Detailed ray-tracing code for capillary optics

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Outline

• Introduction: motivation for developing the capillary ray-tracing model

• main features of our capillary ray-tracing

• simulation versus experiment: far-field images from mono-capillaries

• applications of the code for the optimization of capillary dimensions for submicron focusing/concentration

• the simulation of polycapillary optics
Models for microscopic X-ray fluorescence

Aim: calculation of the full spectral response via the simulation of photon-matter interactions
Main types of mono-capillary optics

- parallel bore-hole (straight) capillary
- tapered bore-hole (conical) capillary
- ellipsoidal (single-bounce) capillary
Polycapillary Optics

Polycapillary optics

Hundreds of thousands of glass fibers having internal diameters of 3-10 µm => X-rays are guided by multiple total reflections within the fibers towards a common focal point

Polycapillary Optics

Polycapillary optics

Point source (X-ray tube)

(a)

Parallel beam (SR beam)

(b)

Point source

(c)

Focus

Parallel output beam

Critical angle of total reflection for glass at X-ray energy $E$:

$$\theta_c \approx \frac{30}{E[\text{keV}]} \text{[mrad]}$$

Reflectivity $\approx 1$ for $\theta \leq \theta_c$

Figure 3.3.1 Polycapillary X-ray optics that produce a focused (a, b) or parallel beam (c), starting from a X-ray point source (micro-focus X-ray tube (a, c)) or a quasi-parallel X-ray source (synchrotron (b)).

Figure 3.3.2 Schematic representation of the principles of capillary optics. $\theta_c$ is the critical angle for total reflection.
Main features of the capillary ray-tracing

• Based on geometrical optics

• uses the Monte Carlo method: (pseudo) random selection of the initial parameters of the photons \((E_0, P_0, \mathbf{r}_0, \mathbf{k}_0)\)

• simulates photon trajectories in 3D, assuming circular or rectangular capillary cross-section

• numerically defined capillary shapes:
  • arbitrary shape distortions, including bent axis

• surface roughness/waviness considered:
  • (reduction of specular reflectivity & diffuse scattering)

Vincze et al., Detailed ray-tracing code for capillary optics
Modeled physics

- Total external reflection on the internal surface including surface roughness modeling => Fresnel reflectivity calculated using scattering factors by Henke et al. [1]; absorption coefficients from McMaster et al [2].
  
- Compton and Rayleigh scattering within the capillary material
  => by atomic (bound) electrons; atomic form factors F(x,Z) and incoherent scattering functions S(x,Z) by Hubbell et al [3].

  => polarization dependent scattering cross sections

- arbitrary multi-element composition (H to U)

- X-ray energy range 1-80 keV

- simplified sources: Gaussian or uniform/isotropic

References


Simulated geometry:

• arbitrary 3D axis
• numerically defined shape
• circular or rectangular cross-section

Ray-tracing corresponding to a measured capillary profile
The ray-tracing model

Necessity to simulate in 3D!

much larger number of reflections then estimated in 2D for extended sources.

Simulated capillary:

10 → 2 µm; L = 10 cm
source: 10 × 10 µm² @ 5 cm
Photon transmission through the capillary wall

Penetration of the photons through the capillary wall

=> can have a significant contribution to the generated beam in case of thin-walled optics at higher X-ray energies => ‘halo effects’
Comparison with an analytical model

Conical capillary: $31 \rightarrow 5 \, \mu\text{m}$, $L = 7 \, \text{cm}$, $d_{\text{sou}} = 5 \, \text{cm}$


Simulated far-field images @ 11 cm

- Point source
- True beam
- $100 \times 100 \, \mu\text{m}^2$ source, $E = 17.4 \, \text{keV}$
- Halo
- Misaligned conical capillary
Intensity loss along the capillary at a photon energy of 17.4 keV

Concentrated versus ‘leaked’ intensity as a function of photon energy

Capillary: 31 $\rightarrow$ 5 $\mu$m, L = 7 cm, $d_{\text{source}}$ = 5 cm
Capillary far-field images

Capillary #29: 42 $\rightarrow$ 20 $\mu$m; l = 10 cm

- perfect conical capillary, 0.3 mrad misalignment
- + wavy surface, max. deviation 0.15 $\mu$m, corr. length 5 mm

**simulation**

experimental CCD image @ 11 cm, E = 8.9 keV

Recorded at the ESRF Optical beamline (P. Engström, A. Rindby)

Simulated and experimental output images from a misaligned tapered capillary having a length of 10 cm, reducing the beam from 100 µm to 10 µm. The experimental image was recorded at the Microfocus beamline of the ESRF (ID13).

Simulated far field image of a tapered capillary having rectangular cross-section.

assumed source: ESRF ID13, capillary: 15 → 3 µm, L = 10 cm.
Surface roughness model

Surface characterized by: roughness ($\sigma_R$) and correlation length ($s$)

Surface roughness model

Ideal surface
Energy = 10 keV

$\sigma_R = 30 \text{ Å}, s = 10 \text{ µm}$

$\sigma_R = 50 \text{ Å}, s = 10 \text{ µm}$

Capillary: 100 $\rightarrow$ 10 µm; length = 20 cm

experimental CCD image from a well-aligned capillary @ 11 cm
capillary: 70 $\rightarrow$ 12 µm, l = 23 cm
e = 8.9 keV (ESRF Optical Beamline)
ESRF Microfocus beamline (ID13), before upgrade

**Source**
- Size (H x V): 134*24 µm²
- Divergence (H x V): 0.21*0.02 mrad²

**Focus**
- Size (H x V): 20*40 µm²
- Divergence (H x V): 2.1*0.2 mrad²

Measured efficiency at 13 keV: 0.27 %
ray-tracing, assuming $\sigma_R = 30 \text{ Å}$: 0.28 %

Add-on capillary optics
- Capillary #61

- Mirror focus
- Undulator
- Si (111)
- Ellipsoidal mirror

Divergence (H x V)
- 0 29.4 31 34.1 m from the source
Possible causes for the low experimental efficiency

Effects of surface roughness

\[ \sigma_R \leq 30 \text{ Å} \]

Effects of capillary bending

\[ \Delta z \leq 4 \text{ µm} \]

Probably the combination of the above factors + waviness
Intensity loss on the capillary internal surface

capillary: #61, 77 → 2 µm, L = 12.3 cm
source: 20 x 40 µm², 2.1 x 0.2 mrad²
(focused beam by ellipsoidal mirror)
E = 13 keV (ESRF ID13)
Halo effects

Intensity distribution at 100 µm from the capillary exit:

Capillary #61

Perfect conical capillary, equivalent dimensions

1 order of magnitude higher level of halo!
Low-beta undulator source

Case study: ESRF Microfocus (ID13) beamline

Optimum parameters of tapered capillary optics providing a 100 nm beam assuming pre-focusing with Kirkpatrick-Baez mirrors producing beam dimensions at the capillary entrance: 0.35 x 0.42 $\mu m^2$, 2.8 x 1.6 $mrad^2$ (HxV, FWHM)
Optimization of capillary dimensions for sub-micron focusing

Beam line: ID13
Expected beam dimensions at the capillary entrance:
0.35 x 0.42 \( \mu m^2 \), 2.8 x 1.6 \( mrad^2 \) (HxV, FWHM)

Capillary length optimization:
a) entrance diameter: 0.5 \( \mu m \); exit = 100 nm

Capillary entrance optimization:
b) exit diameter: 100 nm; length = 2 mm

Case study: single-bounce ellipsoidal capillary @ ESRF BM5 (Snigirev et al.)

Secondary source produced by an FZP: 2.2 µm vertically and 5 µm horizontally

Ray-tracing results corresponding to the above experimental conditions

Two-step hard X-ray focusing combining Fresnel zone plate and single-bounce ellipsoidal capillary,

Polycapillary test experiments

- Full lens: point-to-point focusing

Manufactured at the Department of Low-energy Nucl. Physics, Beijing Normal University,
Y. Yan et al.
First polycapillary tests at HASYLAB beamline L (1999)

Collaboration: Gerald Falkenberg, HASYLAB

- X-ray source: bending magnet (HASYLAB Beam line L)
- Monochromator: Si(111) channel-cut
  - energy range: 5 - 24 keV
- test optics: monolithic polycapillary, half-lens
  - beam size: 34 - 53 μm, depending on the energy

Polycapillary lenses currently applied at BL L: XOS optics (beamsize ~ 5 - 20 μm)
Measured vs. simulated polycapillary efficiency

polycapillary half-lens:

\( d_0 = 7.3 \text{ mm} \)

\( d_1 = 3.6 \text{ mm} \)

\( L = 5.1 \text{ cm} \)

Source: 1.30 x 0.51 mm\(^2\), 0.40 x 0.024 mrad\(^2\) @ 20 m, illuminated area on the capillary entrance: 3 \(\times\) 1 mm\(^2\)

Confocal detection using polycapillary optics

Conventional detection

Intersection X-ray beam and sample

X-ray beam (100 nm)

Confocal detection: 10-20 \( \mu \text{m} \)

Sample on glass tip

Submicron elemental imaging at ESRF ID22NI using bent multilayer beam focusing and confocal detection mode

High resolution RGB-map of the K, Ca and Ni intensity of a series of micrometer-sized inclusions immediately below the surface of a Koffiefontein diamond.

XRF sum spectrum
Conclusions

Our capillary ray-tracing model:

- uses the Monte Carlo method for ray-tracing within the framework of geometrical optics
- treats capillaries having arbitrary shapes, composition
- considers photon penetration through and scattering by the capillary wall
- ray-tracing of polycapillaries is possible
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