Aberrations and finite focal sizes of a bent-crystal polychromator

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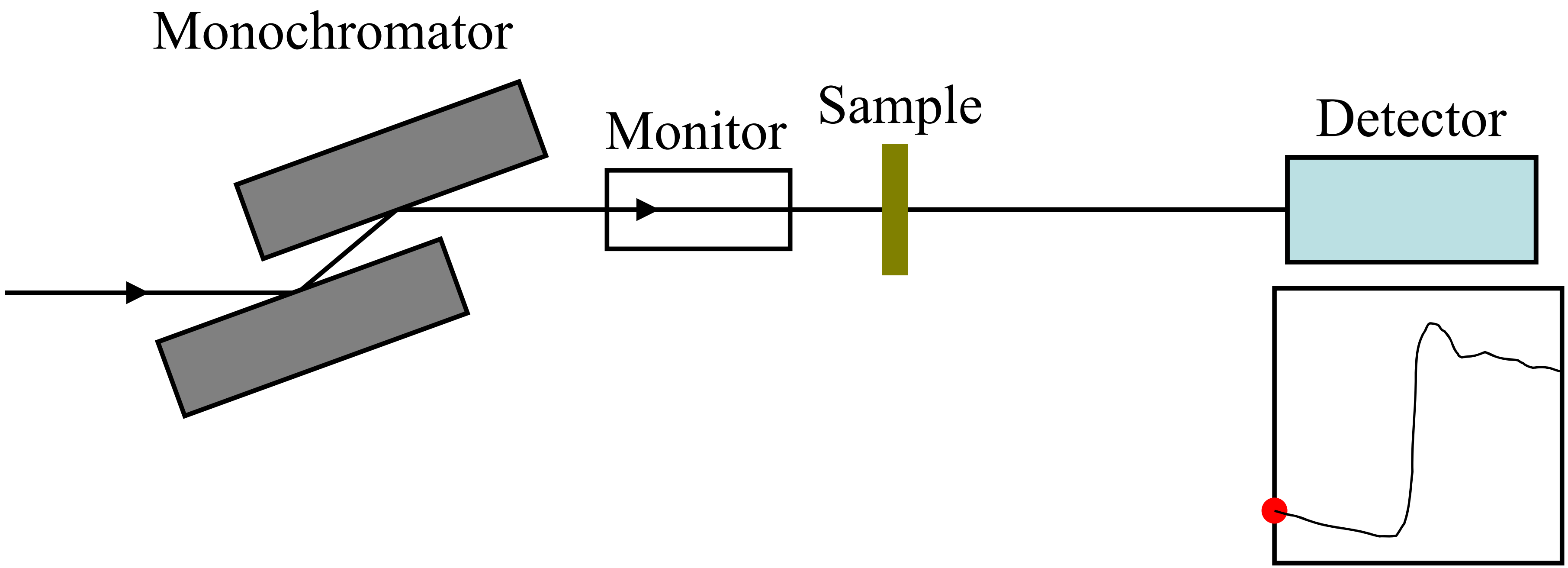
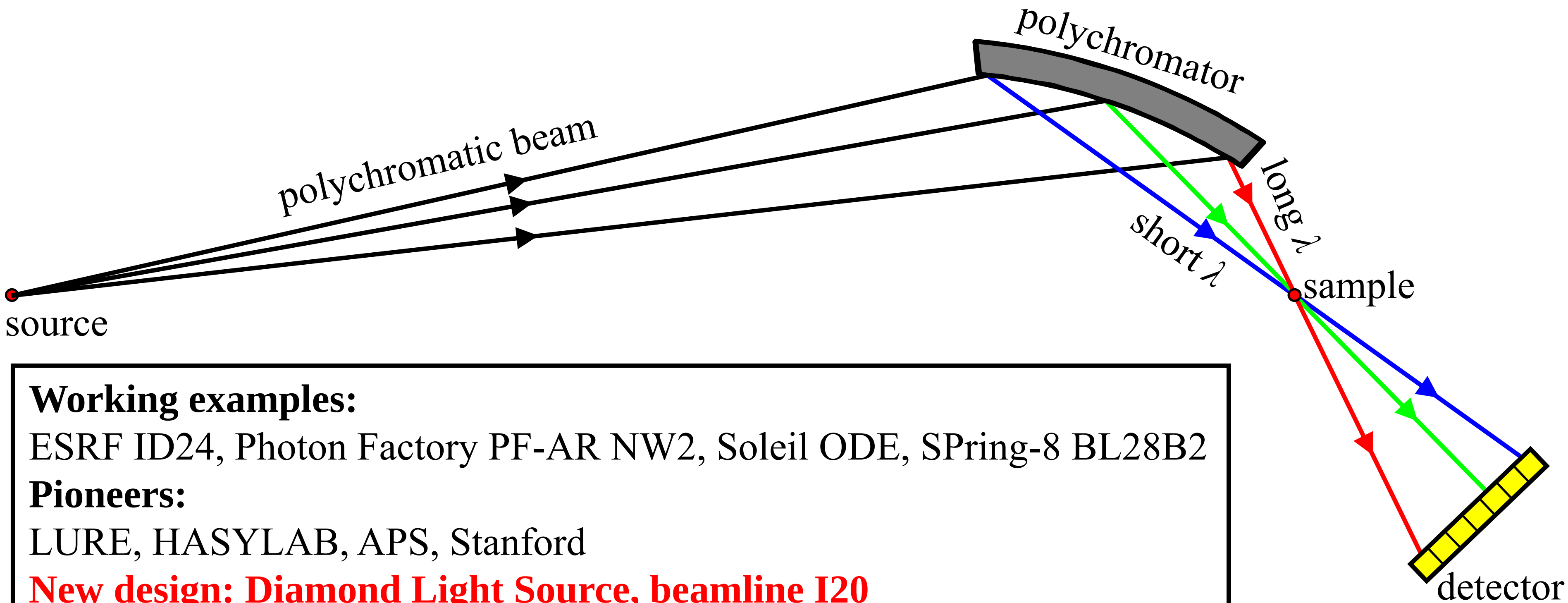
The most common type of X-ray absorption spectroscopy requires the sample to be illuminated by a monochromatic beam.

The monochromator has to be scanned to vary the X-ray photon energy. This is effective but time-consuming.



An alternative is to use a bent crystal to focus a broad-bandwidth beam onto the sample.

A position-sensitive detector behind the sample then receives X-rays whose position is correlated with their energy.

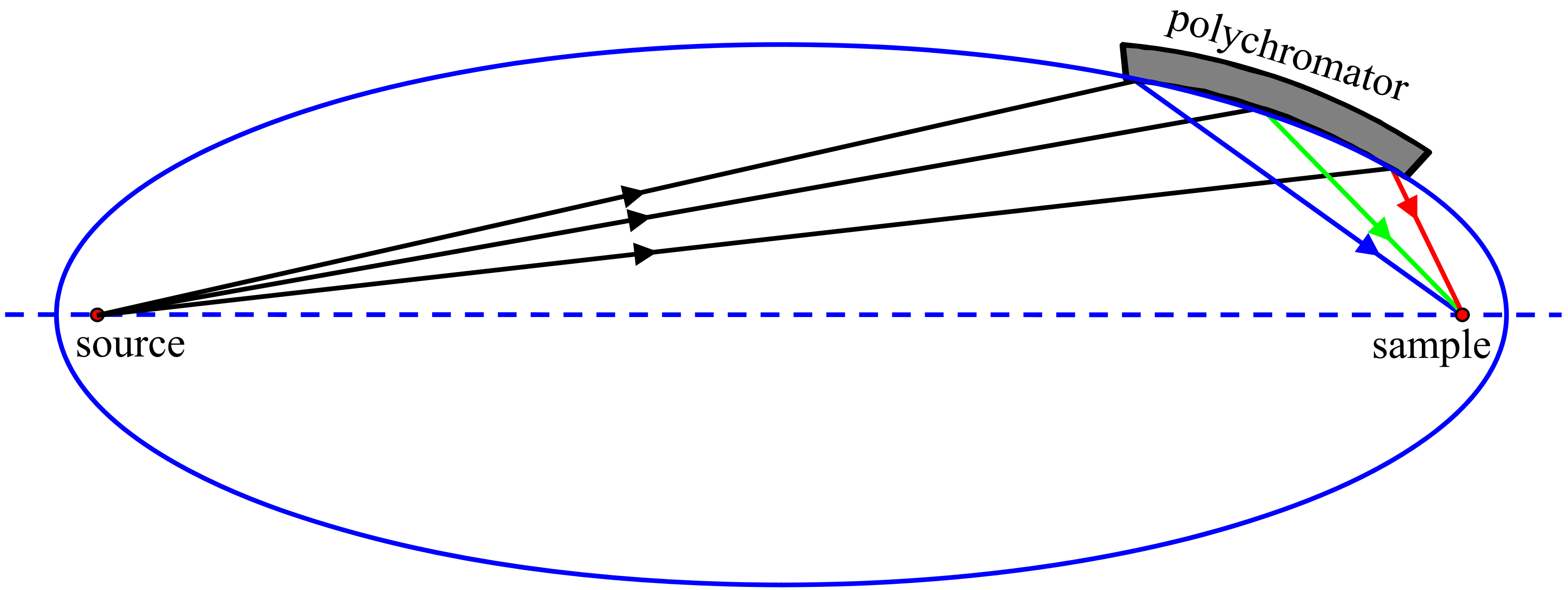


Working examples:
ESRF ID24, Photon Factory PF-AR NW2, Soleil ODE, SPring-8 BL28B2
Pioneers:
LURE, HASYLAB, APS, Stanford
New design: Diamond Light Source, beamline I20

→ an X-ray absorption spectrum can be taken in a short time, without any scanning required.

Quality of focus

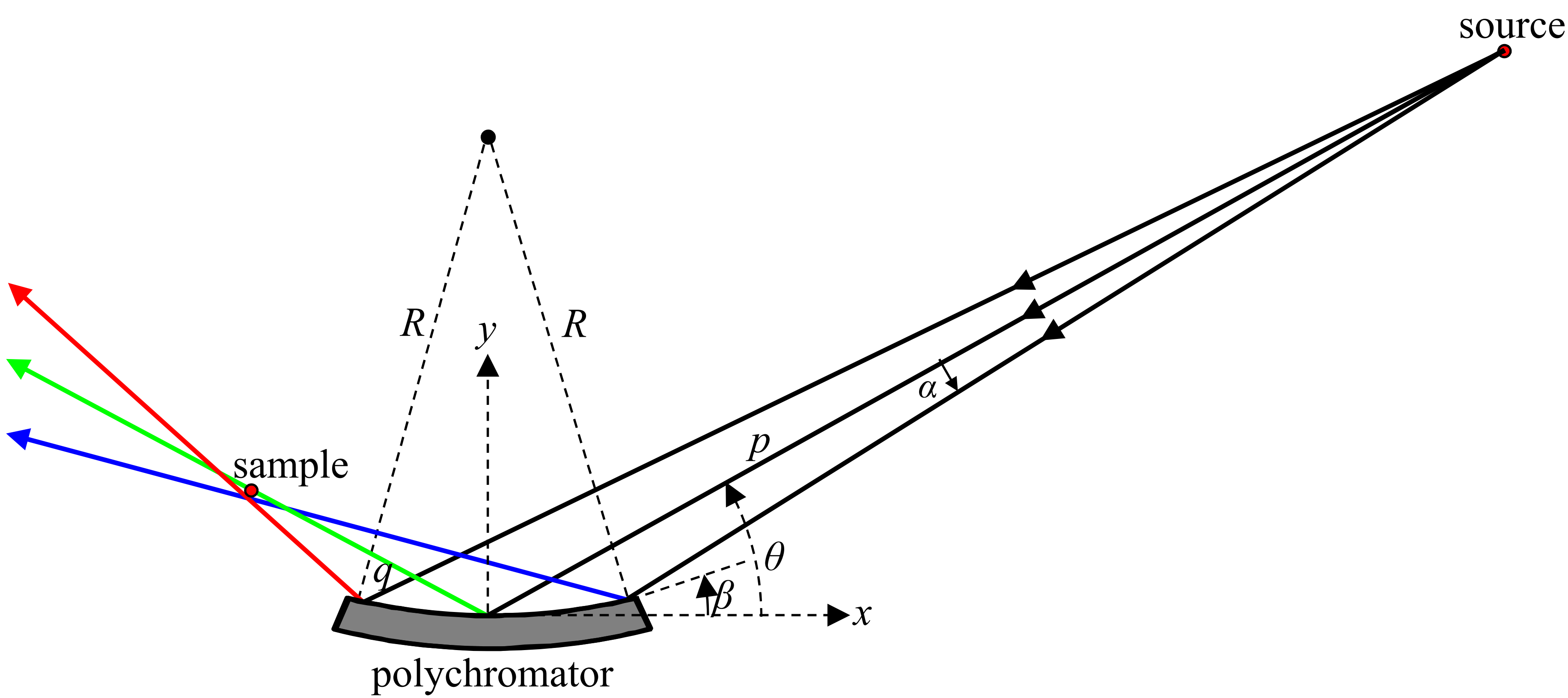
If a polychromator is to focus a point source to a point image,
it must be an arc of the ellipse whose foci lie at the source and the image.



Specified elliptical bends can be approximated by cylindrical bends, which are easier to perform but introduce aberrations.

The effect on the image can be determined by ray tracing.

In the following, the penetration depth is ignored (*for the moment*).
The crystal surface is treated like a mirror.
The Bragg reflection is assumed to be symmetric.



We find that the diffracted rays do not all meet at one point.

The fact that a cylindrically bent mirror/crystal does not focus the rays from a point source into a point image is the "spherical aberration" of this optic.

We can calculate the point at which the reflected ray produced by the incident ray at α intersects the central reflected ray ($\alpha = 0$).

An exact formula exists but is complicated. But the distance $q(\alpha)$ of this intersection point from the crystal can be approximated:

$$q(\alpha) \approx \frac{pR\sin\theta}{|R\sin\theta - 2p|}\left[1 - \frac{3p\cos\theta}{R\sin^2\theta}\left(1 + \frac{p}{R\sin\theta - 2p}\right)\alpha\right]$$

NOTE: Let $q_0 = \lim q(\alpha)$ as $\alpha \to 0$.
If $2p > R\sin\theta$, then $p^{-1} + q_0^{-1} = 2(R\sin\theta)^{-1}$ as shown in previous literature, e.g. H. Tolentino et al., *J. Appl. Cryst.* **21**, 15–21 (1998).

Examples:

$p = 45.1$ m, $q_0 = 1.0$ m (taken from Diamond XAS beamline I20)

Si (111) @ 7000 eV: $\theta = \theta_B = 16.406$ deg, $R = 6.9268$ m

NOTE: $x_{int}(\alpha)$ = x-coordinate of point at which the incident ray at α intercepts the mirror/crystal

$q(\alpha)$ = exact value

$\delta q(\alpha)$ = percent error of the approximate formula for $q(\alpha)$ from the exact value

α (deg)	x_{int} (m)	q (m)	δq (%)
−0.06	−0.1614	1.1157	+0.4
+0.06	+0.1740	0.8744	+0.6

Si (311) @ 26000 eV: $\theta = \theta_B = 8.372$ deg, $R = 13.438$ m

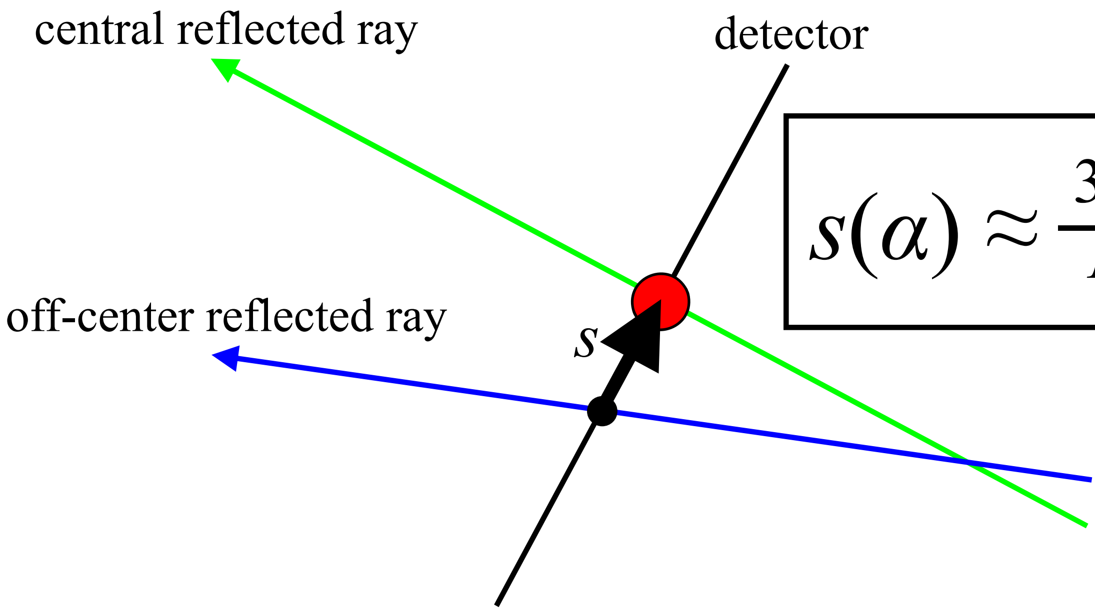
α (deg)	x_{int} (m)	q (m)	δq (%)
−0.06	−0.3033	1.2246	+1.3
+0.06	+0.3534	0.7373	+3.0

The variations in *q* show a large lengthwise broadening of the polychromatic focus!

The approximate expression for $q(\alpha)$ is accurate to within a few percent for reasonable mirror/crystal lengths.

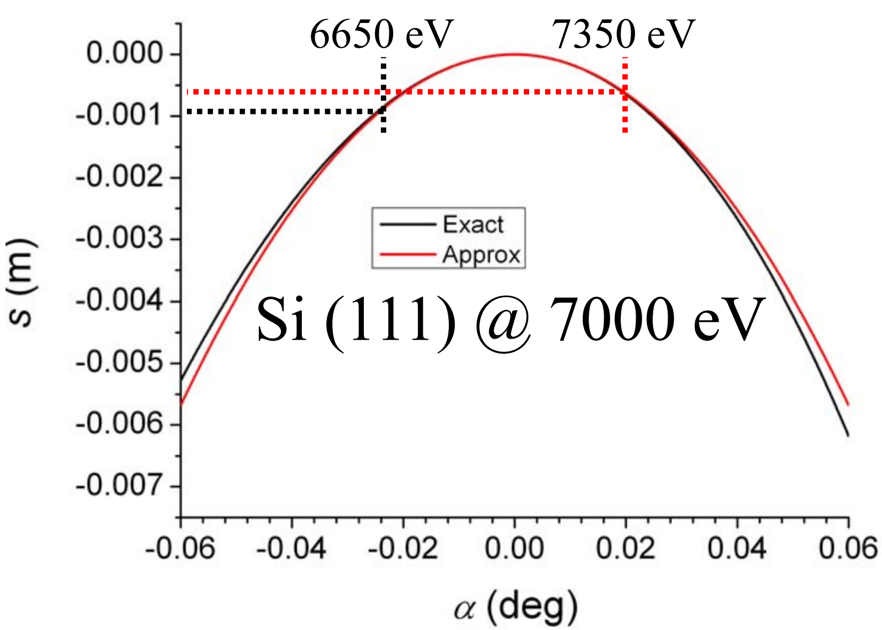
Next, we calculate where each reflected ray falls on a screen perpendicular to the central reflected ray,
and passing through the ideal focus at q_0.

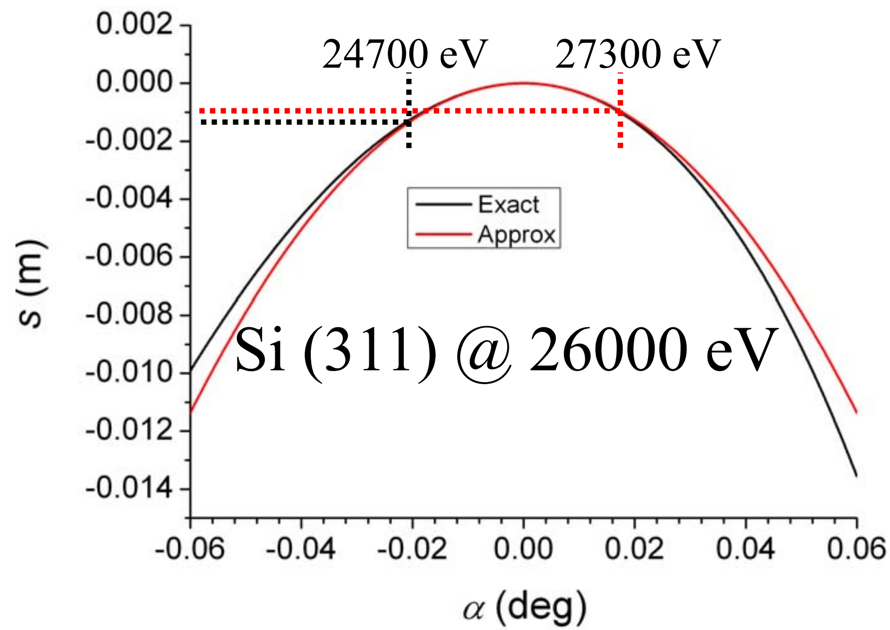
Again, the complicated exact formula can be approximated:



$$s(\alpha) \approx \frac{3p^2 \cos\theta}{R \sin^2\theta}\left(\frac{R \sin\theta - p}{|R \sin\theta - 2p|}\right)\alpha^2$$

Note that all off-center reflected rays hit the detector on the same side of the central reflected ray!

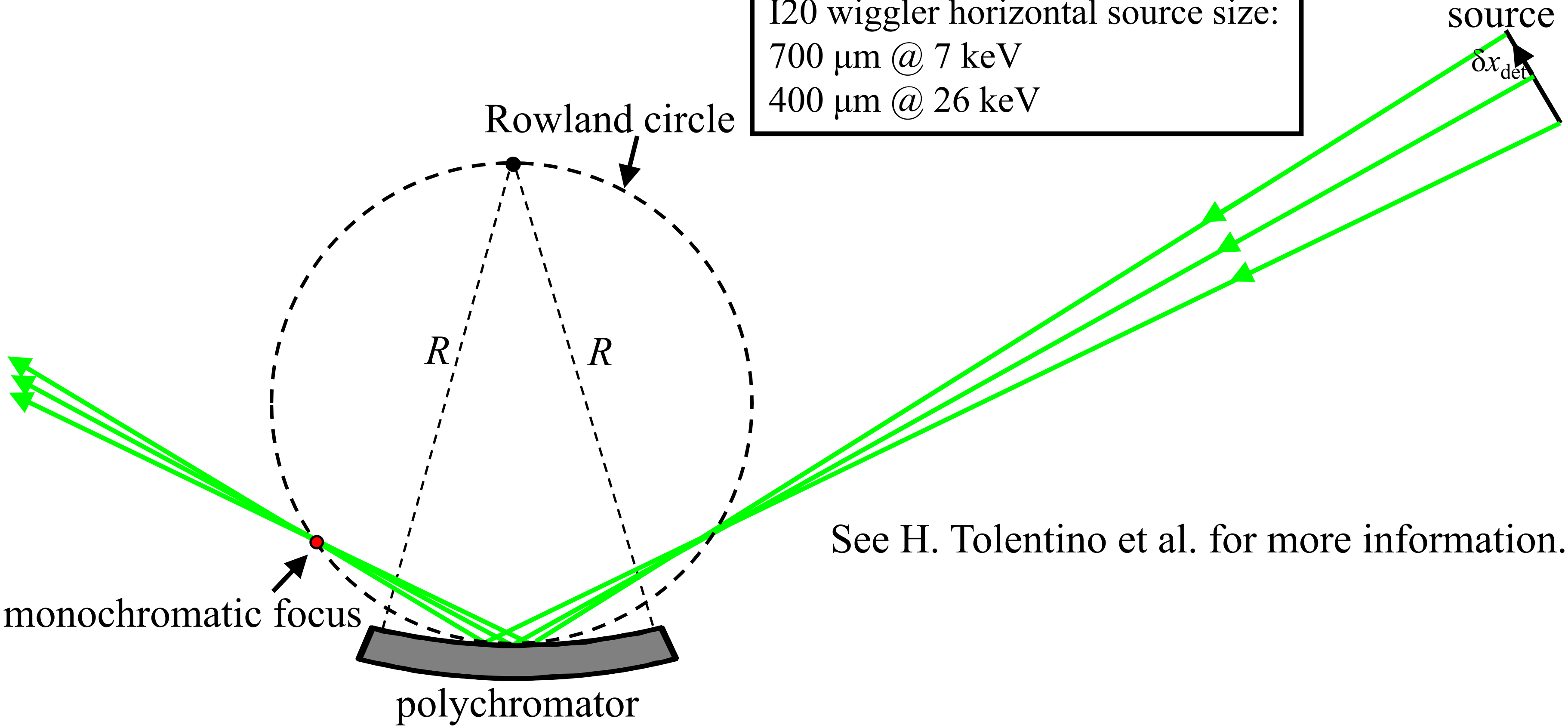




Monochromatic focus (brief explanation):

- Here, we account for the non-zero size of the source.
- Each wavelength has a monochromatic focus.
- All diffracted rays of that wavelength come together at that focus, no matter where on the source they start.

I20 wiggler horizontal source size:
700 μm @ 7 keV
400 μm @ 26 keV



See H. Tolentino et al. for more information.

The distance of the monochromatic focus from the crystal = $R \sin\theta \approx 2q$.

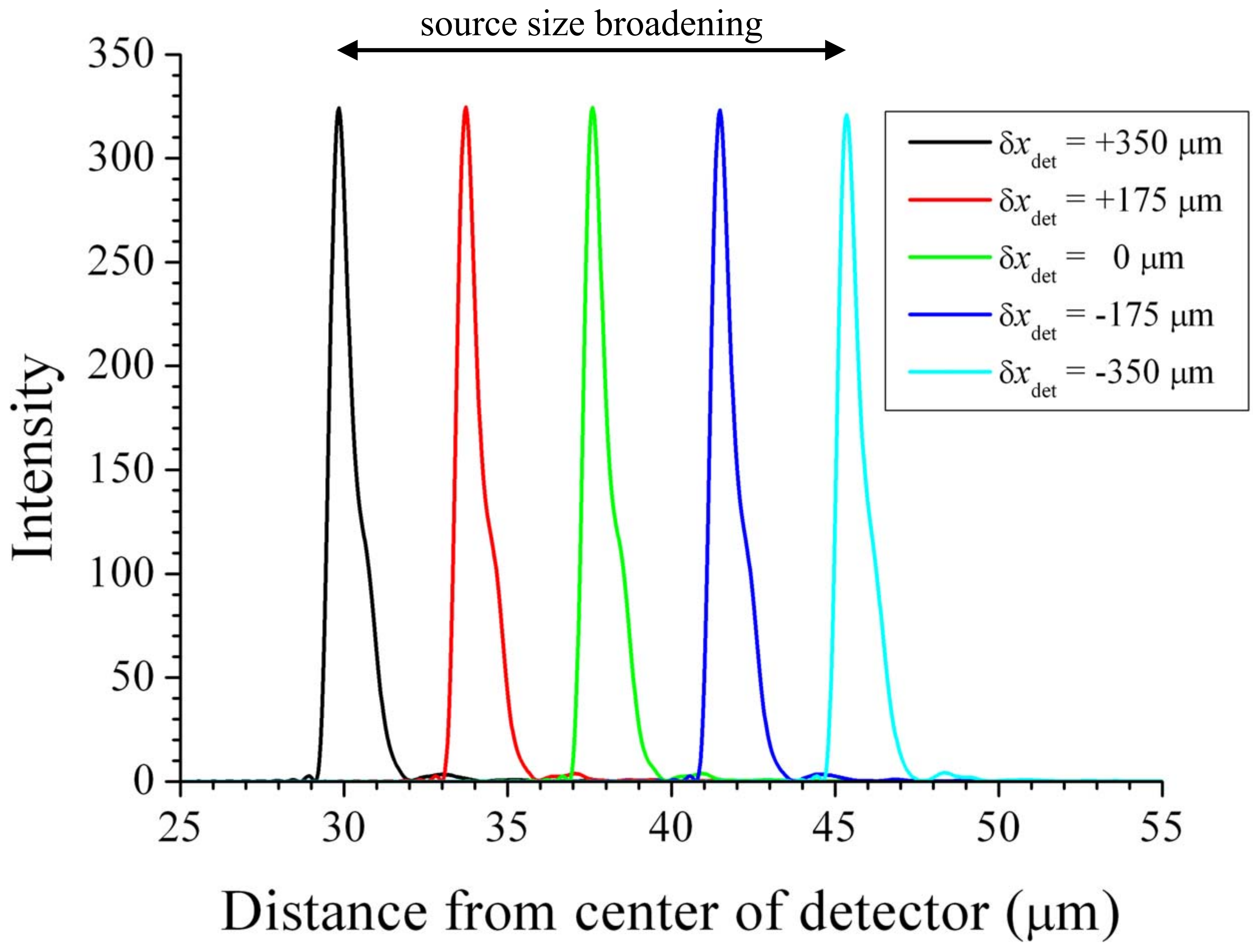
Ray-tracing alone is not adequate!

- Diffraction from a crystal ≠ reflection from a mirror!
  Crystal diffraction allows a small but nonzero penetration of the waves into the crystal.
  → **Takagi-Taupin theory**

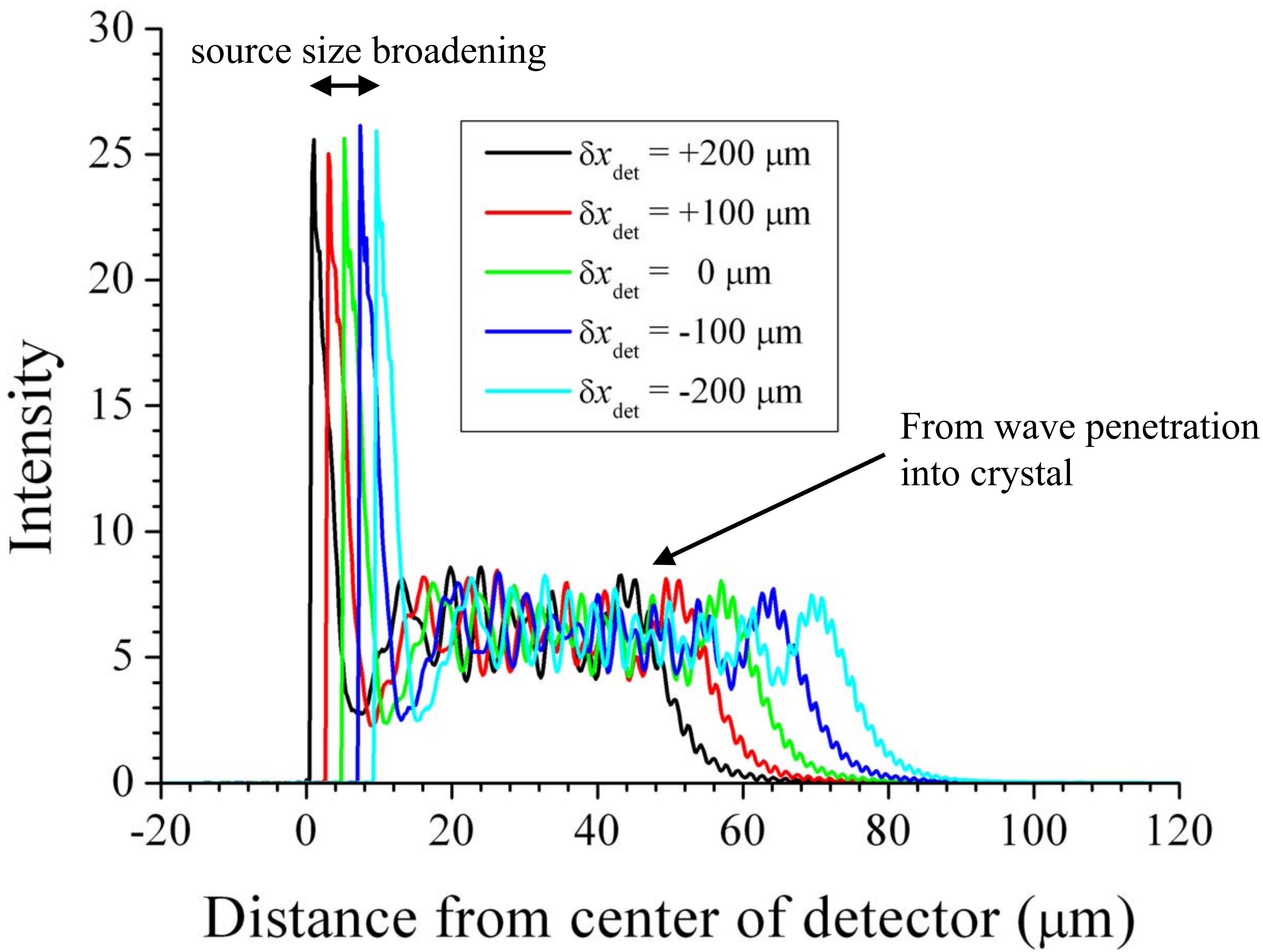
- The wave diffracted by the crystal continues to experience diffraction on its way to the detector.
  This diffraction limits the achievable focal spot size even if all geometrical factors in the resolution are removed.
  → **Fresnel diffraction**

Ya. I. Nesterets and S. W. Wilkins (*J. Appl. Cryst.* **41**, 237-248, 2008):
a wave treatment of focusing from bent Laue crystals
yields considerable differences from geometrical theory.

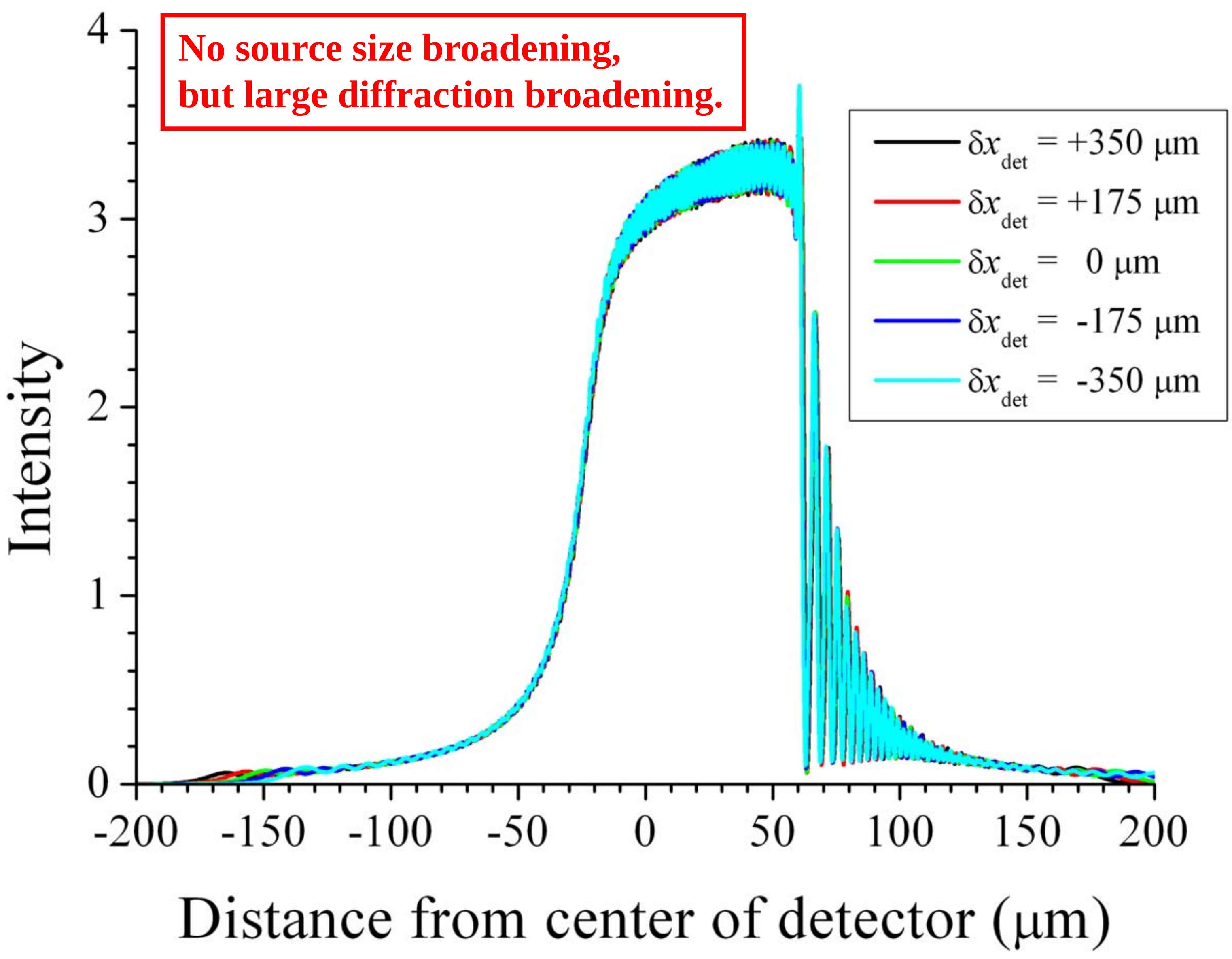
Si (111) @ 7000 eV at polychromatic focus



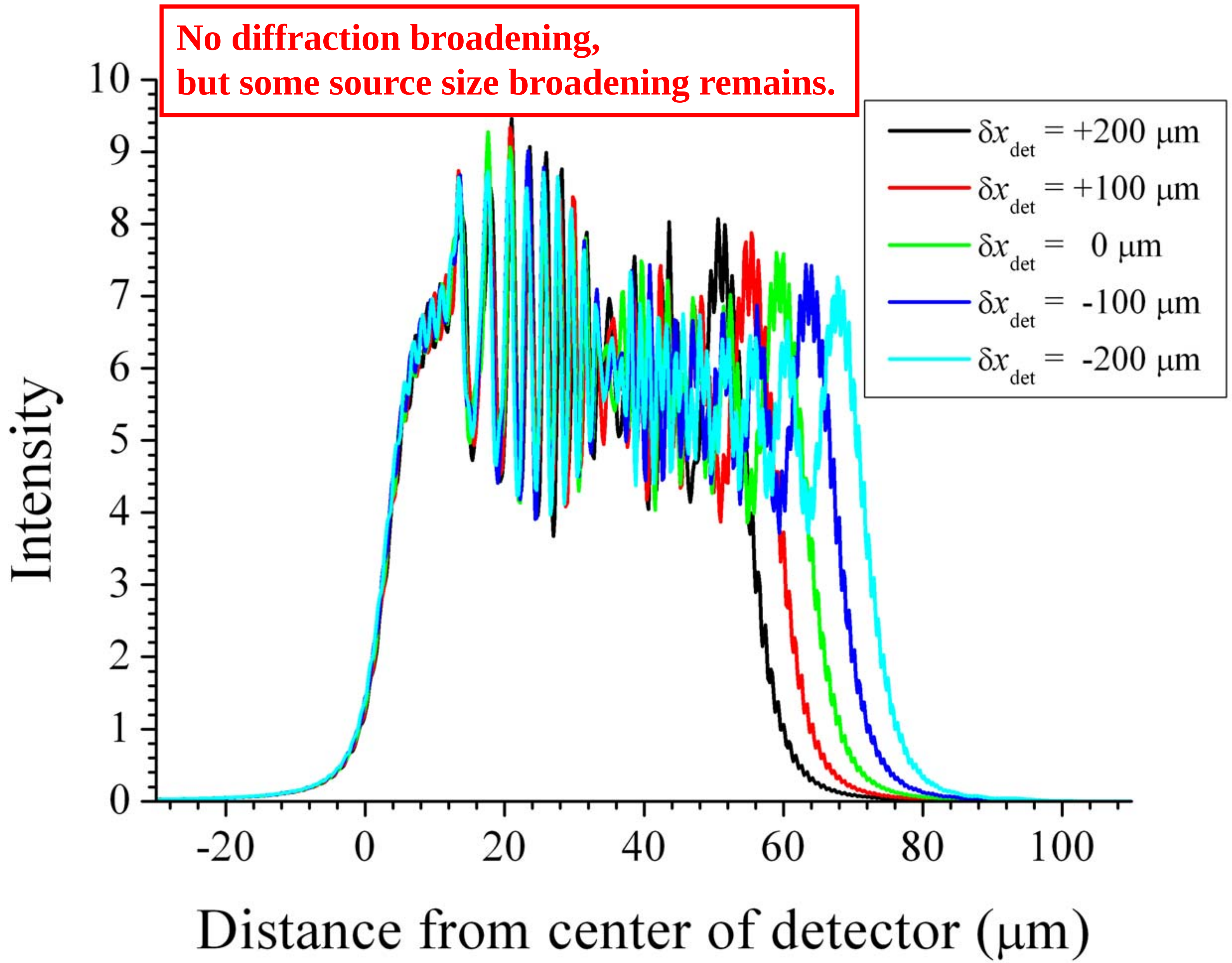
Si (311) @ 26000 eV at polychromatic focus



Si (111) @ 7000 eV at monochromatic focus



Si (311) @ 26000 eV at monochromatic focus



Conclusions

- Spherical aberration at the polychromatic focus is considerable even for moderate bandwidths.

- Diffraction effects on the beam spot size at the polychromatic and monochromatic focus can now be determined.

- The wave-optical method can be extended to polychromators deformed by heat load.