Detailed ray-tracing code for capillary optics

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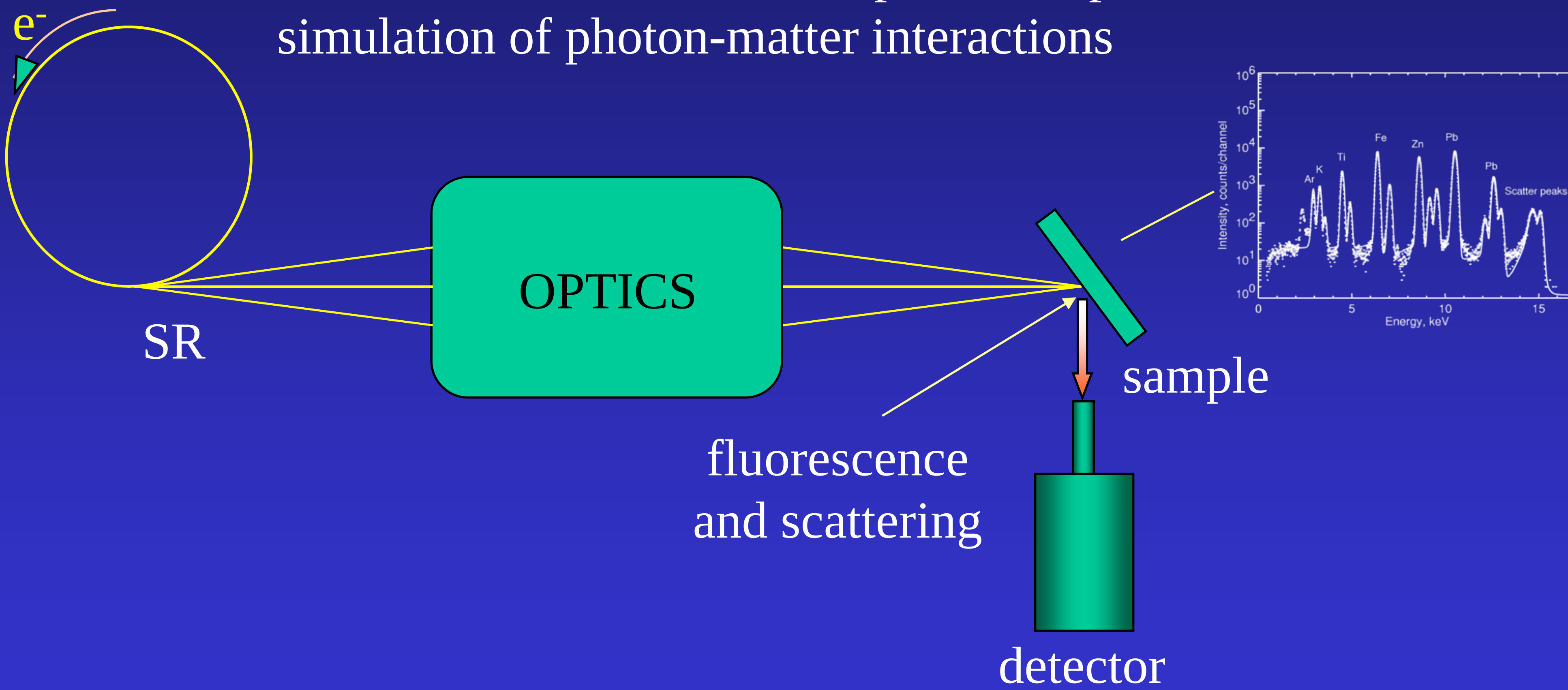
Outline

- 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

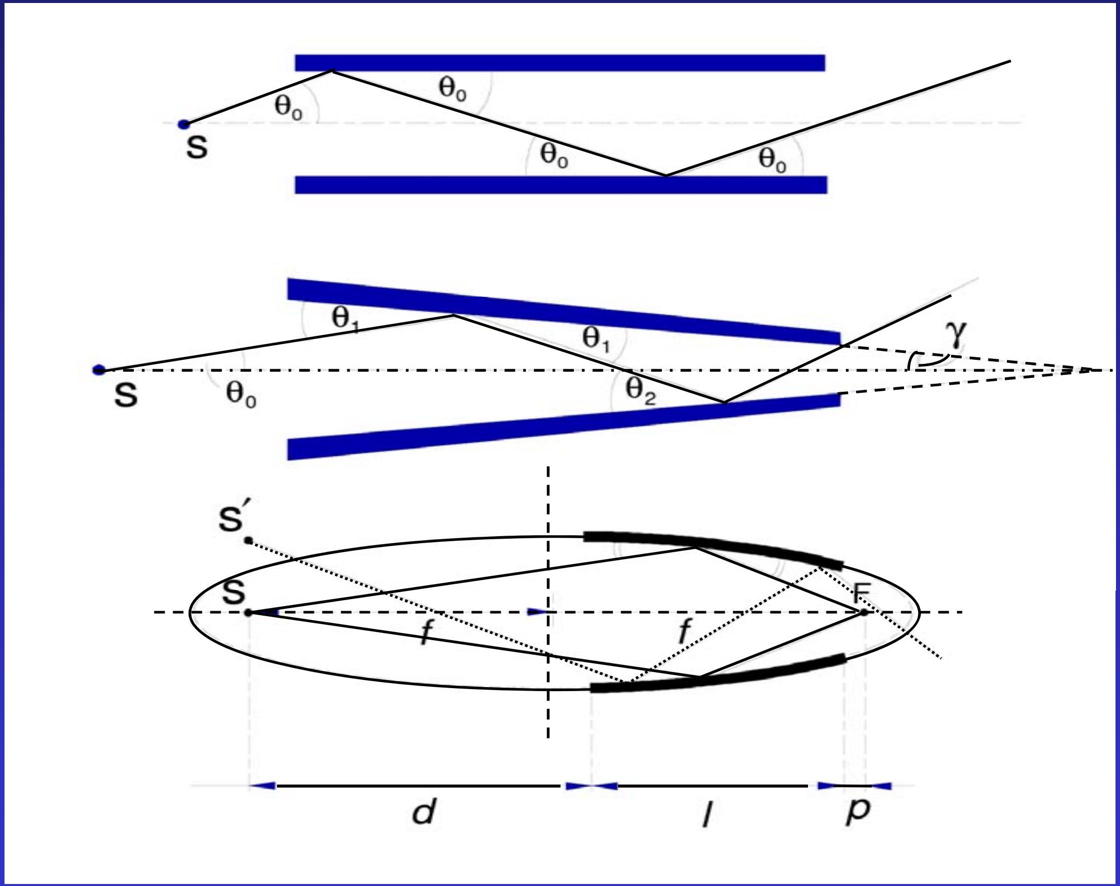


Main types of mono-capillary optics

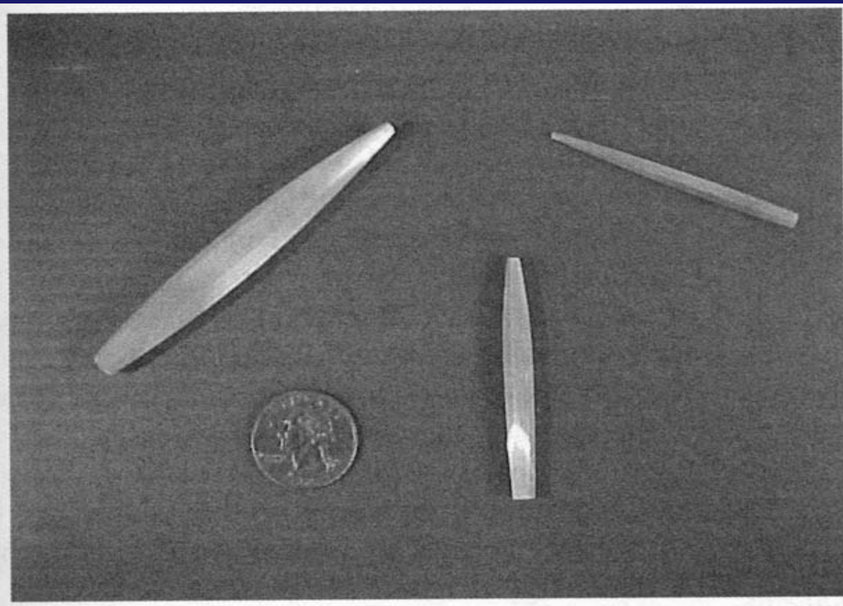
parallel bore-hole (straight) capillary

tapered bore-hole (conical) capillary

ellipsoidal (single-bounce) capillary



Polycapillary Optics



<u>Polycapillary optics</u>

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

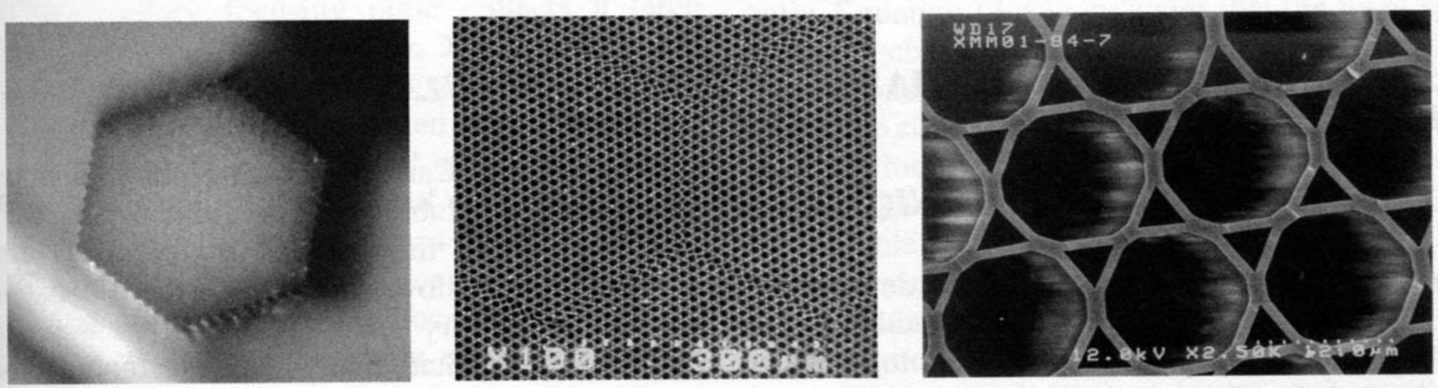


Figure 3.3.4 Photographs and SEM images showing the typical size of monolithic polycapillary optics and their cross-section

K. Tsuji, J. Injuk, R. Van Grieken (eds.), X-ray Spectrometry: Recent Technological Advances, Chapter 3.3 (2004).

Polycapillary Optics

90

Polycapillary optics

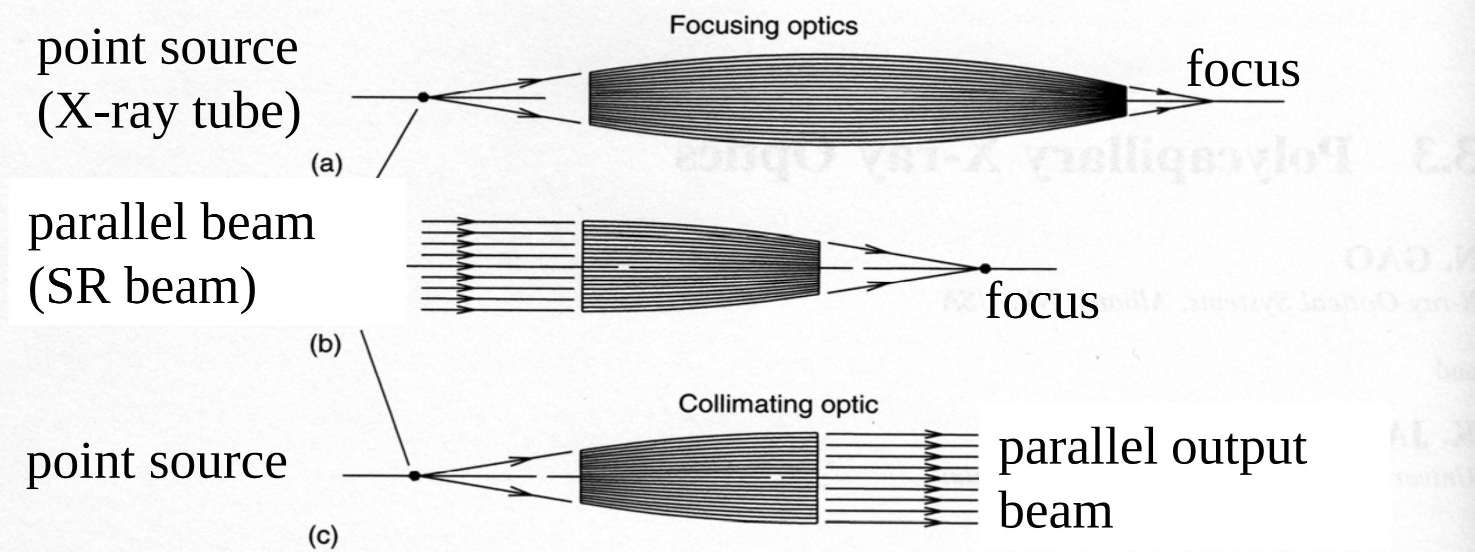


Figure 3.3.1 Polycapillary X-ray optics that produce a focused (a,b) or parallel beam (c), starting from a X-ray point source (micro-focus X-ray tube (a, c)) or a quasi-parallel X-ray source (synchrotron (b))

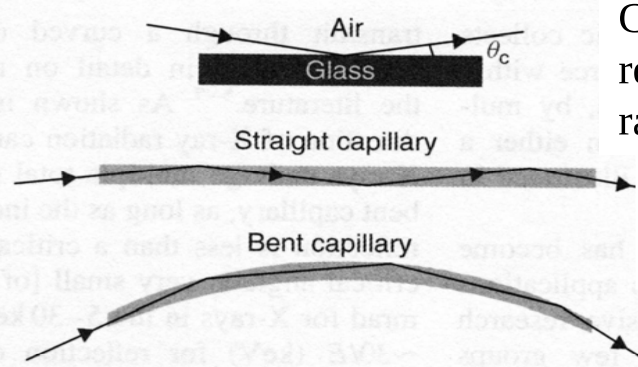


Figure 3.3.2 Schematic representation of the principles of capillary optics. θ_c is the critical angle for total reflection

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

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

reflectivity ≈ 1 for $\theta \le \theta_C$

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 $(E_0, P_0, \vec{r}_0, \vec{k}_0)$

- 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

X-Ray Spectrometry, Volume 24 Issue 1, Pages 27 – 37, 1994.

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

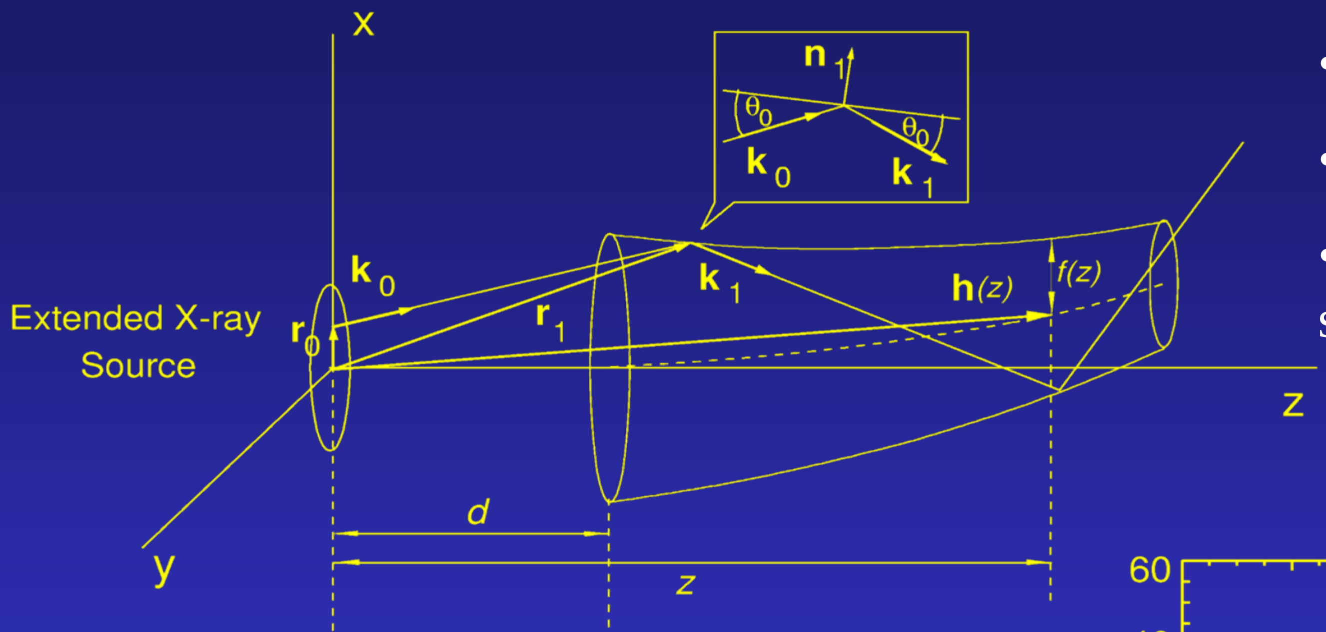
References

[1] B.L. Henke, E.M. Gullikson, and J.C. Davis. X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30000 eV, Z=1-92, Atomic Data and Nuclear Data Tables Vol. 54 (no.2), 181-342 (July 1993)

[2] McMaster, W.H., Kerr del Grande, N., Mallett, J.H., and Hubbell, J.H., Lawrence Livermore National Laboratory Report UCRL-50174 (1969), S2.

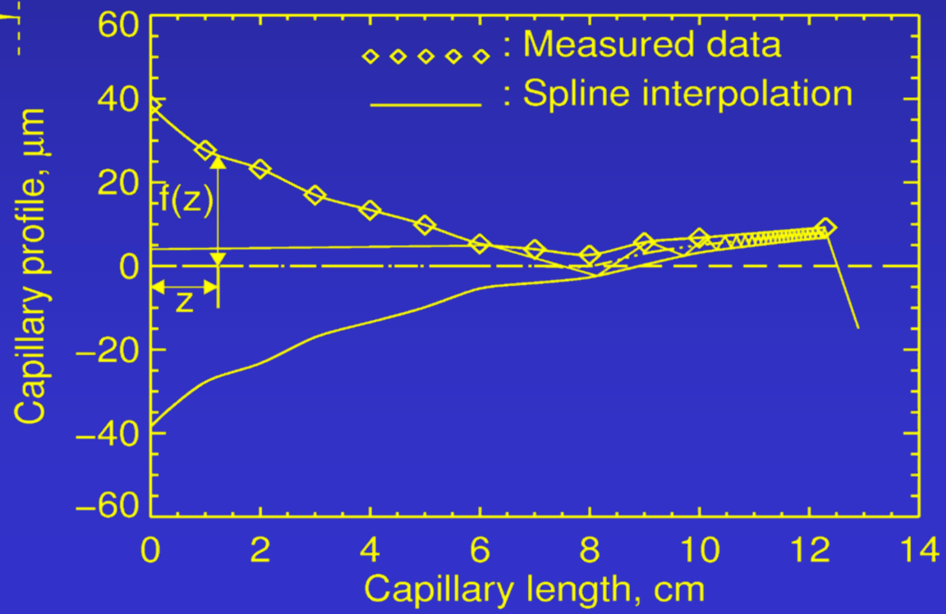
[2] Hubbell, J.H., Veigele, Wm.J., Briggs, E.A., Brown, R.T., Cromer, D.T., and Howerton, R.J., "Atomic form factors, incoherent scattering functions, and photon scattering cross sections," J. Phys. Chem. Ref. Data 4, 471-538 (1975).

Simulated geometry:



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

Ray-tracing corresponding to a measured capillary profile



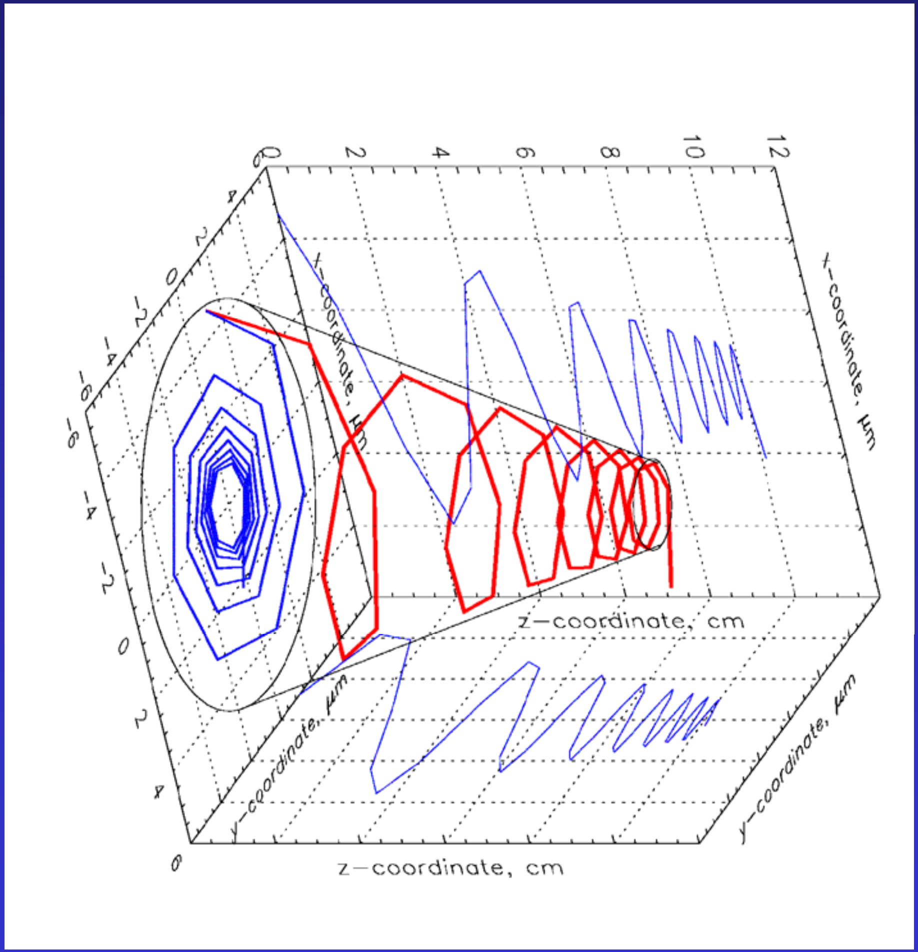
The ray-tracing model

Necessity to simulate in 3D!

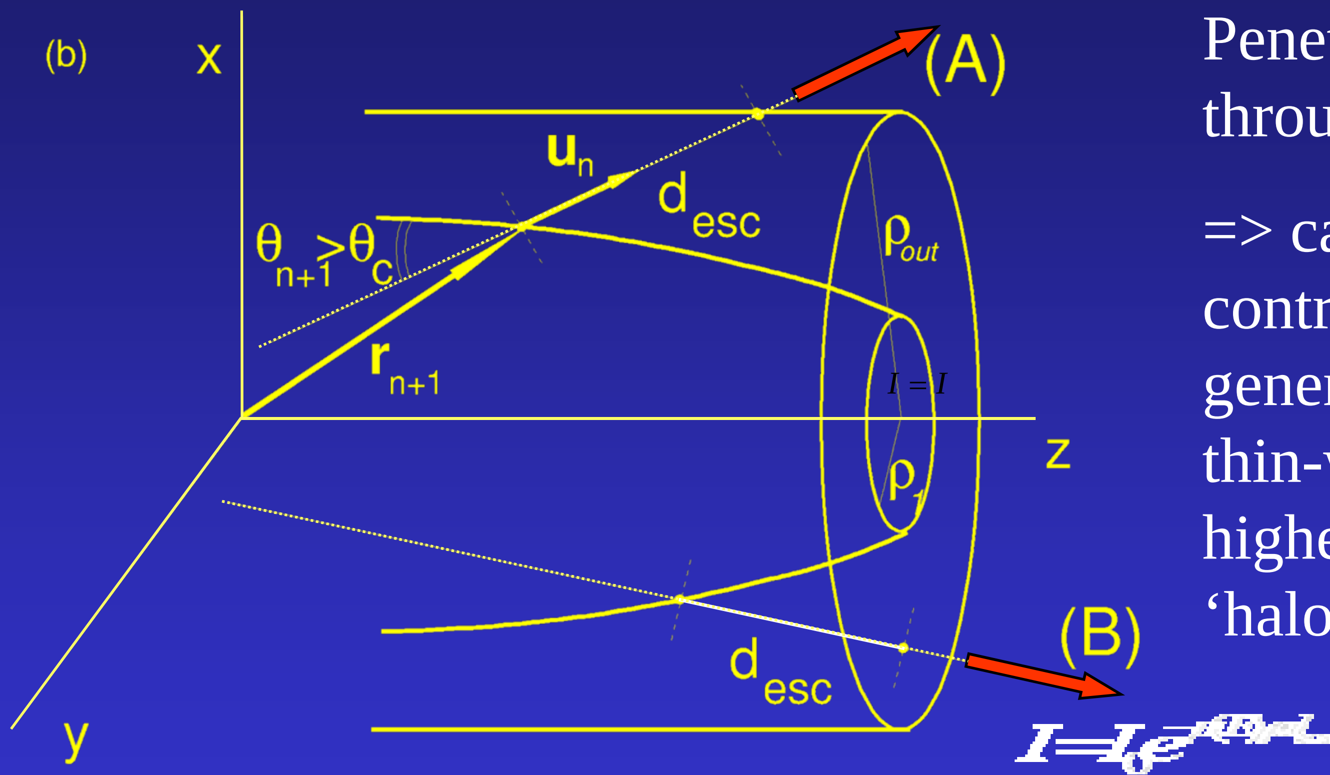
➡ much larger number of reflections then estimated in 2D for extended sources.

Simulated capillary:

10 ⟶ 2 µm; L = 10 cm
source: 10 × 10 µm^2 @ 5 cm



Photon transmission through the capillary wall

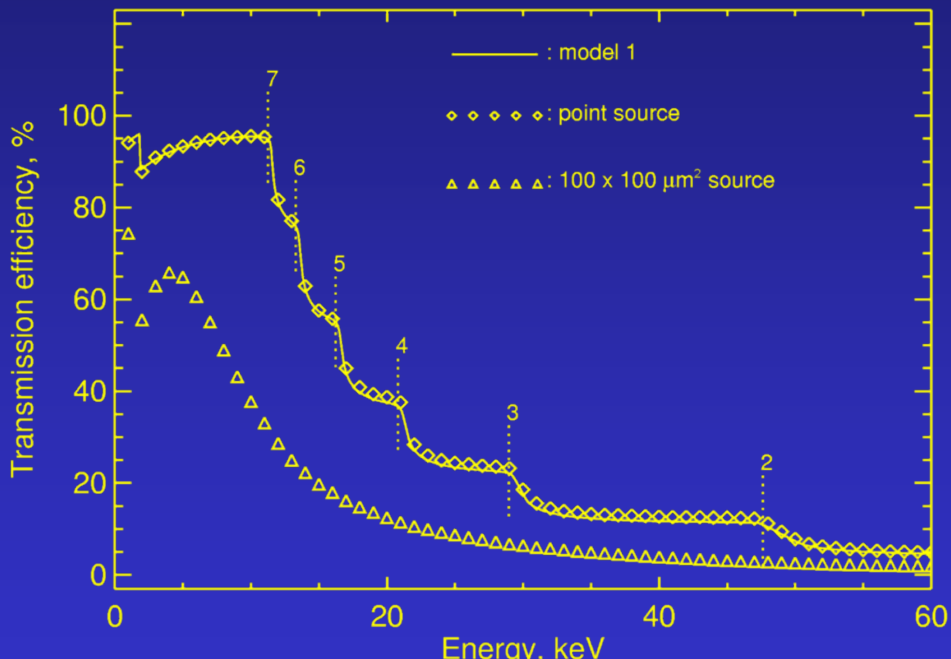


Penetration of the photons through the capillary wall

=> 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 → 5 μm, L = 7 cm, d_{sou} = 5 cm

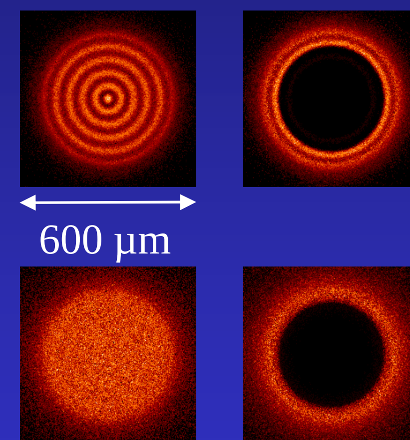


Analytical model: P. Engström, Ph.D. thesis, Chalmers Univ. of Technology (1991).

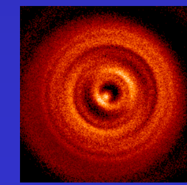
Simulated far-field images @ 11 cm

Point source

100 × 100 μm² source, E = 17.4 keV

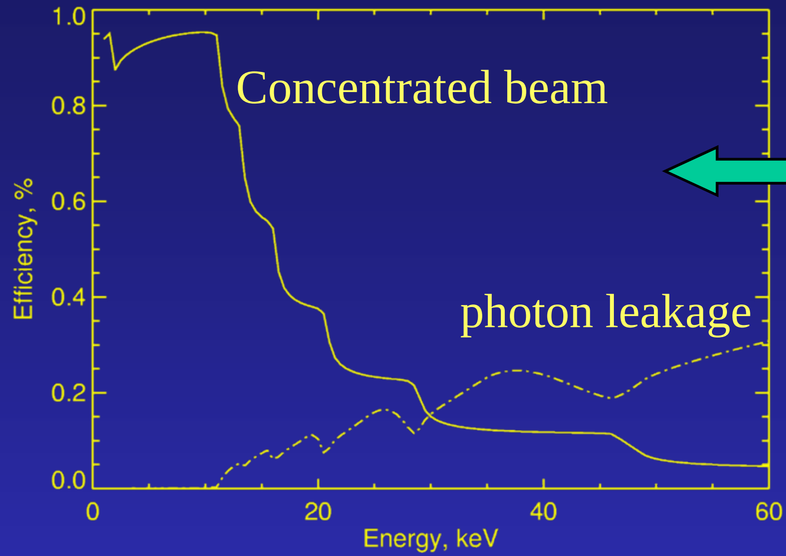


True beam halo



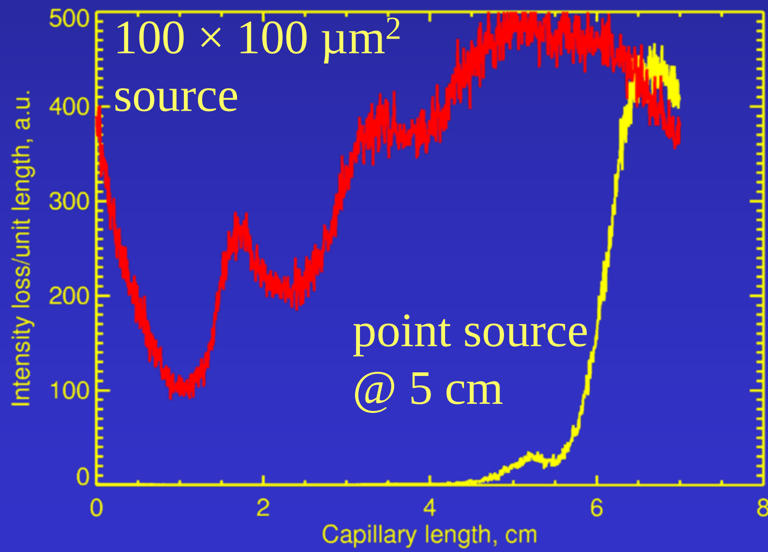
misaligned conical capillary

Capillary: 31 → 5 µm, L = 7 cm, d_{sou} = 5 cm



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

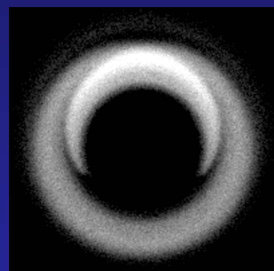
Intensity loss along the capillary at a photon energy of 17.4 keV



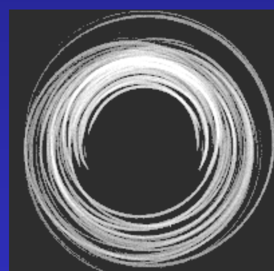
Capillary far-field images

Capillary #29: 42 → 20 µm; l = 10 cm

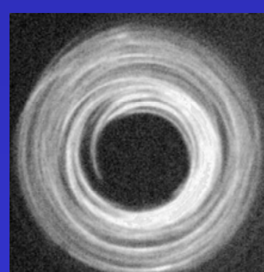
simulation



perfect conical capillary,
0.3 mrad misalignment



+ wavy surface,
max. deviation 0.15 µm,
corr. length 5 mm



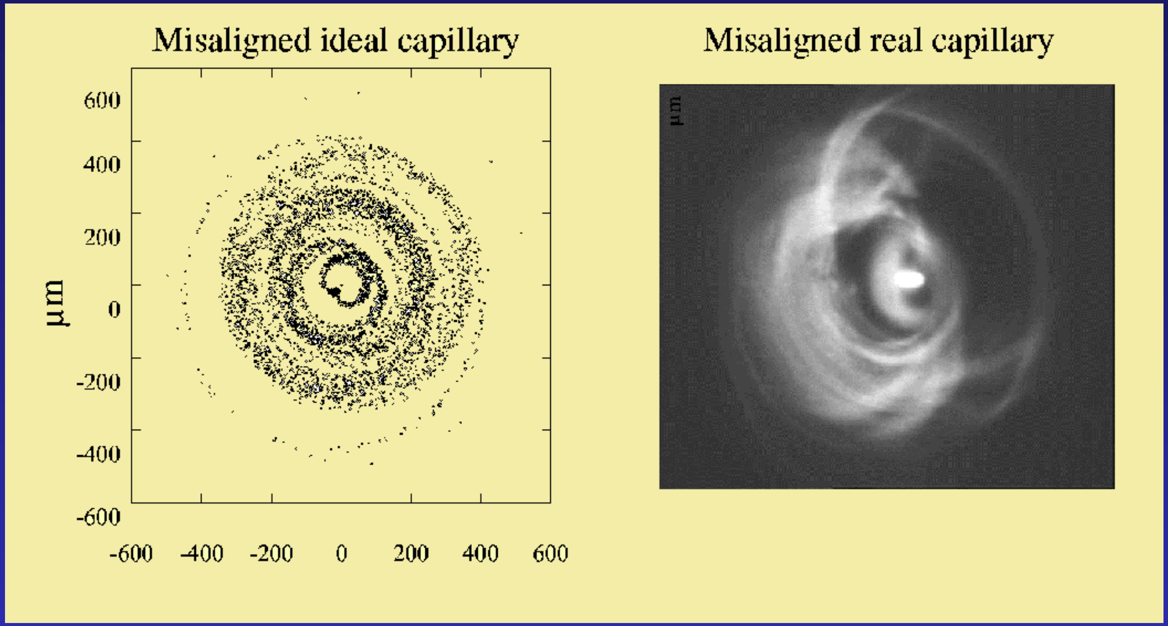
200 µm

experimental CCD image @ 11 cm,
E = 8.9 keV

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

Rev. Sci. Instrum. 69, 3494 (1998) L. Vincze,, K. Janssens, F. Adams, A. Rindby, P. Engström

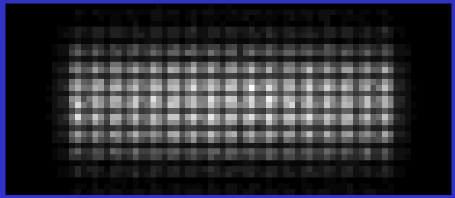
Capillary far-field images



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).

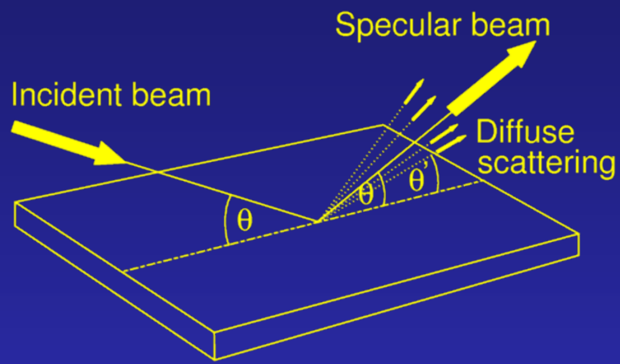
Simulated far field image of a tapered capillary having rectangular cross-section.

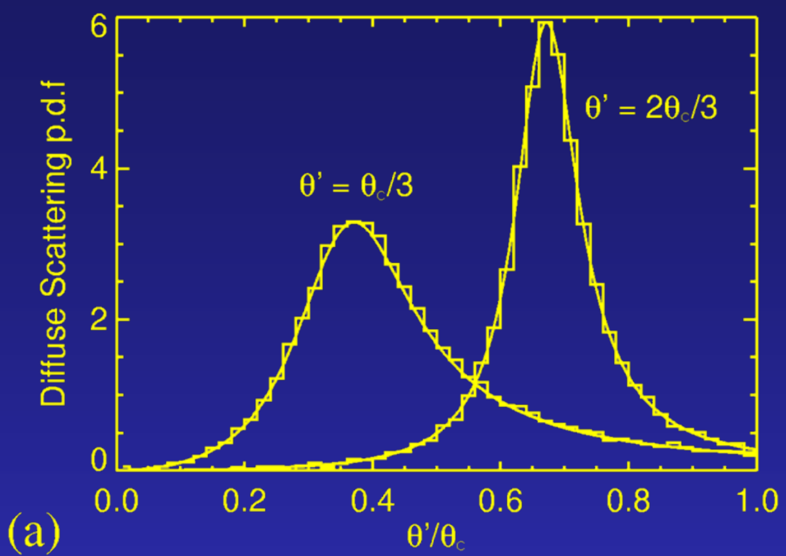
assumed source: ESRF ID13, capillary: 15 → 3 µm, L = 10 cm.

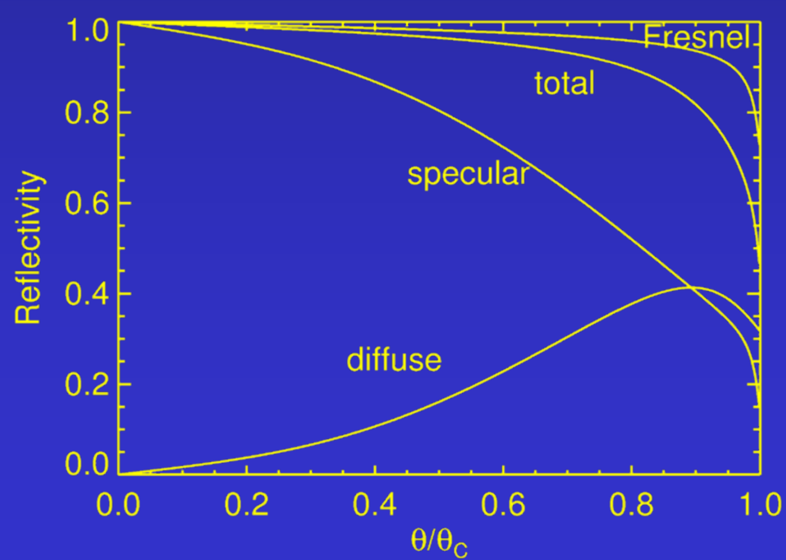


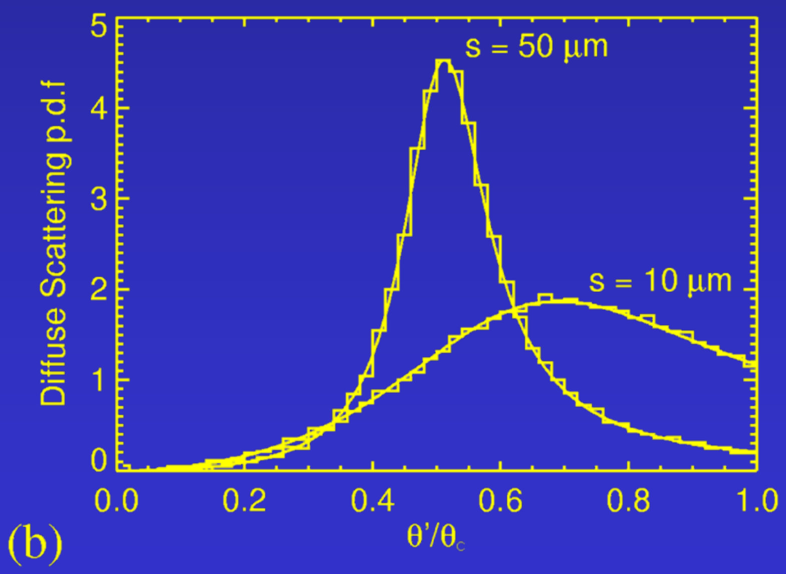
Surface roughness model

Surface characterized by: roughness (σ_R) and correlation length (s)



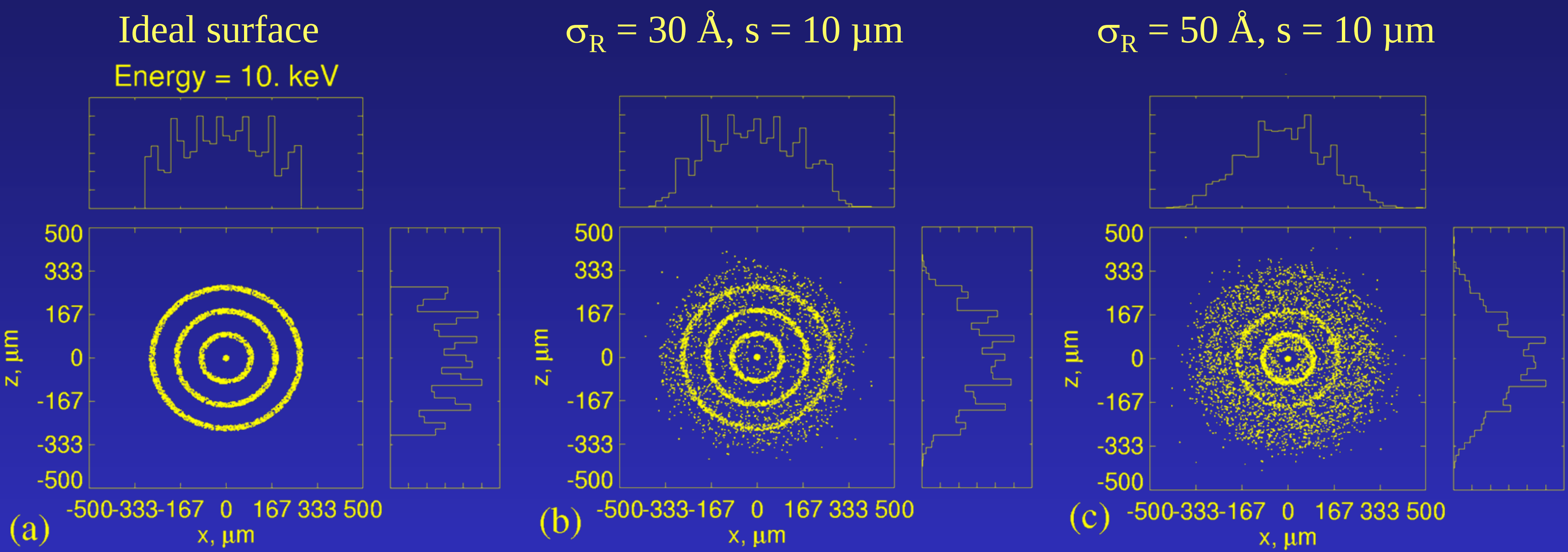




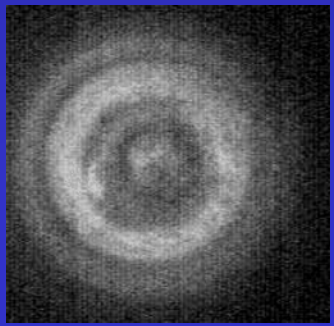


J. C. Kimball and D. Bittel, J. Appl. Phys. 74, 877 (1993)

Surface roughness model

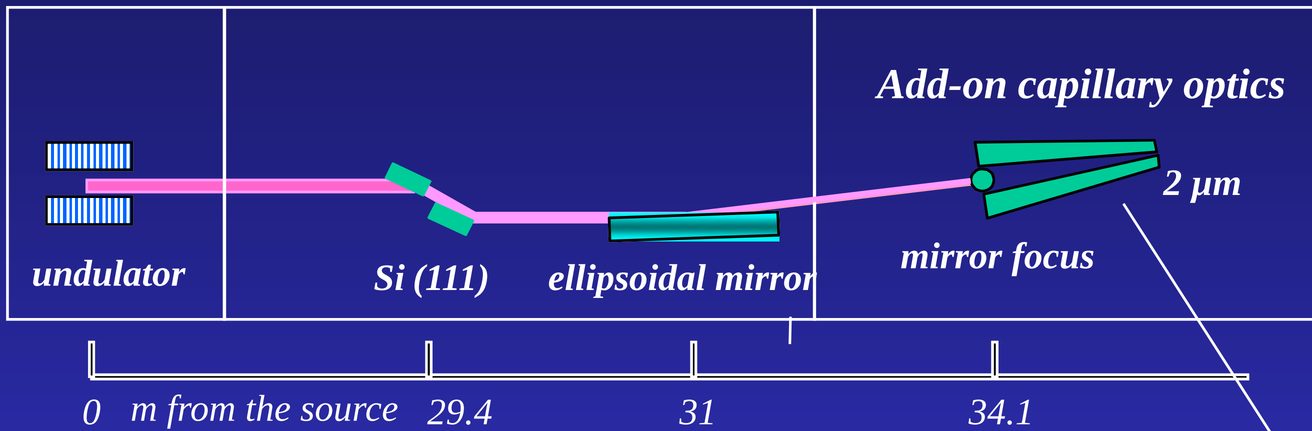


Capillary: 100 → 10 µm; length = 20 cm

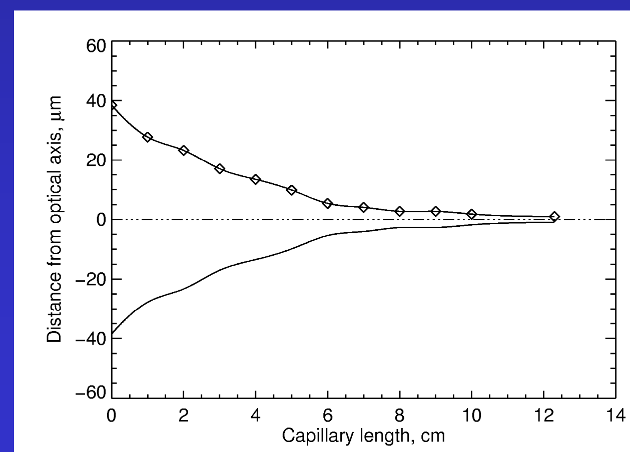


experimental CCD image from a well-aligned capillary @ 11 cm
capillary: 70 → 12 µm, l = 23 cm
E = 8.9 keV (ESRF Optical Beamline)

ESRF Microfocus beamline (ID13), before upgrade



Capillary #61



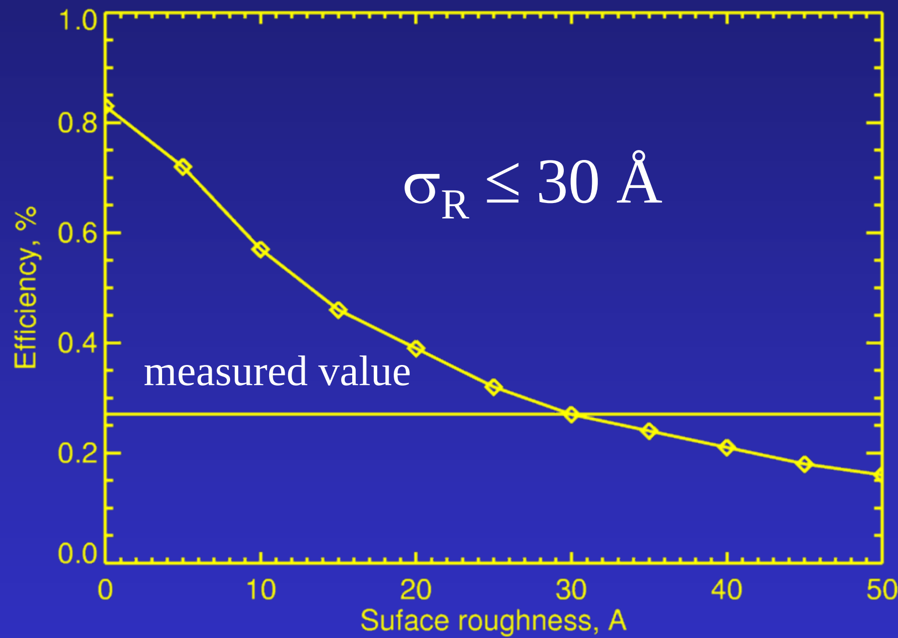
source		focus
134*24 µm²	***Size (H x V)***	***20*40 µm²***
0.21*0.02 mrad²	***Divergence (H x V)***	***2.1*0.2 mrad²***

Measured efficiency at 13 keV: 0.27 %

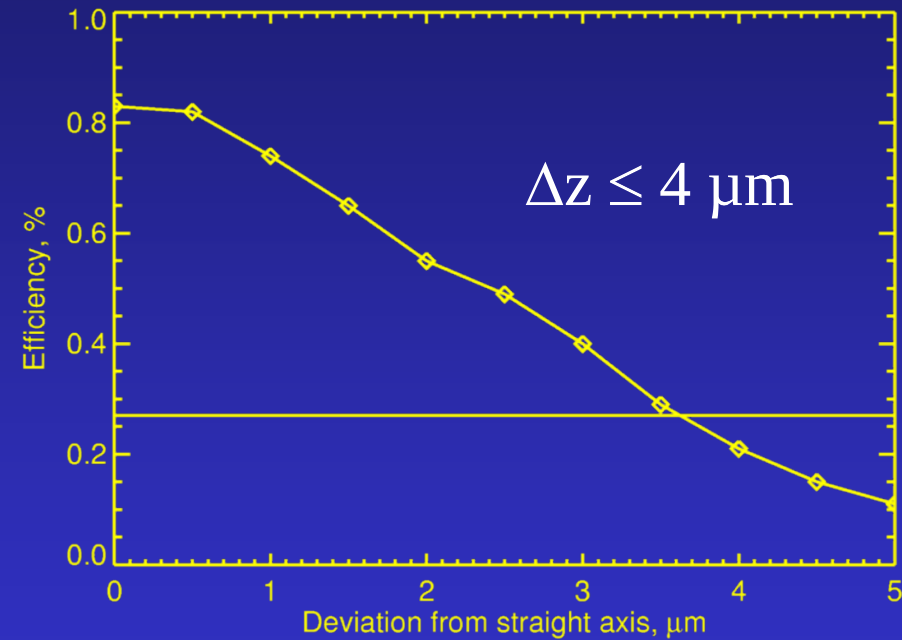
ray-tracing, assuming σ_R= 30 Å: 0.28 %

Possible causes for the low experimental efficiency

Effects of surface roughness



Effects of capillary bending



⇒ Probably the combination of the above factors + waviness

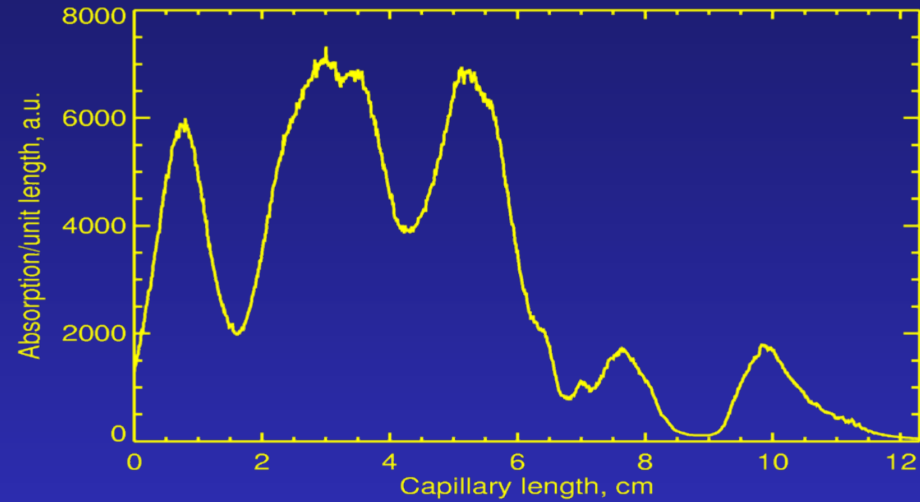
Intensity loss on the capillary internal surface

capillary: #61, 77 → 2 μm, L = 12.3 cm

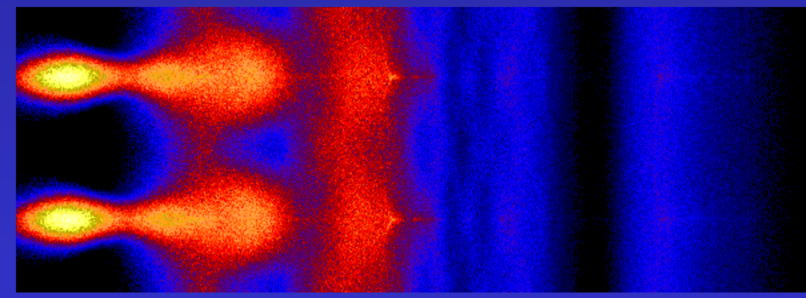
source: 20 x 40 μm^2, 2.1 x 0.2 mrad^2
(focused beam by ellipsoidal mirror)

E = 13 keV (ESRF ID13)

Intensity loss along the capillary



transversal direction

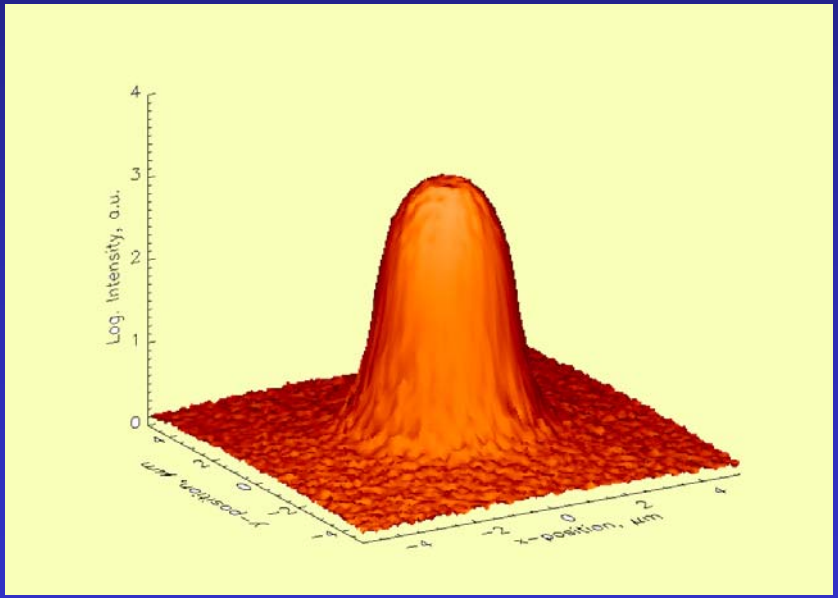


longitudinal direction

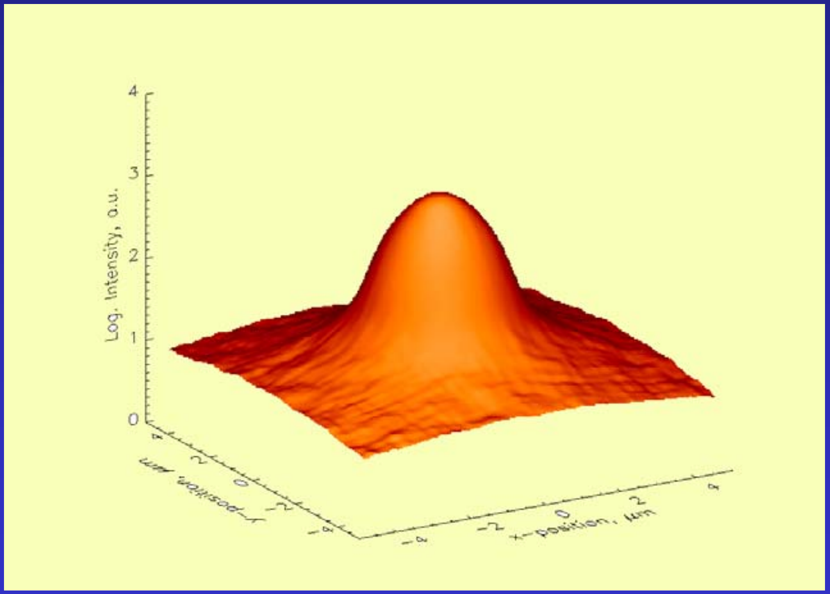
Halo effects

Intensity distribution at 100 µm from the capillary exit:

Capillary #61

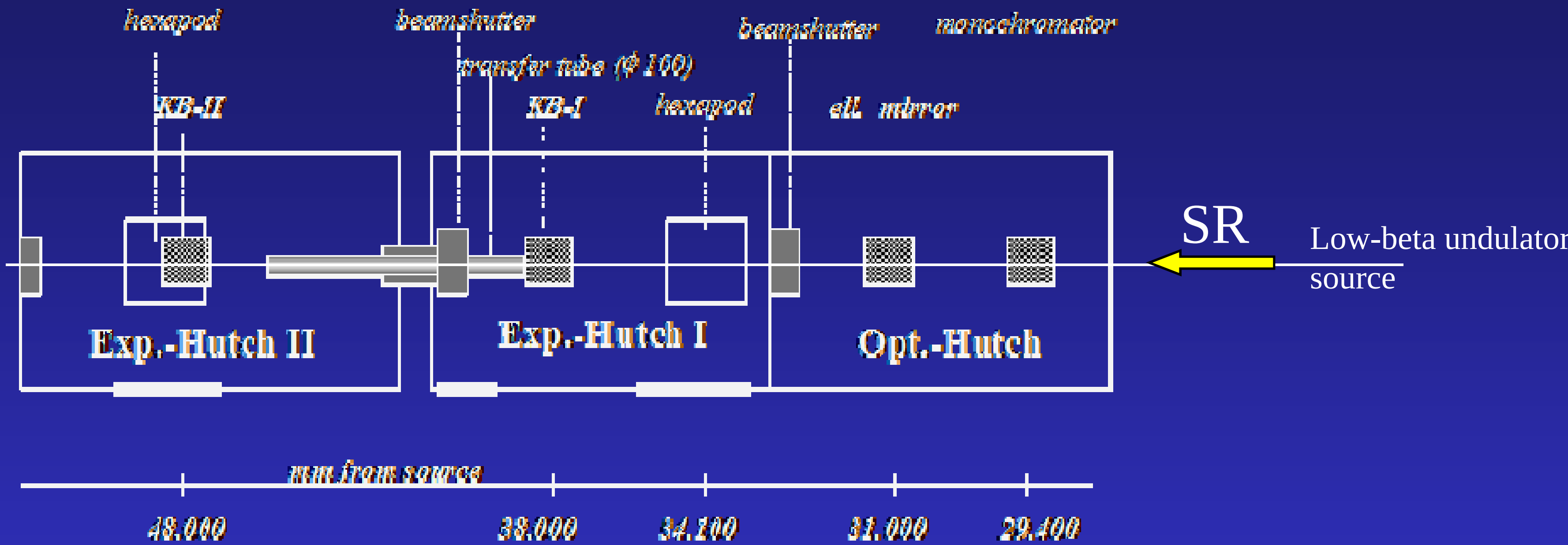


Perfect conical capillary, equivalent dimensions



➡ 1 order of magnitude higher level of halo!

Case study: ESRF Microfocus (ID13) beamline

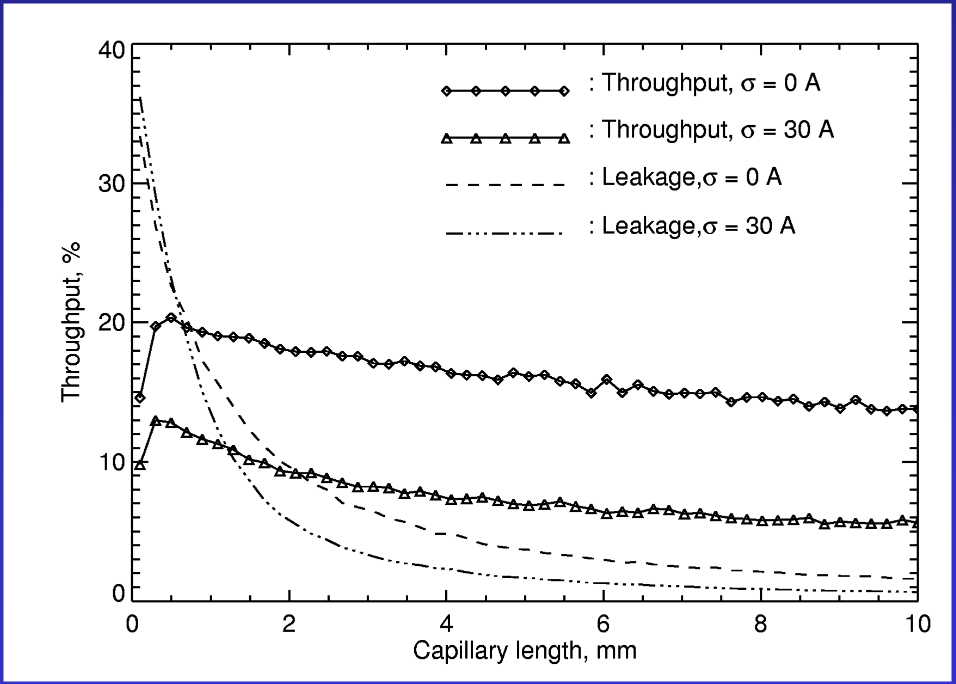


Optimum parameters of tapered capillary optics providing a 100 nm beam assuming pre-focusing with Kirkpatrick-Baez mirrors producing beam dimensions at the capillary entrance: 0.35 x 0.42 μm^2 , 2.8 x 1.6 $mrad^2$ (HxV, FWHM)

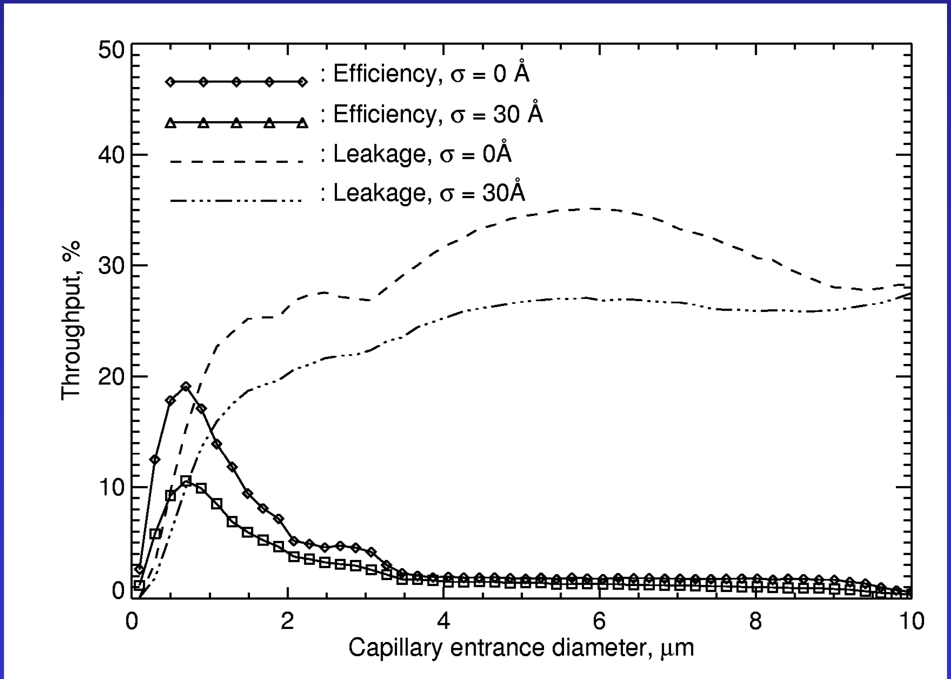
Optimization of capillary dimensions for sub-micron focusing

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

Capillary length optimization:
a) entrance diameter: 0.5 µm; exit = 100 nm

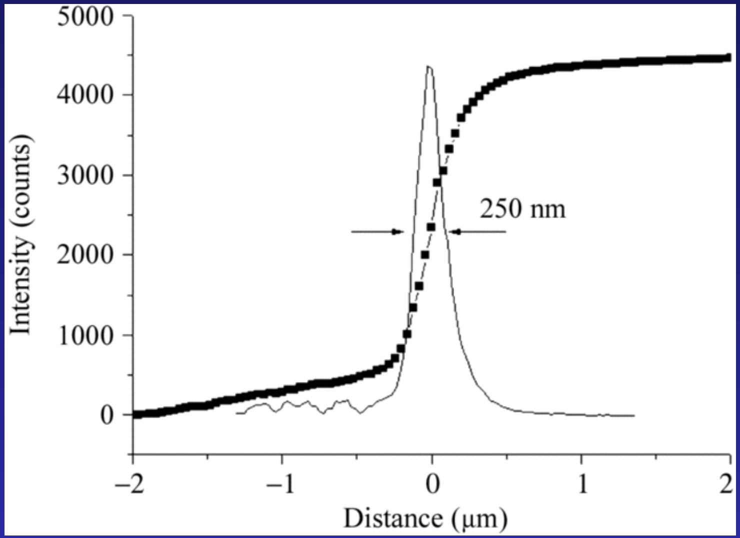


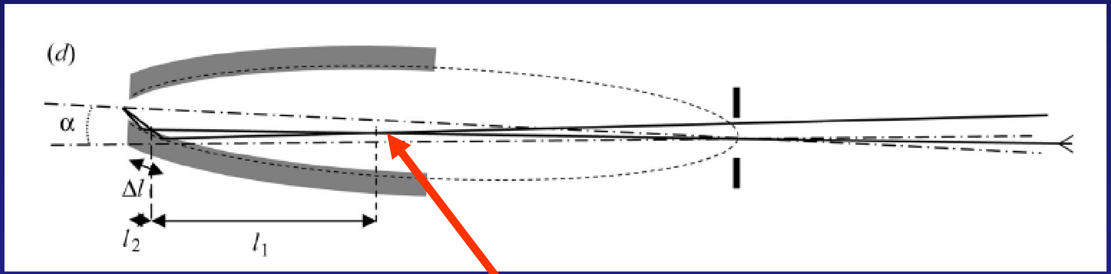
Capillary entrance optimization:
b) exit diameter: 100 nm; length = 2 mm



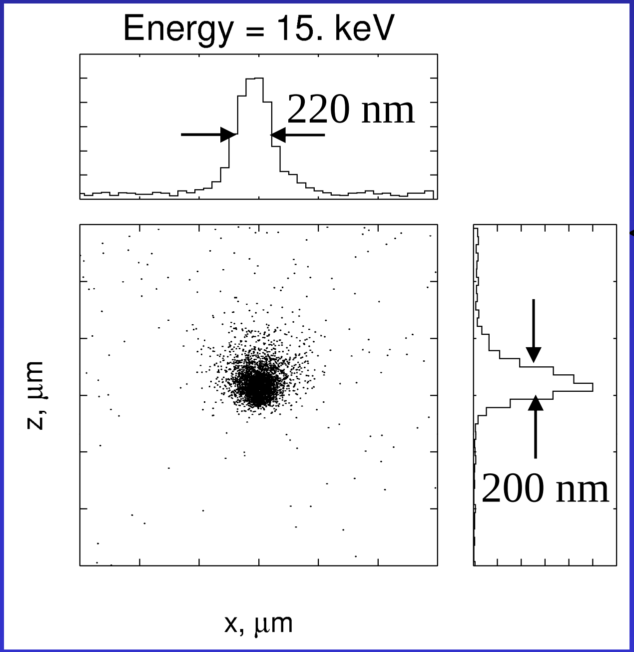
L. Vincze and C. Riekel, X-Ray Spectrom. 2003; 32: 208–214, Status and perspectives of capillary optics at a third-generation synchrotron radiation source

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

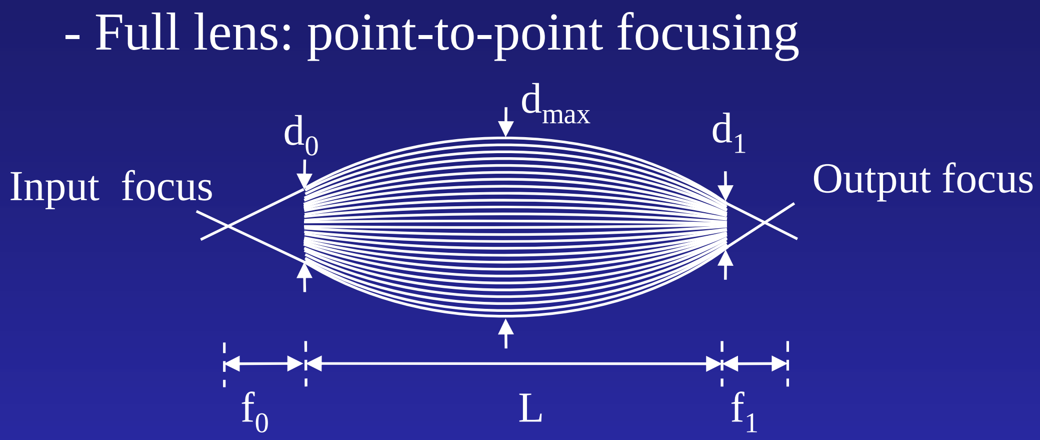


Ray-tracing results corresponding to the above experimental conditions

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

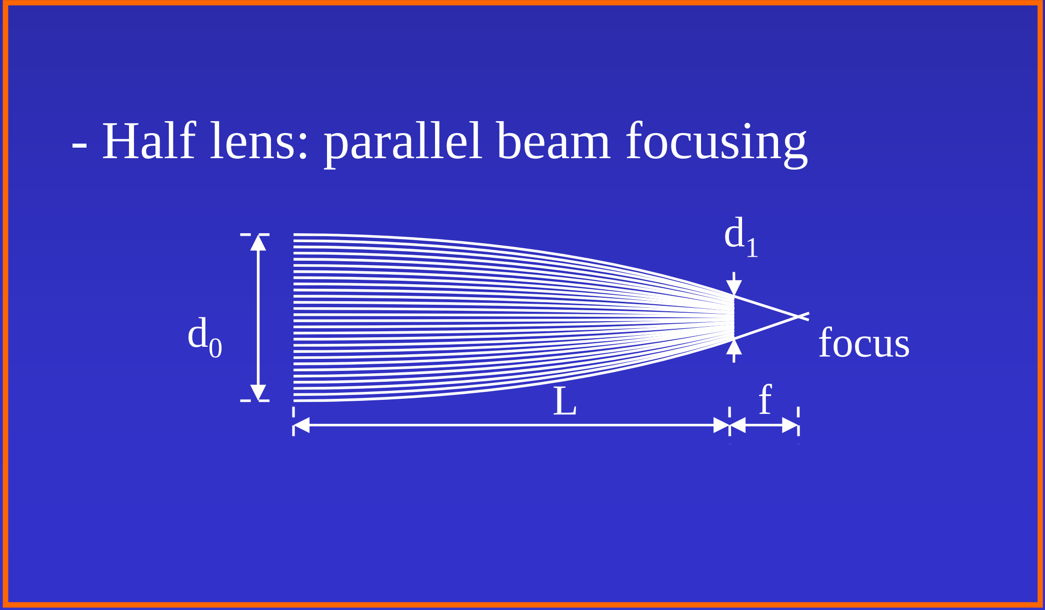
A. Snigirev, A. Bjeoumikhov, A. Erko, I. Snigireva, M. Grigoriev, V. Yunkin, M. Erkob and S. Bjeoumikhovae, J. Synchrotron Rad. (2007). 14, 326–330.

Polycapillary test experiments



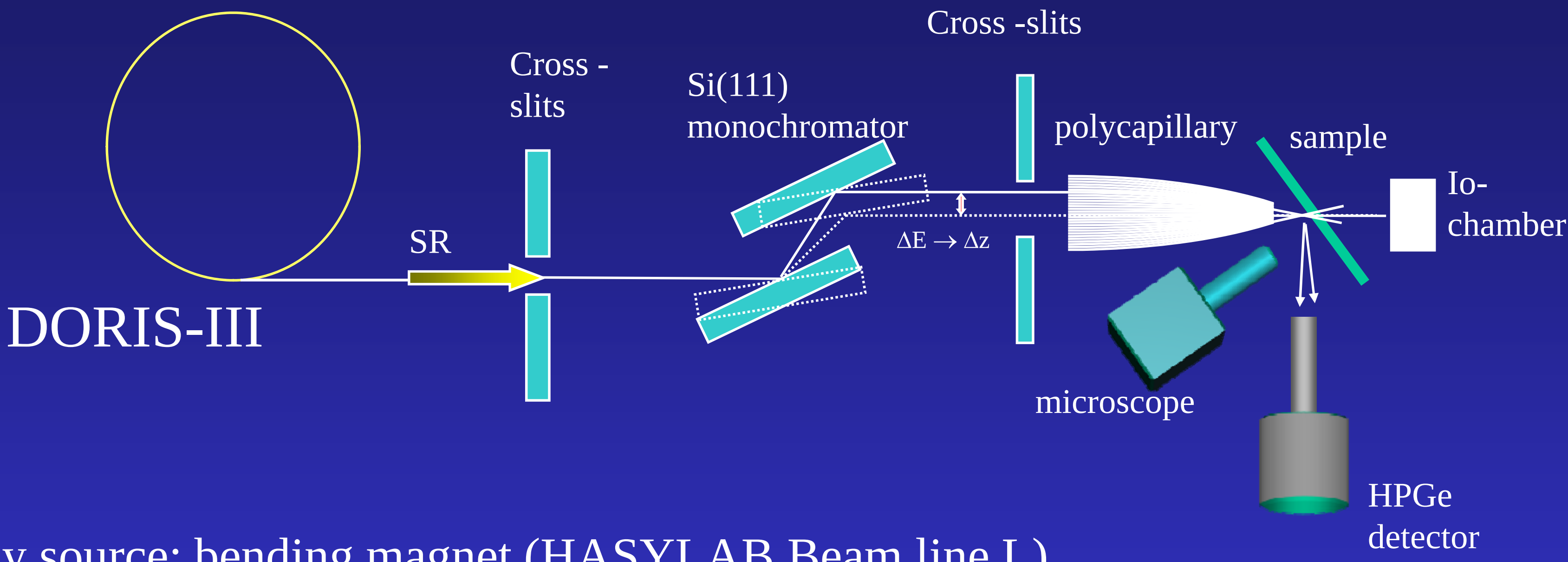
Manufactured at the Department of Low-energy Nucl. Physics, Beijing Normal University,

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

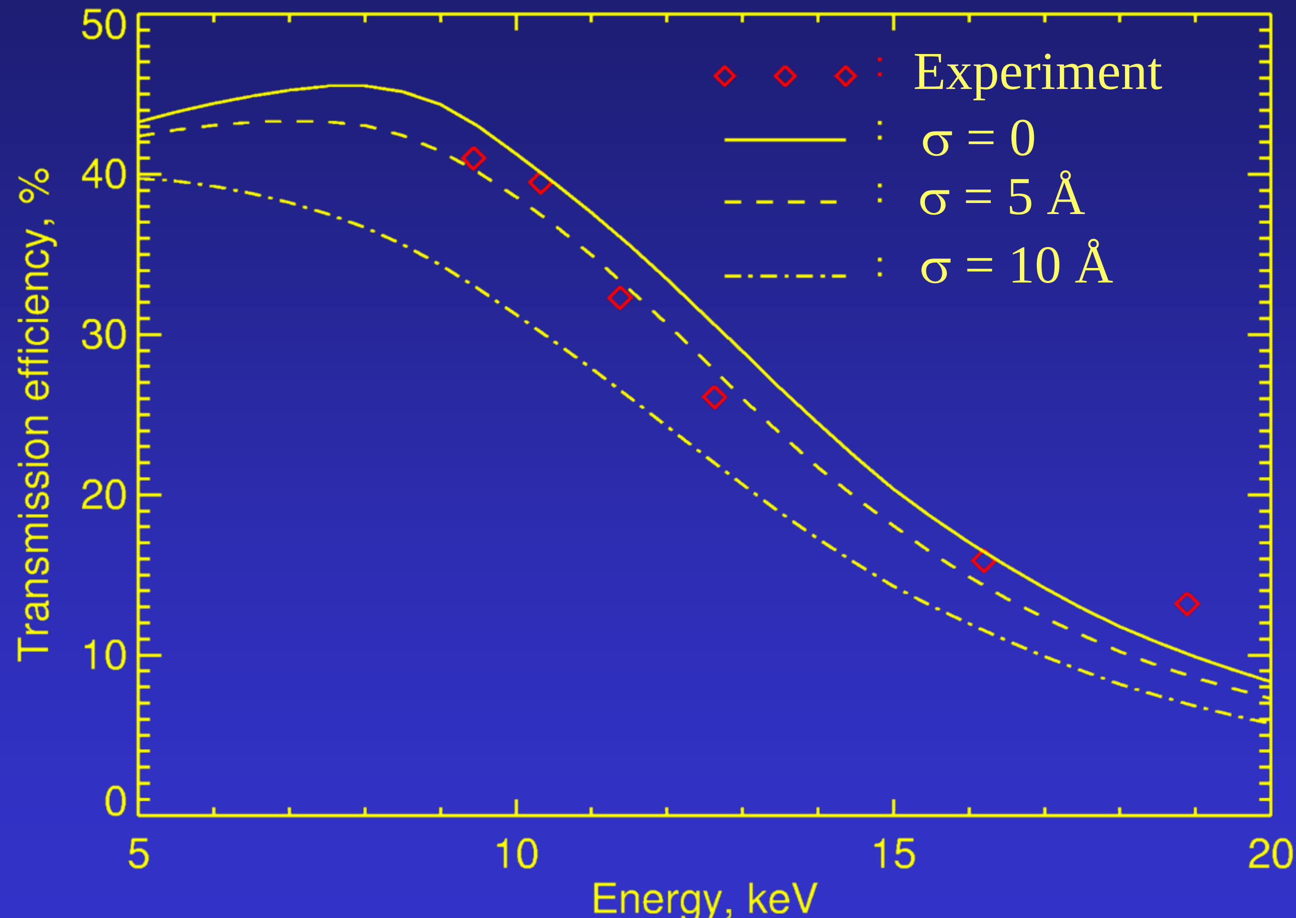
polycapillary half-lens:

d_0 = 7.3 mm

d_1 = 3.6 mm

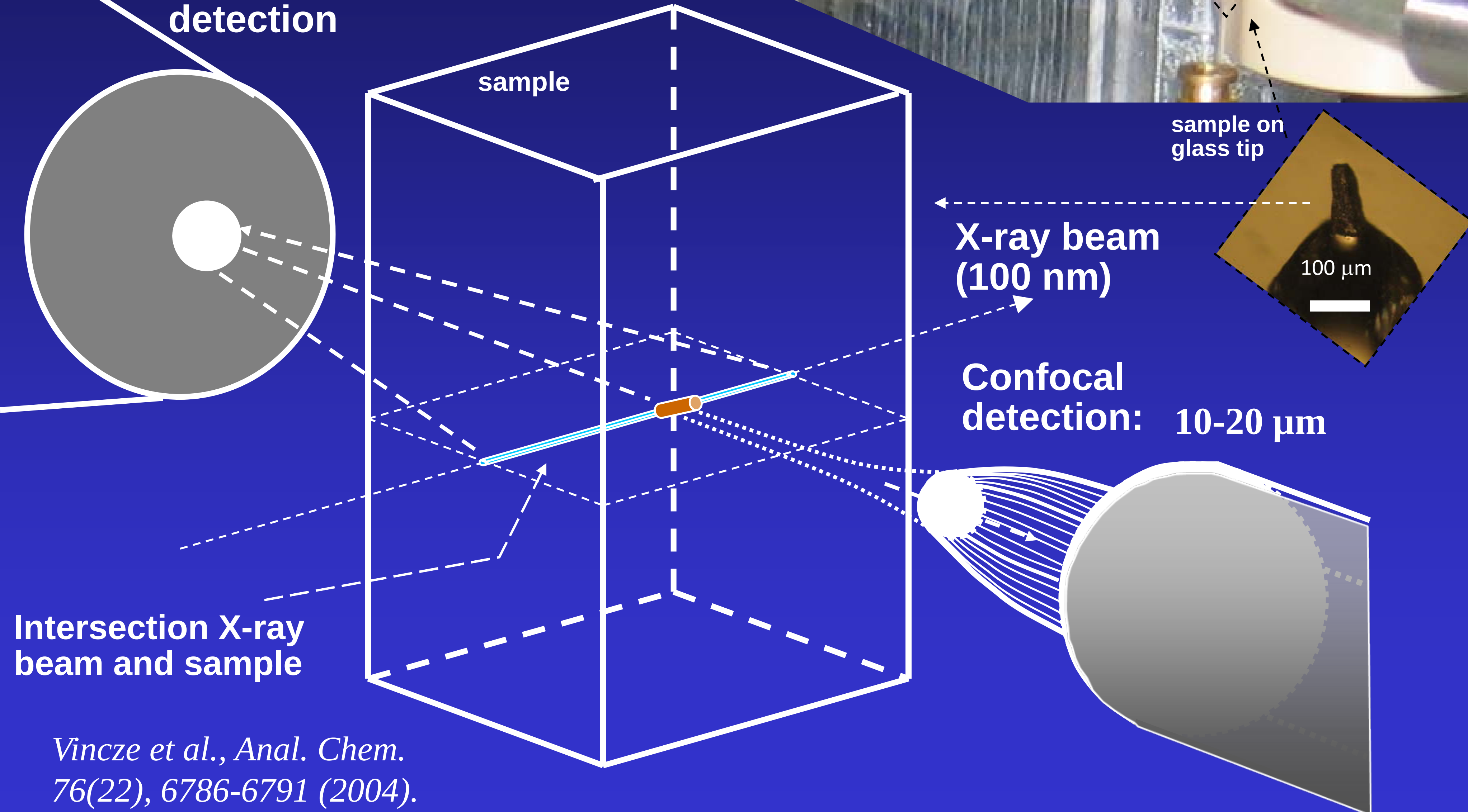
L = 5.1 cm

Source: 1.30 x 0.51 mm^2, 0.40 x 0.024 $mrad^2$ @ 20 m, illuminated area on the capillary entrance: 3 × 1 mm^2



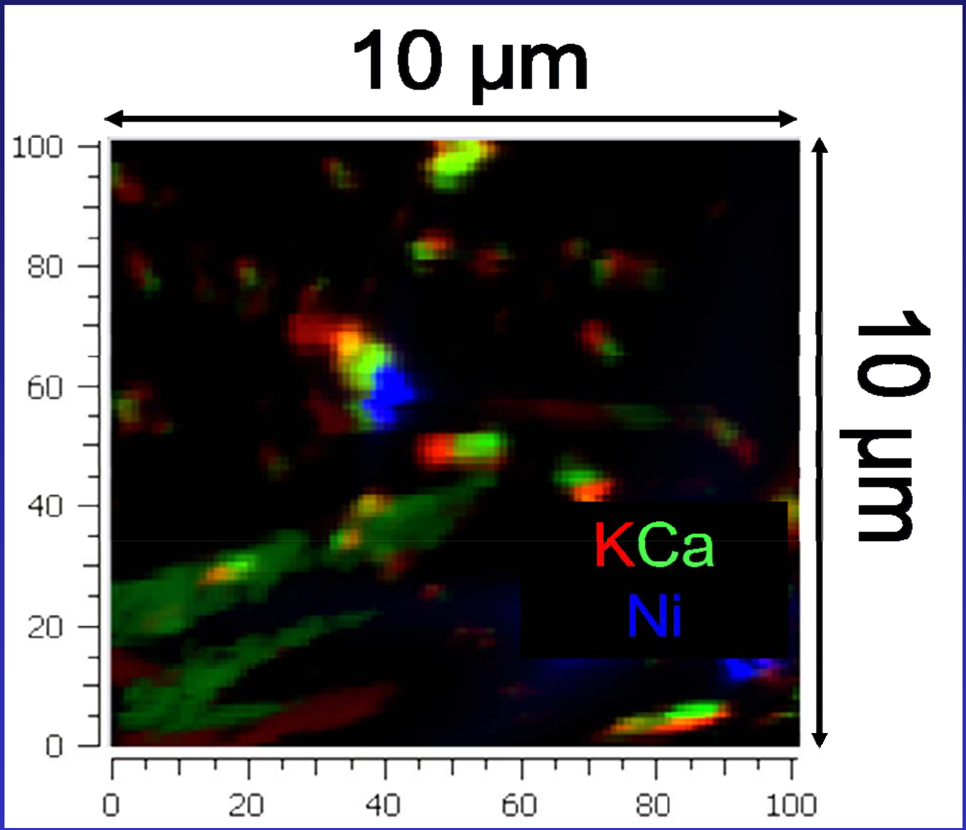
Vincze et al., J. Anal. At. Spectrom., 2002, 17, 177 - 182

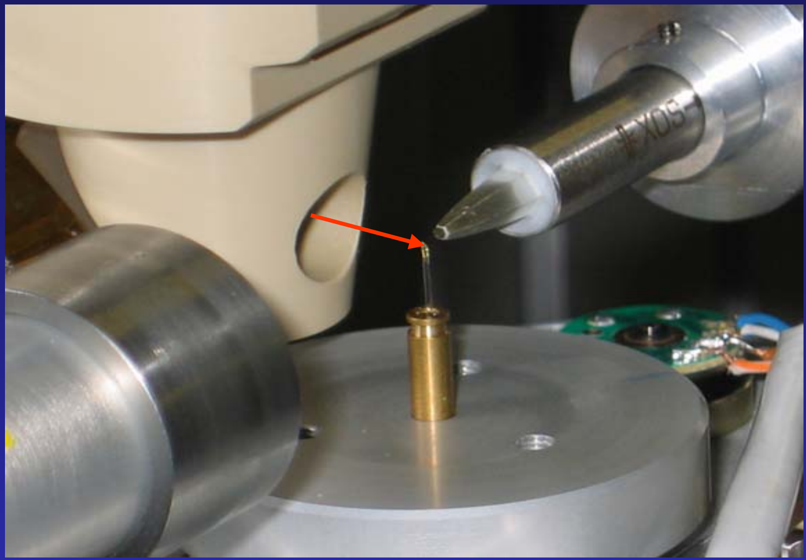
Confocal detection using polycapillary optics

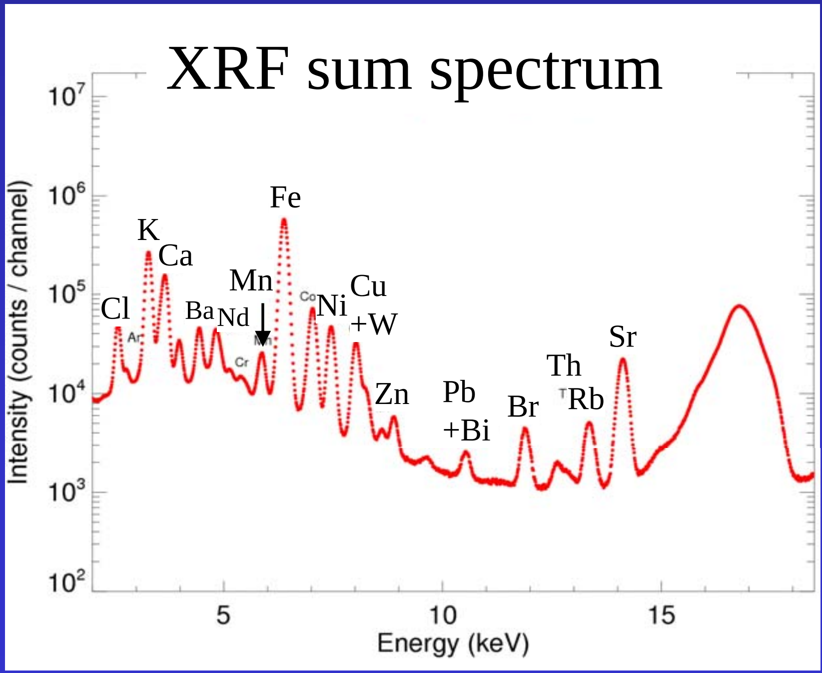


Vincze et al., Anal. Chem. 76(22), 6786-6791 (2004).

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.

Conclusions

<u>Our capillary ray-tracing model:</u>

• *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*

Acknowledgements

A. Rindby	Chalmers Univ. of Technology, Gothenburg, Sweden
P. Engström	Chalmers Univ. of Technology, Gothenburg, Sweden
C. Riekel	ESRF ID13, Grenoble, France
M. Burghammer	ESRF ID13, Grenoble, France
J. Morse	ESRF, Grenoble, France
F. Adams	University of Antwerp, Belgium
B. Vekemans	University of Ghent, Belgium
J. Susini	ESRF ID21, ID22, ID18F Grenoble, France
P. Cloetens	ESRF ID22NI, Grenoble, France
G. Falkenberg	PETRA-III, Hamburg, Germany