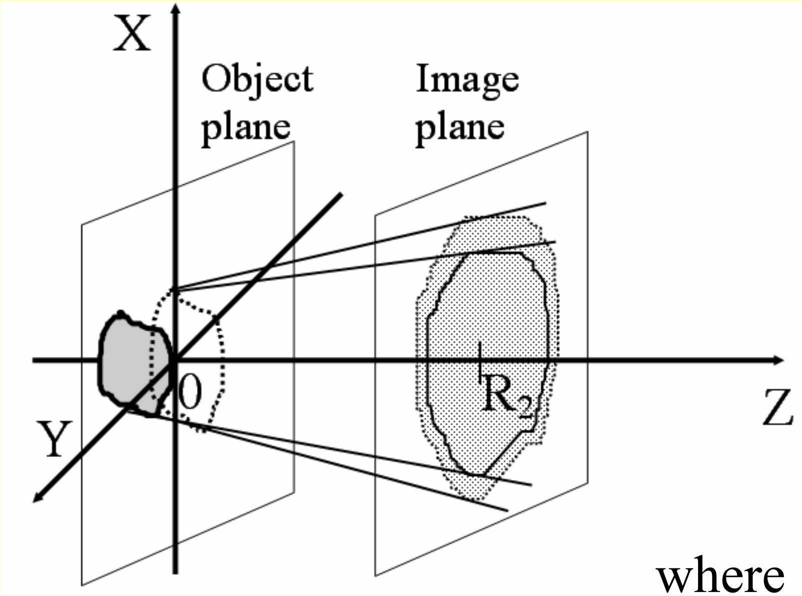
When also $[S^{\text{in}}(\mathbf{r},\nu)]^{1/2}[S^{\text{in}}(\mathbf{r}',\nu)]^{1/2} = S^{\text{in}}((\mathbf{r}'+\mathbf{r})/2,\nu)$, => quasi-homogeneous illumination

When also $S^{\text{in}}(\mathbf{r},\nu)$=const($\nu$) => spatially incoherent source

When $\breve{g}(\mathbf{r},\nu)$=1, this model includes plane and spherical coherent incident waves

This model also describes incident radiation on a sample for typical bending magnet beamlines

SPECTRAL DENSITY OF PROJECTION IMAGES IN THE CASE OF SCHELL-MODEL-TYPE ILLUMINATION



For Schell-model-type incident illumination, the expression for the *spectral density in the image plane has the same general form as in the case of an extended spatially incoherent source:*

image plane   imaging system   coherent image

$$\hat{S}(\mathbf{u}, R_2, \nu) = \hat{P}(\mathbf{u}, M, \nu)\hat{S}^{\text{coh}}(M\mathbf{u}, R', \nu)$$

where $\hat{P}(\mathbf{u}, M, \nu) = \hat{S}_{\text{n}}^{\text{src}}(-(M-1)\mathbf{u}, \nu)\,\hat{D}(\mathbf{u}, \nu)$

is the *total MTF of the system,*

$\hat{S}_{\text{n}}^{\text{src}}(\mathbf{u}, \nu)$ is a rescaled Fourier transform of $\breve{g}(\mathbf{r}, \nu)$ (it is related to the *normalized spectral density in the source plane*).

$\hat{D}(\mathbf{u}, \nu)$ is the MTF of the detector, and

$$\hat{S}^{\text{coh}}(\mathbf{u}, R', \nu) = \iint e^{-i2\pi\,\mathbf{r}\cdot\mathbf{u}}\tilde{Q}^*(\mathbf{r}+\alpha\mathbf{u}, \nu)\tilde{Q}(\mathbf{r}-\alpha\mathbf{u}, \nu)d\mathbf{r}, \quad \tilde{Q} = (S^{\text{in}})^{1/2}e^{ik\psi^{\text{in}}}Q,$$

expn of phase => Guigay type condition   includes coherent aberrations

is the *spectral density* in the image plane corresponding to *coherent quasi-plane incident illumination* (it reflects both object properties and "coherent aberrations" of the incident illumination)

SOLUTION TO THE DIRECT PROBLEM IN THE CASE OF SCHELL-MODEL-TYPE ILLUMINATION

The previous formulae can be easily converted into *real-space representations:*

$$S(\mathbf{r}, R_2, \nu) = M^{-2} \iint S^{\mathrm{coh}}(\mathbf{r}''/M, R', \nu) P(\mathbf{r} - \mathbf{r}'', \nu) \mathrm{d}\mathbf{r}''$$

where $P(\mathbf{r}, M, \nu) = \iint S_{\mathrm{n}}^{\mathrm{src}}(\mathbf{r}', \nu) D(\mathbf{r} + (M-1)\mathbf{r}', \nu) \mathrm{d}\mathbf{r}'$

is the *total PSF of the system*. Integrating over ν we obtain the following expression for the *time-averaged intensity distribution in the detector plane:*

coherent image (pw) ⟵ instrument ⟶

$$I(\mathbf{r}, R_2) = \frac{1}{M^2} \int \iiint \iint S^{\mathrm{coh}}\left(\frac{\mathbf{r}'' + (M-1)\mathbf{r}'}{M}, R', \nu\right) S_{\mathrm{n}}^{\mathrm{src}}(\mathbf{r}', \nu) D(\mathbf{r} - \mathbf{r}'', \nu) \mathrm{d}\mathbf{r}' \mathrm{d}\mathbf{r}'' \mathrm{d}\nu$$

This formula has the *same general form as the corresponding formula for an extended spatially incoherent source*. However, partial coherence of the incident illumination results in a non-trivial distribution of incident spectral density and phase, which are both included in S^{coh} via the modified transmission function.

A MODEL FOR THE MODIFIED TRANSMISSION FUNCTION

Having obtained the general formulae for the spatial distribution of the spectral density and polychromatic intensity of a projection image under the Schell-model-type illumination, we now consider relevant properties of the object under investigation. We assume that the modified transmission function (which describes the object transmission properties as well as coherent aberrations of the incident wave) can be represented as

$$\tilde{Q} \equiv \exp(-\tilde{\mu} + i\tilde{\varphi}) \cong Q_h(1 + \chi_h)$$

TIE+Born model

where $Q_h = \exp(-\bar{\mu}_h + i\bar{\varphi}_h)$ is a slowly varying function, and

$$\chi_h = -\Delta\mu_h + i\Delta\varphi_h \text{ is } \textbf{\textit{assumed}} \text{ to be small, i.e. } |\chi_h| << 1.$$

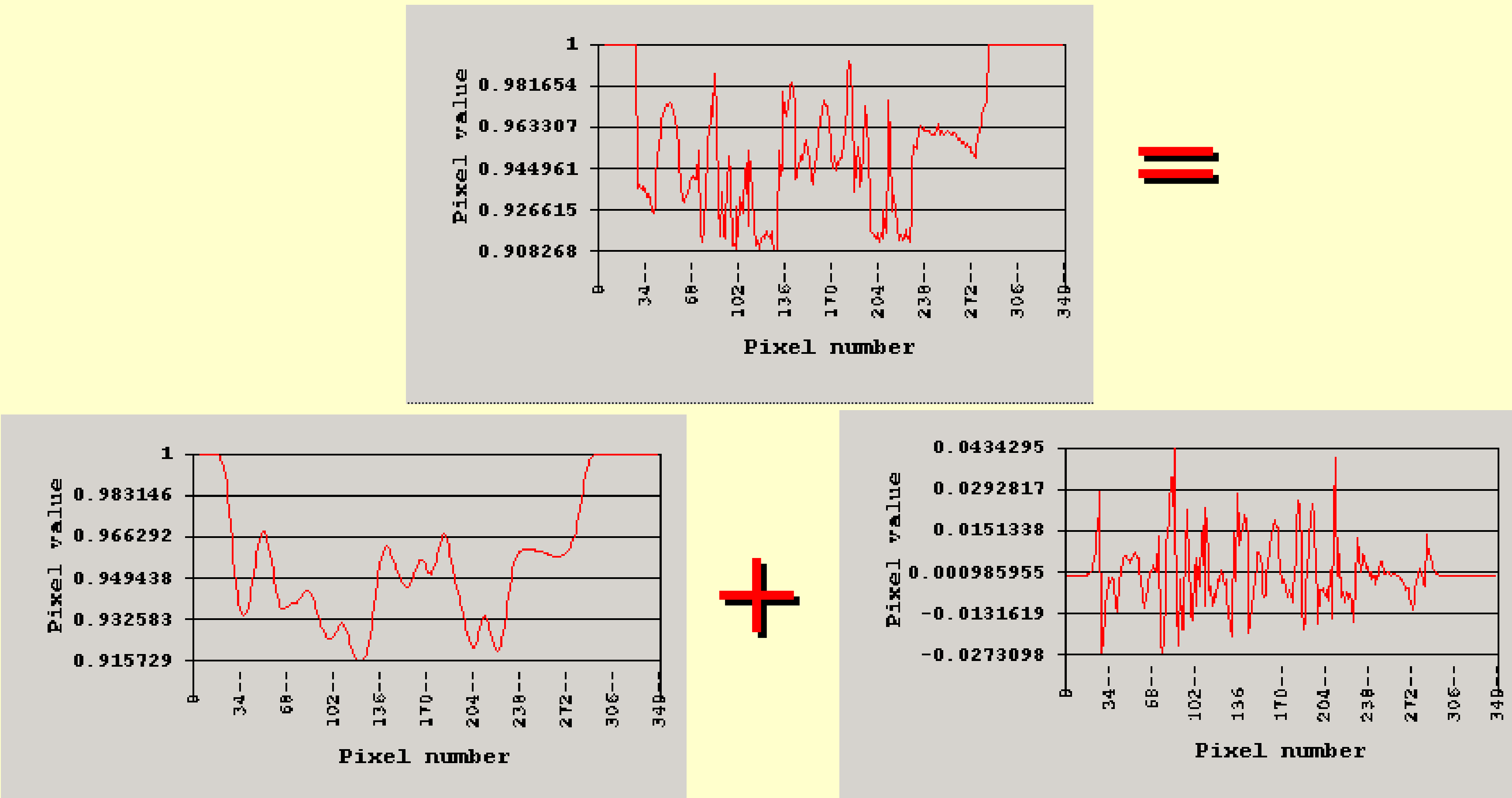
Here the slowly varying components, $\bar{\mu}_h$ and $\bar{\varphi}_h$, are defined as running averages

$$\bar{f}_h(x, y, \nu) = h^{-2} \int_{-h/2}^{h/2} \int_{-h/2}^{h/2} f(x + x', y + y', \nu) \mathrm{d}x' \mathrm{d}y', \;\; f = \bar{f}_h + \Delta f_h,$$

over distance $h=\lambda R'/d$, where d is the smaller of the spatial resolution of the imaging system and the minimal feature size present in the object.

A MODEL FOR THE MODIFIED TRANSMISSION FUNCTION. 2

In other words, a function is assumed to be representable as a sum of its slowly varying (smoothed over distances ~h) version and a rapidly varying residual, which is small in magnitude. Note that the TIE and the 1-st Born (Fourier Optics) approximations correspond to the cases χ_h=0 and Q_h=const, respectively.



COHERENT SPECTRAL DENSITY FOR THE TIE+BORN MODEL

If the *modified transmission function* with amplitude q_h satisfies the TIE+Born model, then the general non-linear formula for the spectral density distribution of a projection image can be linearized with respect to the transmitted phase :

←――― **TIE (slowly varying)** ―――→

$$\hat{S}^{coh}(\mathbf{u},R',\nu)=[\,q_h^2\,]^{\wedge}(\mathbf{u},\nu)-(R'/k)[\nabla_\perp\cdot(q_h^2\nabla_\perp\overline{\varphi}_h)]^{\wedge}(\mathbf{u},\nu)-$$

$$2\cos[\pi\lambda R'u^2)][\,q_h^2\Delta\mu_h\,]^{\wedge}(\mathbf{u},\nu)+2\sin[\pi\lambda R'u^2\,][\,q_h^2\Delta\varphi_h\,]^{\wedge}(\mathbf{u},\nu)$$

Note:

$q_h = |Q_h|$

Here the first line corresponds to the TIE-type approximation applied to the slowly varying function Q_h, while the second line corresponds to the scattered wave in the first-Born-type approximation applied to the small function $|Q_h|^2\chi_h$

Note that both the phase and the intensity terms in this equation contain contributions from the incident wave, as well as the object, as by definition

$$\widetilde{\varphi}=k\psi^{in}+\arg Q \quad\text{and}\quad \widetilde{\mu}=-\ln(S^{in})/2-\ln|Q|$$

include both coherent aberrations & object properties

The total spectral density, $\hat{S}(\mathbf{u},R_2,\nu)=\hat{P}(\mathbf{u},M,\nu)\hat{S}^{coh}(M\mathbf{u},R',\nu)$,

is also ***linear with respect to the transmitted phase***.

IMPORTANT SPECIAL CASES OF THE GENERAL FORMULAE

I. Illumination conditions that are treated

I.1. Partially coherent standard Schell-model illumination: $\psi^{in} = 0$

partially coherent quasi-homogeneous illumination, then also

$$(S^{in})^{1/2}(\mathbf{r},\nu)(S^{in})^{1/2}(\mathbf{r}',\nu) = (S^{in})^{1/2}((\mathbf{r}+\mathbf{r}')/2\ ,\nu)$$

spatially incoherent source: then also $S^{in}(\mathbf{r},\nu) = S^{in}(\nu)$.

I.2. Coherent quasi-spherical wave: $S_n^{src}(\mathbf{r}, \nu) = \delta(\mathbf{r}-\mathbf{r}_0)$ (including abns)

ideal spherical wave: then also $\psi^{in} = 0$ and $S^{in}(\mathbf{r},\nu) = S^{in}(\nu)$

I.3. Coherent quasi-plane wave: $M = 1$ (see earlier eqn)

Plane wave: then also $\psi^{in} = 0$ and $S^{in}(\mathbf{r},\nu) = S^{in}(\nu)$

II. Object properties that are treated

II.1. Non-absorbing (pure phase) object: $\mu = 0$

II.2. Homogeneous (single material) object: $\varphi(\mathbf{r},\nu) =-\gamma(\nu)\, \mu(\mathbf{r},\nu)$, $\gamma = \delta / \beta$

II.3. Weak object: $\mu << 1$, $|\varphi(\mathbf{r}+\alpha\mathbf{u}, \nu) - \varphi(\mathbf{r}-\alpha\mathbf{u}, \nu)| << 1$ (i.e. slowly varying φ or weak φ but may be rapidly varying <=> Guigay assumption)

II.4. Slowly varying object: $\Delta\mu_h=\Delta\varphi_h= 0$. (TIE)

LINEAR PHASE RETRIEVAL IN THE NEAR-FRESNEL REGION

1. General methods are based on: $\hat{S}(\mathbf{u}, R_2, \nu) = \hat{P}(\mathbf{u}, M, \nu)\hat{S}^{\mathrm{coh}}(M\mathbf{u}, R', \nu)$

Spatial deconvolution removes the effect of the MTF of the imaging system, then the phase retrieval is performed as in the coherent case. Note that coherent "aberrations" of the incident illumination described by S^{in} and φ^{in} are included in S^{coh}. Separate experiments for characterization of the incident illumination need to be carried out in order to quantify these effects.

2. For pure phase and for homogeneous objects the ***total phase***, $\varphi = \overline{\varphi}_h + \Delta\varphi_h$, can be retrieved at once from a single projection image:

$$\hat{\varphi}(\mathbf{u}, \nu) = \frac{[S^{\mathrm{coh}} / S^{\mathrm{in}} - 1]^{\wedge}(\mathbf{u}, R', \nu)}{2\sin(\pi\lambda R' u^2)}$$

pure phase objects with
$|\varphi(\mathbf{r}+\alpha\mathbf{u}, \nu) - \varphi(\mathbf{r}-\alpha\mathbf{u}, \nu)| \ll 1$

$$\hat{\varphi}(\mathbf{u}, \nu) \cong \frac{\gamma}{2}\ln\left(\frac{\hat{S}^{\mathrm{coh}}(\mathbf{u}, R', \nu) / S^{\mathrm{in}}(\nu)}{\cos(\pi\lambda R' u^2) + \gamma\sin(\pi\lambda R' u^2)}\right)$$

homogeneous objects ***(both μ and φ can be large !!!)***

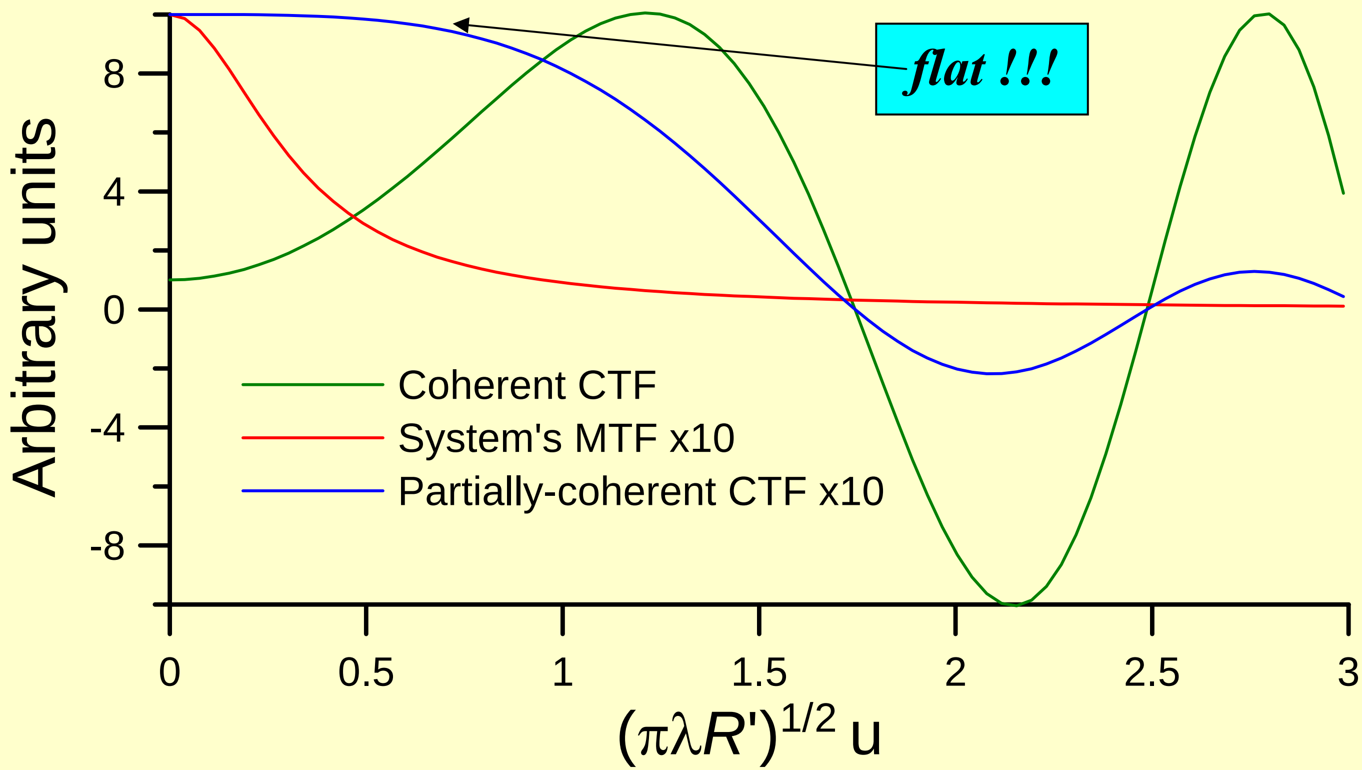
Consider u -> 0

See also re phase retrieval for homogeneous objects: Paganin et al J. Microscopy (2002), 206, 11-40.

CONTRAST TRANSFER FUNCTION FOR HOMOGENEOUS OBJECTS

$$\hat{S}(\frac{\mathbf{u}}{M}, R_2, \nu) = \underbrace{\overbrace{\hat{P}(\frac{\mathbf{u}}{M}, \nu)}^{\text{MTF}} \overbrace{\sqrt{(1+\gamma^2)} \sin[\pi\lambda R' u^2 + \arctan \gamma^{-1}(\nu)]}^{\text{CTF}^{\text{coh}}}}_{\text{CTF}} [q^2]^{\wedge}(\mathbf{u}, R', \nu)$$

When $|\pi\lambda R' u^2| << 1$, $\text{CTF}^{\text{coh}} \cong 1 + \gamma\pi\lambda R' u^2$. Let $\hat{P}(\frac{\mathbf{u}}{M}, \nu) \cong (1 + \gamma\pi\lambda R' u^2)^{-1}$



AUTOMATIC PHASE RETRIEVAL AND DECONVOLUTION

In the case of uniform illumination ($\psi^{\text{in}} = 0$ and $S^{\text{in}}(\mathbf{r},\nu) = S^{\text{in}}(\nu)$), the spectral density distribution of projection images of *homogeneous objects with slowly varying (on the length scale $h=\lambda R'/d$, where d is the size of the smallest resolvable object feature)* and using the modified transmission functions is equal to

$$\hat{S}(\mathbf{u},R_2,\nu)=\hat{P}(\mathbf{u},M,\nu)\,[q_h^2]^{\wedge}(M\mathbf{u},\nu)\,[1+\gamma\pi\lambda R' M^2 u^2]$$

where $\hat{P}$ is the total MTF of the imaging system.

We now assume that the system *PSF is symmetric* and its width is of the same order as *Md*. Then the MTF can be approximated by the second-order Taylor expansion,

$$\hat{P}(\mathbf{u},M,\nu)\cong p_0(M,\nu)-(2\pi)^2 p_2(M,\nu)u^2, \text{ and}$$

$$\hat{S}(\mathbf{u},R_2,\nu)=[q_h^2]^{\wedge}(M\mathbf{u},\nu)\times$$

$$\{p_0(M,\nu)+u^2[\underbrace{\gamma\pi\lambda R' M^2 p_0(M,\nu)-(2\pi)^2 p_2(M,\nu)}_{\text{can be equal to zero !!!}}]\}$$

AUTOMATIC PHASE RETRIEVAL AND DECONVOLUTION. MONOCHROMATIC CASE

Therefore at the defocus distance

$$R'_d(M,\nu) \equiv \sigma^2(M,\nu)k\beta(\nu)/\delta(\nu)$$

$$N_F \equiv \frac{2\pi\sigma^2}{\lambda R'_d} = \frac{\delta}{\beta}$$

where

$$\sigma^2(M,\nu) \equiv \frac{2p_2(M,\nu)}{M^2 p_0(M,\nu)} = \frac{\sigma_D^2(\nu)+(M-1)^2\sigma_S^2(\nu)}{M^2}$$

is the variance of the system's PSF, one has $\gamma\lambda R'M^2 p_0 = 4\pi\, p_2$, and

$$\hat{S}(\mathbf{u},R_2,\nu) = [q_h^2]^{\wedge}(M\mathbf{u},\nu)\,p_0(M,\nu)$$

"ideal" imaging system

i.e. the image coincides with the rescaled modified transmission function. The effects of the convolution with the system PSF and the Fresnel diffraction have cancelled each other (CTF is constant). This condition is analogous to the Scherzer defocus in electron microscopy, where the Fresnel diffraction effects are optimally cancelled by the spherical aberration of an electron microscope.

AUTOMATIC PHASE RETRIEVAL AND DECONVOLUTION. POLYCHROMATIC CASE

The optimal defocus distance generally depends on ν. However, it can be shown that for *weak homogeneous objects*, a projection image at the defocus distance

$$R'_d = \sigma^2(M)\frac{< k\beta >}{< \delta >} \quad < k\beta > = \frac{\int k\beta(\nu)S^{\mathrm{in}}(\nu)\mathrm{d}\nu}{I^{\mathrm{in}}}, < \delta > = \frac{\int \delta(\nu)S^{\mathrm{in}}(\nu)\mathrm{d}\nu}{I^{\mathrm{in}}}$$

is equal to

$$I(M\mathbf{r}, MR'_d) \cong M^{-2}\int p_0(M,\nu)\,|\,Q(\mathbf{r},\nu)\,|^2\, S^{\mathrm{in}}(\nu)\mathrm{d}\nu,$$

and

i.e. spectrally weighted sum over object fnc

$$\varphi(\mathbf{r},\nu_0) = k_0\delta(\nu_0)[M^2 I(M\mathbf{r}, MR'_d) - I^{\mathrm{in}}(\nu)] / \int 2k\beta(\nu)p_0(M,\nu)S^{\mathrm{in}}(\nu)\mathrm{d}\nu$$

By choosing the defocus distance equal to R_d' in the polychromatic case one can achieve an "automatic" simultaneous spatial deconvolution and phase retrieval. The result is achieved by making the Fresnel diffraction counteract the blurring due to the finite size of the PSF of the imaging system. Compared to conventional "post-processing" methods for image deconvolution and phase retrieval, *the above "hardware" method has an obvious advantage of being <u>insensitive to the image detection noise</u>.*

NUMERICAL EXAMPLE OF THE AUTOMATIC PHASE RETRIEVAL AND DECONVOLUTION

Polychromatic case

Incident spectral density corresponding to a W X-ray tube operated at E=30 keV

Apatite sample with a transverse size of 1.6 x 1.6 mm^2 and with maximum thickness variation of ~50 μm (max.absorption ~ 30%, max.phase shift ~10 radians)

Lorentzian source and detector MTFs with σ_S=2 μm and σ_D=10 μm, M=2

Polychromatic projection images $I(M\mathbf{r}, MR'_d) \cong M^{-2} \int |Q(\mathbf{r},\nu)|^2 \, S^{\text{in}}(\nu) \mathrm{d}\nu$

$\sigma_S = 0\,\mu m, \sigma_D = 0\,\mu m$

$R' = 0\,cm$

$\sigma_S = 2\,\mu m, \sigma_D = 10\,\mu m$

$R' = 0\,cm$

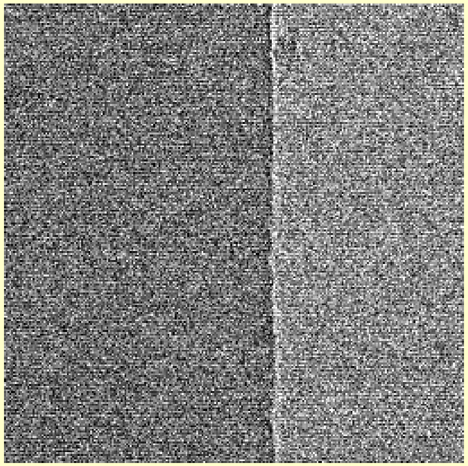
$\sigma_S = 2\,\mu m, \sigma_D = 10\,\mu m, \;\; M = 2$

$R' = R'_d = 2.84\,cm$

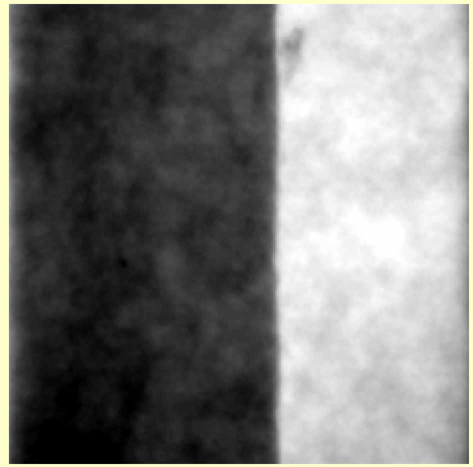
EXPERIMENTAL DEMONSTRATION

Polychromatic case

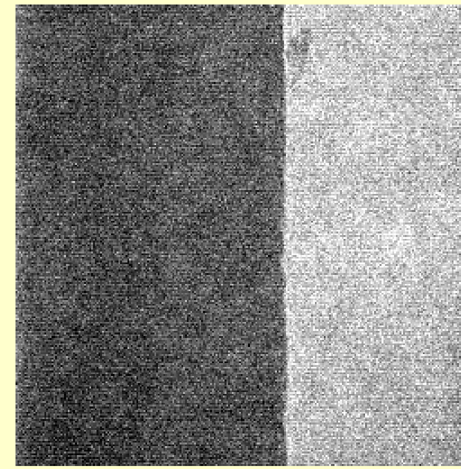
In-line X-ray image of an edge of a 100 μm Polyethylene sheet; microfocus source; W target; $E = 30$ keV; $\sigma_x = 3.5$ μm; $R_1 = 4$ cm, $R_2 = 196$ cm.



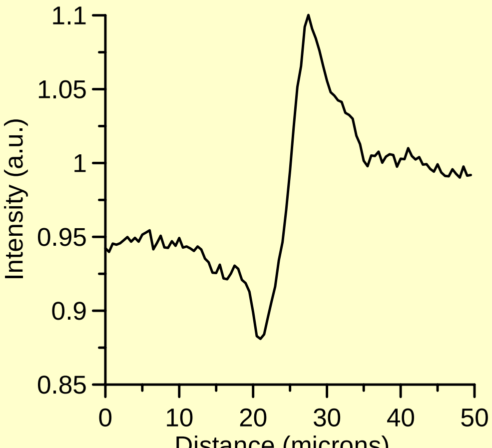
experimental in-line X-ray image



TIE phase-retrieved image



deblurred image



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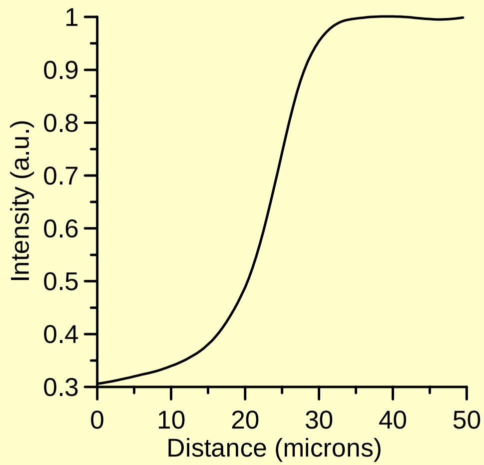

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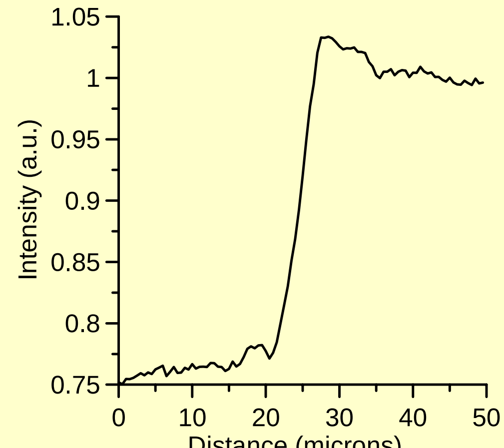

CONCLUSIONS

1. ***Incident problem*****:** We have derived a "general" formula for the spectral density distribution of projection images under partially coherent Schell-model-type illumination that includes: *coherent plane and spherical incident waves, quasi-homogeneous and spatially incoherent sources as special cases*.

2. ***Direct problem:*** We have linearized the formula for partially coherent projection images with respect to the transmitted phase distribution under the assumption that the coherent aberrations of the incident illumination and the object transmission function can be represented as the *sum of a slowly varying plus a rapidly varying but small component* (TIE+Born approximation).

3. ***Inverse problem*****:** We have demonstrated that by appropriately choosing the defocus distance ($\boldsymbol{N_F=\delta/\beta}$), the effects of image blurring due to the finite PSF of the imaging system and the *Fresnel diffraction effects can be made to cancel each other resulting in a simultaneous automatic phase retrieval and spatial deconvolution of partially coherent images of homogeneous objects*.