Beyond the Geometric toward the Wave Optical Approach in the Design of Curved Crystal and Multilayer Optics for EDXAS

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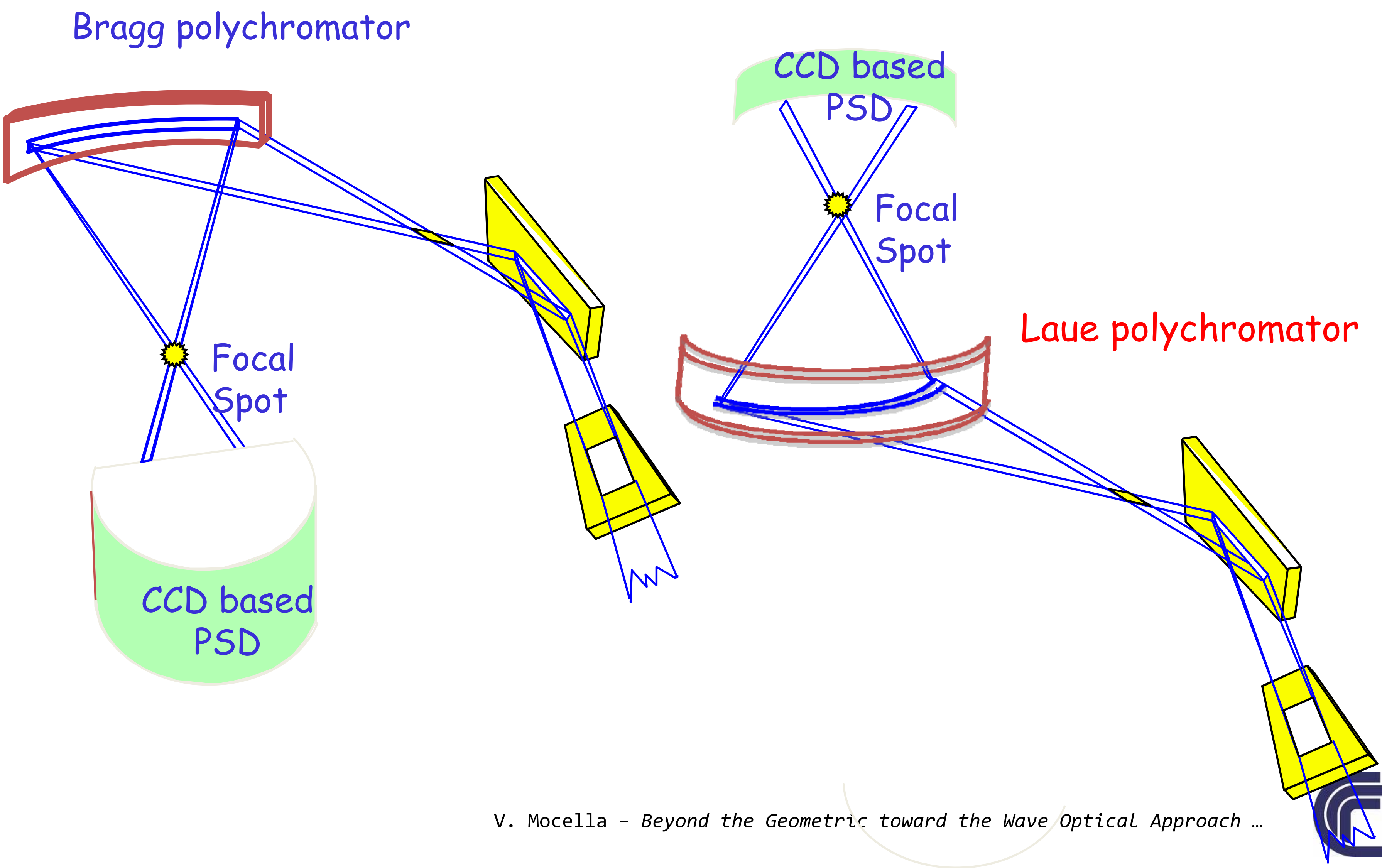
ESRF, Grenoble

Optical scheme



Challenge for new polychromators

The Goal : a sub-micrometer spot size

Homogenous and stable in position and shape

For a review of recent progress on the focal spot at ID24

Pascarelli et al., J. Synchrotron Rad. (2006). 13, 351–358

This is presently possible for multilayers.

Technological limitations

surface roughness,

homogeneous thickness ecc.

Technological limitations are usually considered within a pure geometrical approach estimating their effect.

Intrinsic limitations

beam penetration in Bragg case

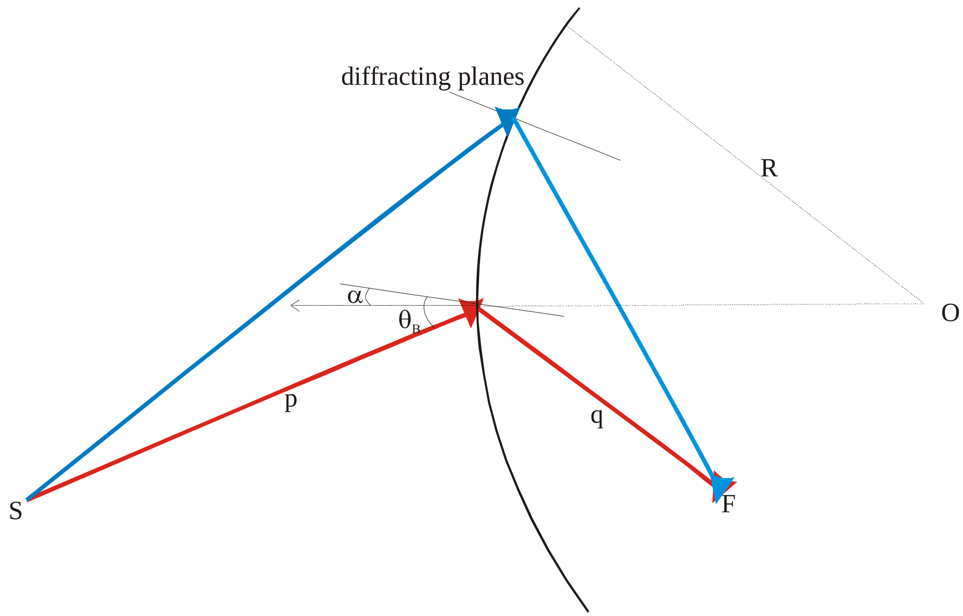
spread over Borrmann triangle in Laue case

Intrinsic limitations are studied with a a wave-optical approach (analytic, semi-analytic and numerical solution of Takagi equations and related derivations

Laue Case

Polychromatic dynamical focusing

A typical example of counterintuitive result if only geometrical approach is used



Geometrical focusing

Lens equation for polychromatic beam in symmetric case

$$\frac{2}{R\cos\theta_B} = \frac{1}{p} + \frac{1}{q}$$

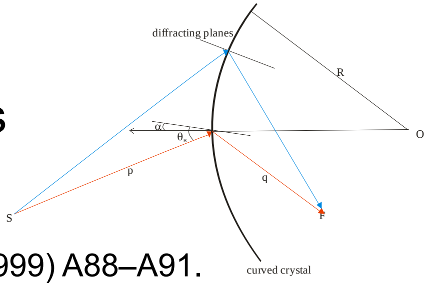
In lab $R = \infty$ ⇒ $p = q$

synchrotron $p >> q$ ⇒ $R \approx \dfrac{2q}{\cos\theta_B}$

Geometrical Focusing Approximations

Infinitely narrow beam: *Incident radiation ➡ composed of rays each associated to the wavelength obeying the Bragg law at the corresponding entrance point.*
Apparently this is an approximation because actually the crystal “sees” the whole accepted angular divergence (Darwin width) for each wavelength.
Only apparently .... because from polychromaticity derives incoherence.

Infinitely narrow beam ⟺ incoherent source-points
Is **not** an approximation for a white incident beam

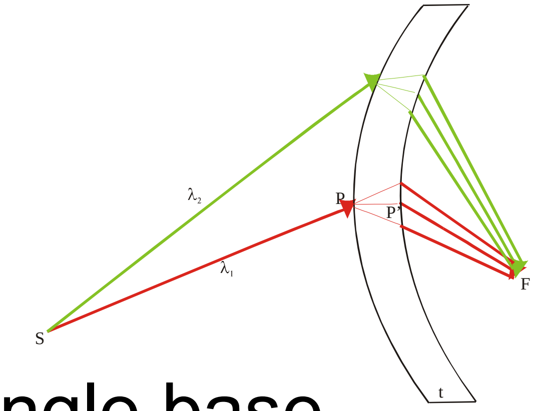


Mocella, V., Epelboin, Y., *J. Appl. Cryst*. **32**, 154-159 (1999); Mocella et al., J. Phys. D: Appl. Phys. 32 (1999) A88–A91.
Epelboin, Y., Mocella, V.,. Soyer, A., *Phil. Trans. R. Soc. A* **357**, 2731 (1999). Mocella, V.et al. *J. Appl. Cryst*. 36, 129 (2003).

Infinitely thin crystal : Intuitive picture

Spreading over the Borrmann triangle for each wavelength

How is it possible to reduce the spreading ?

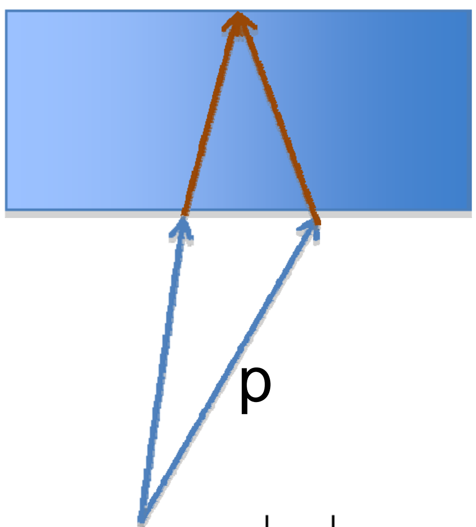


Dynamical focusing of the Borrmann triangle base

Tichkness effect: Counterintuitive picture

Dynamical focusing: a flat lens for Monochromatic wave

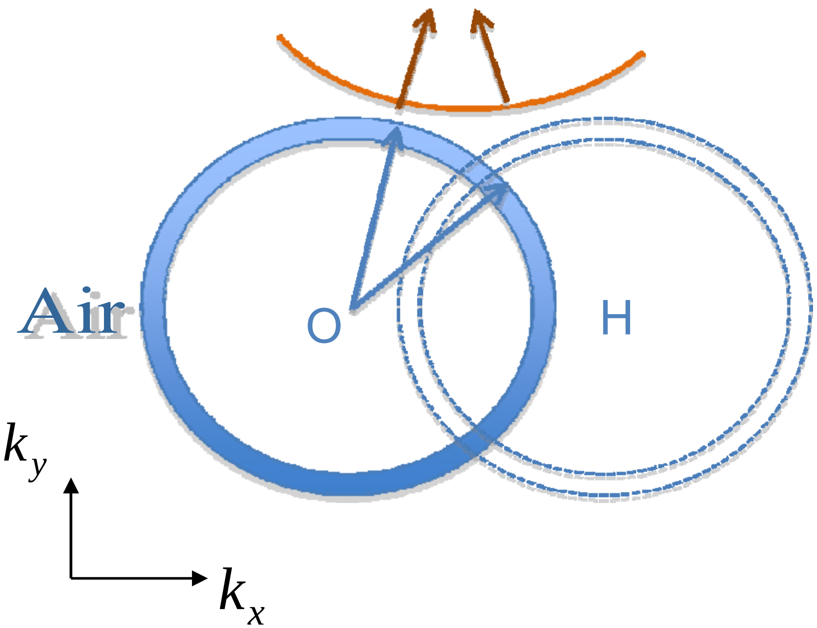
Direct space



$$t_{foc} = p \frac{|\chi_h|}{2\sin^2\theta_B \cos\theta_B}$$

Reciprocal space

From Dynamical diffraction theory



Afanas'ev A.M., Khon V. G, Sov. Phys. Solid State, 19, 1035-1040 (1977) Aristov et al., Acta Cryst. A36, 1002-1013 (1980).

A typical analitical derivation from dynamical diffractiont theory (a wave optical approach) that cannot be undestood and studied using geometrical approach

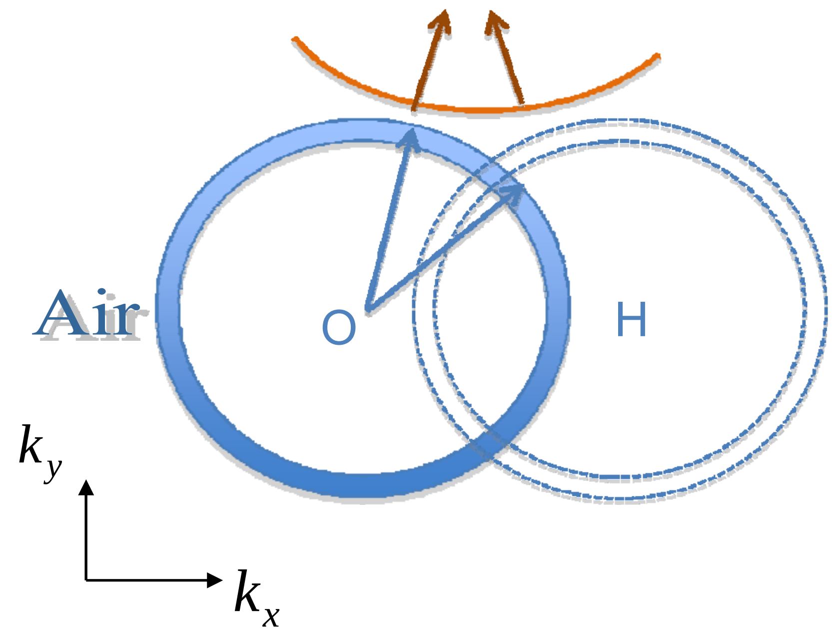
Dynamical focusing :
a precursor of negative refraction

VOLUME 85, NUMBER 18 PHYSICAL REVIEW LETTERS 30 OCTOBER 2000

Negative Refraction Makes a Perfect Lens

J. B. Pendry

Photonic crystals are presently the most efficient negative index metamaterials

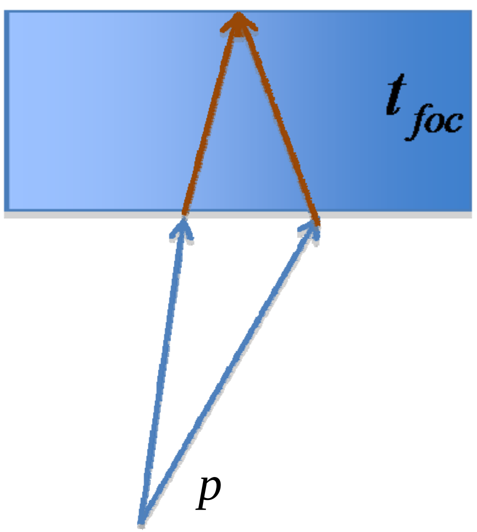


Our proposition

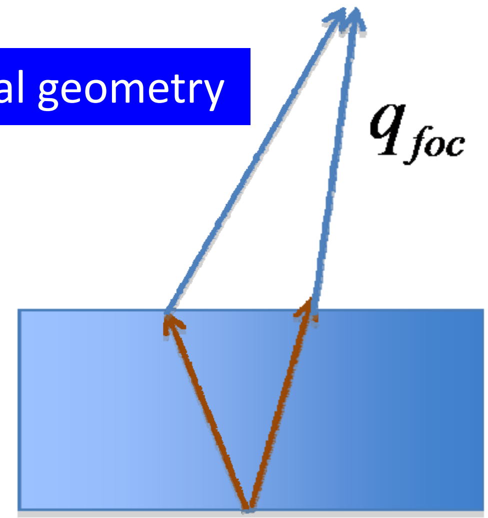
Monocromatic dynamical focusing in reciprocal geometry

Direct geometry

$$t_{foc} = p\frac{|\chi_h|}{2\sin^2\theta_B\cos\theta_B}$$



Reciprocal geometry



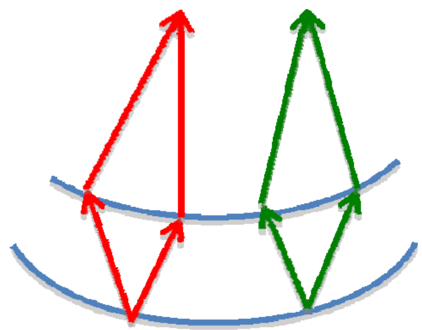
$$q_{foc} = \frac{2\sin^2\theta_B\cos\theta_B}{|\chi_h|}t$$

Mocella et al., J. Appl. Cryst. ***37****, 941-946 (2004).*

The monocromatic dynamical focusing in reciprocal geometry is the keypoint for polychromatic dynamical focusing

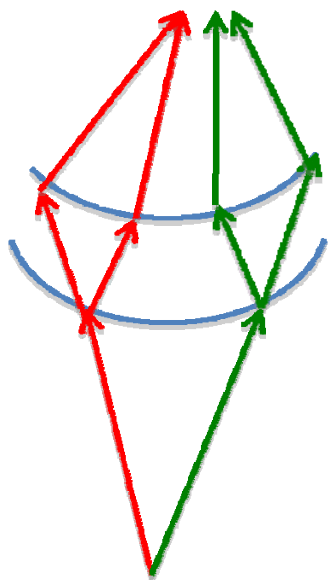
Polycromatic dynamical focusing

Polichromaticty
+ reciprocal
dynamical focusing



Combining geometrical polychromatic focusing with reciprocal dynamical focusing

$$R \approx \frac{2q}{\cos\theta_B}$$



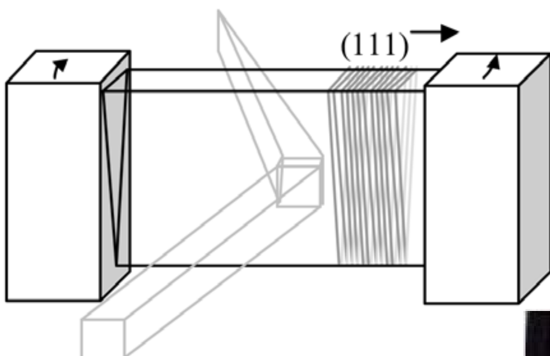
$$t_{foc} = q\frac{|\chi_h|}{2\sin^2\theta_B\cos\theta_B}$$

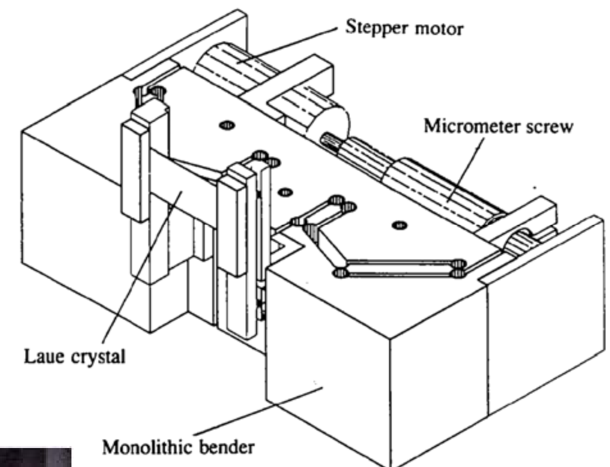
Thickness is a key parameter for polychromatic focusing

Mocella et al., J. Appl. Cryst. ***37****, 941-946 (2004).*

Experimental results of dynamical polychromatic focusing

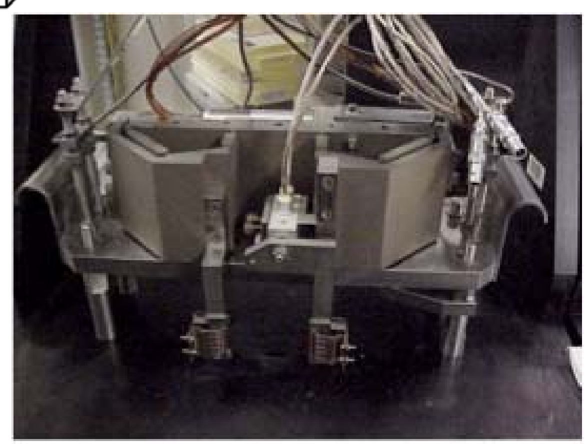
Wedge shaped bent Silicon Laue
Crystal, diffracting in horizontal plane





White beam

ESRF (ID11 and BM5)



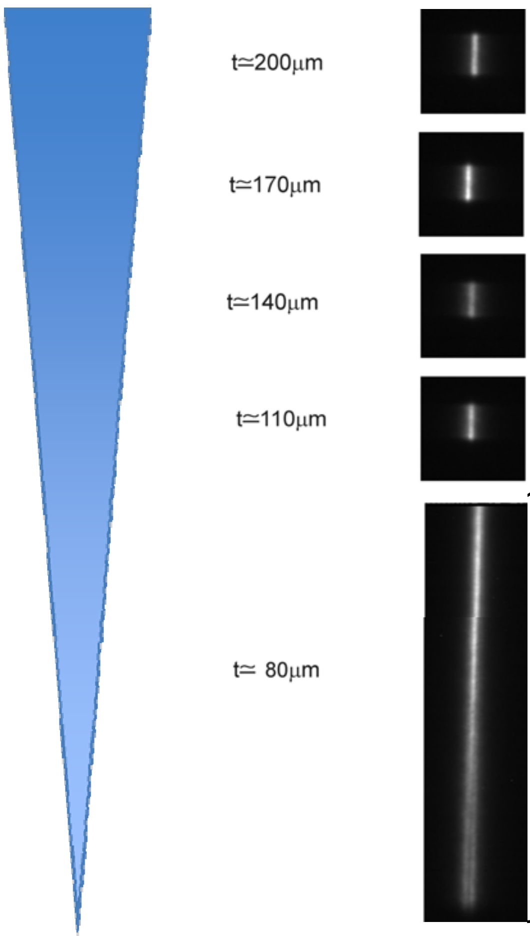
ID24 bender

Dynamical polychromatic focusing: experimental results

BM5

horizontal source size s_h=*270 mm* FHWM

E=25 keV *p*= 30 m *q* =*1.28 m.*



$$t_{foc} = 168\,\mu m$$

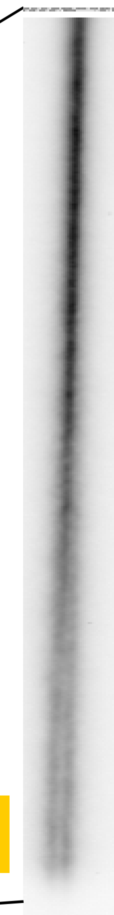
FWHM=16 µm

Demagnified source size

$s_h\, q/p$=11.5 μm

CCD camera PSF about 5 μm

Defocusing of the Borrmann triangle



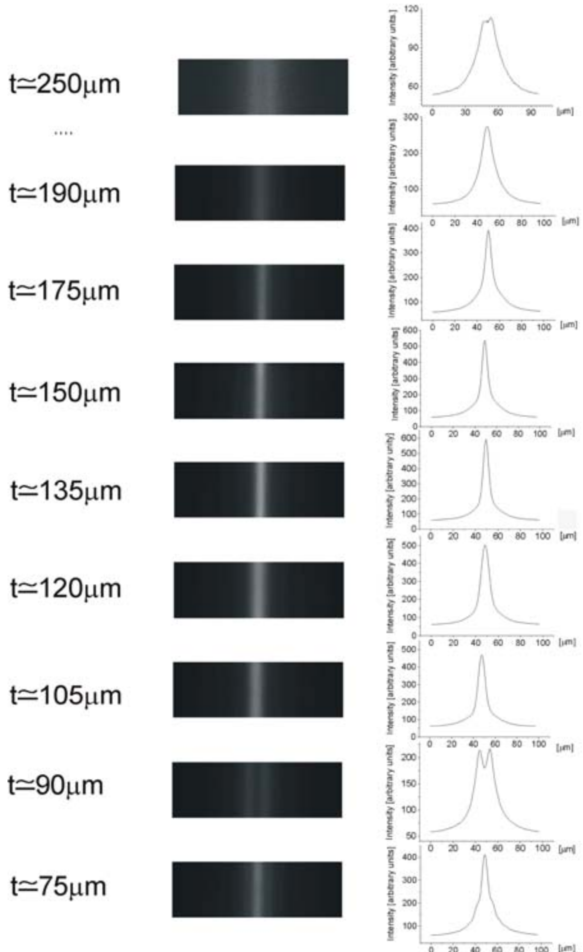
Mocella et al., J. Appl. Cryst. ***41****, 695-700 (2008).*

Dynamical polychromatic focusing: experimental results

ID11

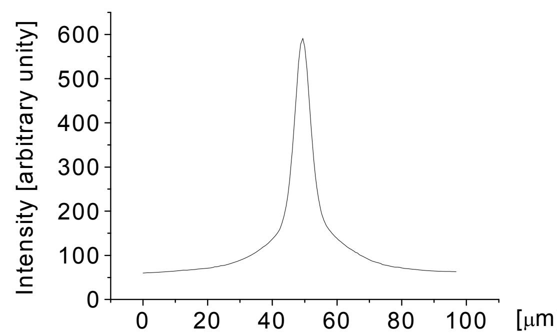
E=50 keV

$$t_{foc} = 133\,\mu m$$



p = 54 m q=0.75 m

incident beam
1 x 0.5 mm (V x H)



FWHM=6.8 µm

$$s_{hp} = s_h \frac{q}{p} \approx 0.8\mu m$$

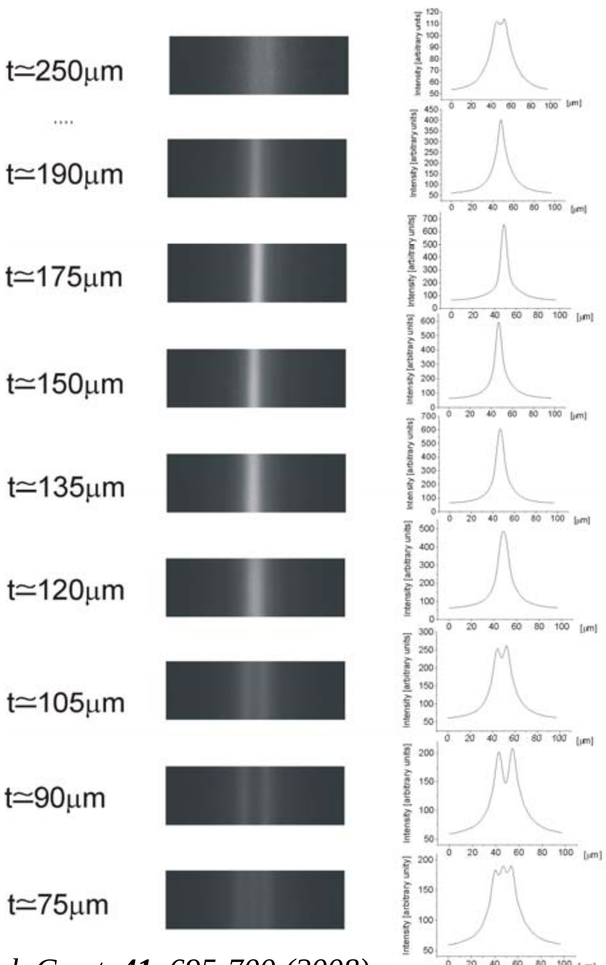
CCD camera PSF about 5 μm

Mocella et al., J. Appl. Cryst. ***41****, 695-700 (2008).*

Dynamical polychromatic focusing: experimental results

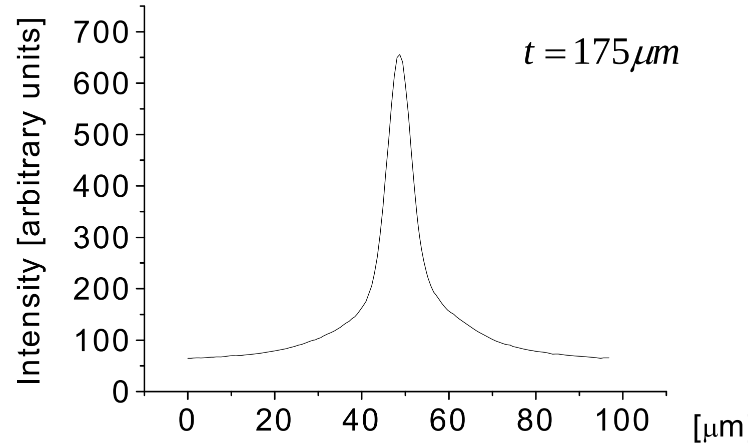
ID11 E=50 keV

$t_{foc} = 177\,\mu m$



p = 54 m q=1 m

incident beam
1 x 0.5 mm (V x H)



FWHM=8.0 µm

$$s_{hp} = s_h \frac{q}{p} \approx 1\mu m$$

CCD camera PSF about 5 μm

Mocella et al., J. Appl. Cryst. ***41****, 695-700 (2008).*

Dynamical polychromatic focusing: summary

- The focus size with a symmetrically cut bent crystal in Laue geometry is strongly improved by an adequate choice of the crystal thickness.
- When different focal distances or energies are required for experiments, a wedge shaped crystal offers a useful thickness tuning tool to obtain the minimum focal spot size.
- The Borrmann fan contribution is at least reduced to the order of a few micron i.e. the same order as the source demagnification due to the presence of the dynamical focusing.

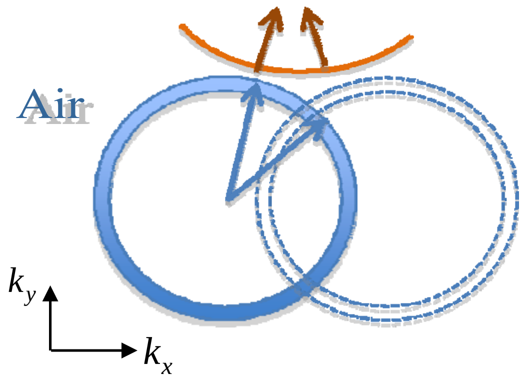
Theory *Mocella et al., J. Appl. Cryst.* ***37****, 941-946 (2004).*

Experiments *Mocella et al., J. Appl. Cryst.* ***41****, 695-700 (2008).*

Improve the Dynamical Focusing

Aberration from the projection of the circular dispersion surface

in air on the hyperbolic dispersion surface in the crystal



This can be compensated for by refraction on a suitably shaped entrance surface of the crystal,

using a diffractive–refractive lens in Laue geometry.

J. Hrdý, V. Mocella, P. Oberta, L. Peverini and K. Potlovskiy, J. Synchrotron Rad., **13**, 392-396 (2006).

Combining Dynamical Focusing and polarizer

A Laue polychromator can also integrate an efficient polarizer, using the polarization dependence of the dispersion surface

V. Mocella, P. Dardano, L. Moretti, and I. Rendina Optics Express, **13**, Issue 19, pp. 7699-7707 (2005)

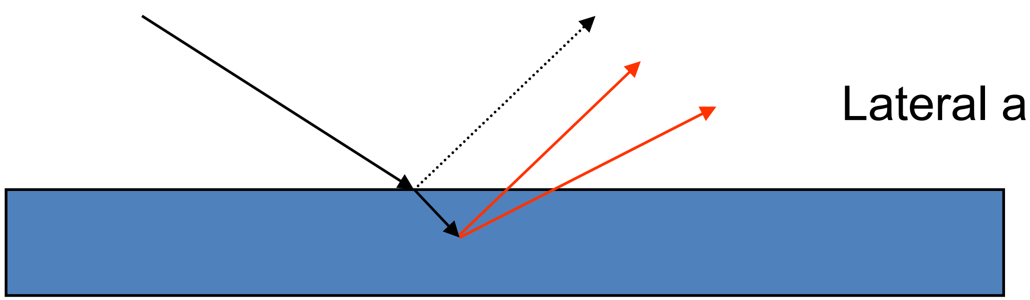
Optical wave approach for polychromator analysis in reflection geometry

- Elliptically curved crystals in Bragg geometry
- Multilayers (elliptically curved and graded)

First results

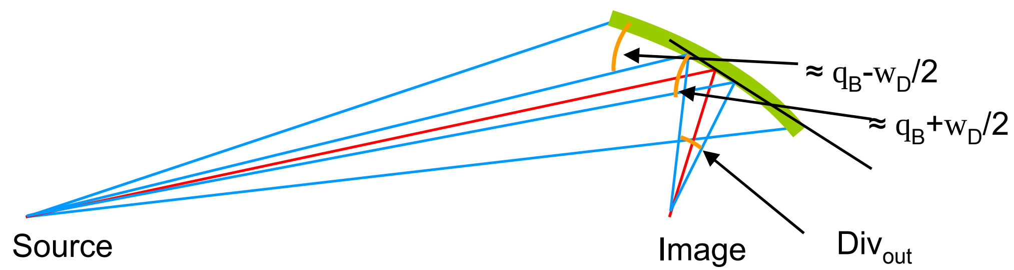
In both cases the penetration of the beam inside the crystal (or the ML) is the origin of a deviation from geometric behavior and affects the focusing performance.

In general for reflection geometry, total reflection of Bragg reflection, the deviation from specular reflection can be classified as a generalized Goos-Hänchen effect.



Lateral and angular shift

Elliptically curved crystals in Bragg geometry preliminary results of an optical wave approach



Intuitive picture

Diffraction limit estimation of focal size

$$\Delta x \cdot w_D \approx \lambda$$

Si(111) 7 keV (λ = 1.8 Å) $w_D = 79\,\mu rad$

the focal spot size is limited to: $\Delta x \approx 2\,\mu m$

Two approaches

i) Semi-analytic solution of the integral form of the TT-equations, leading to a series expansion of the wave amplitudes at the crystal surface.

ii) a fully numerical solution of the partial-differential form of the TT-equations based on a code already validated in the case of heat loaded crystals and surface acoustic wave fields in Si crystals

Semi-analytic derivation

Standard Takagi equations in the case of a quadratic phase factor, due to a parabolic or elliptic shape of the incident wave

$$\frac{\partial E_o}{\partial s_o} = iu_{-h} E_h(s_o, s_h) \exp(-iAs_o s_h - iBs_o^2 - iCs_h^2)$$

$$\frac{\partial E_h}{\partial s_h} = iu_h E_o(s_o, s_h) \exp(iAs_o s_h + iBs_o^2 + iCs_h^2)$$

using

$$E_h = \exp(iBs_o^2) D_h \quad \text{and} \quad E_o = \exp(-iCs_h^2) D_o$$

$$D_o = G_o \quad \text{and} \quad D_h = \exp(iAs_o s_h) G_h$$

$$\frac{\partial G_o}{\partial s_o} = iu_{-h} G_h \quad ; \quad \frac{\partial G_h}{\partial s_h} = iu_h G_o - iAs_o G_h$$

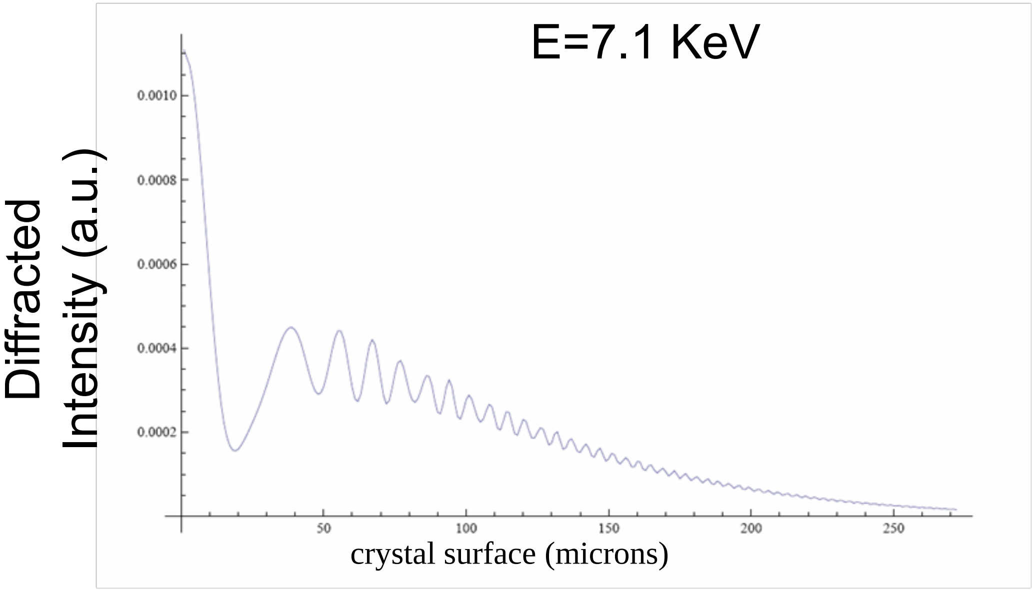
These equation can be put in a integral form and solved by iteration leading to a series expansion of the wave amplitudes at the crystal surface...

$$G_{h,1}(s_o, s_h) = iu_h$$

$$G_{h,2}(s_o, s_h) = iu_h[-(iA + u^2) s_o s_h + \gamma u^2 \frac{s_h^2}{2}]$$

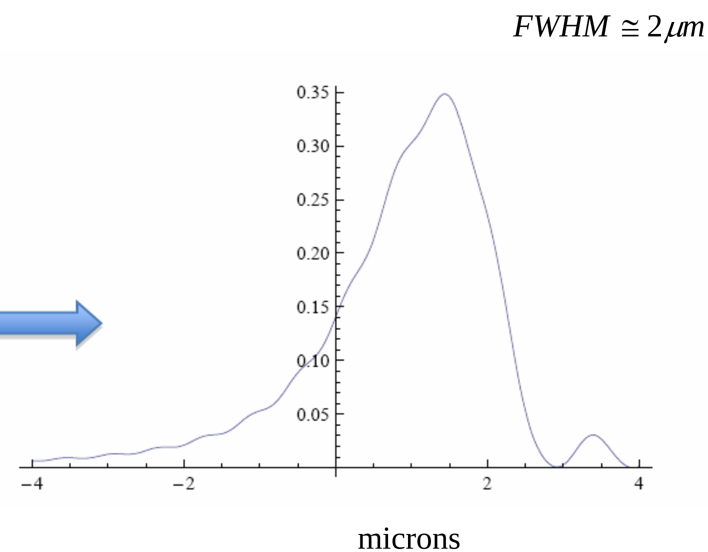
…. evaluating such expansion we get th diffracted wave at exit surface

Preliminary results from a comparison between a semi-analytic model and a fully numerical solution of the TT eqs, with an elliptically bent crystal



p=45 m
q=0.5 m

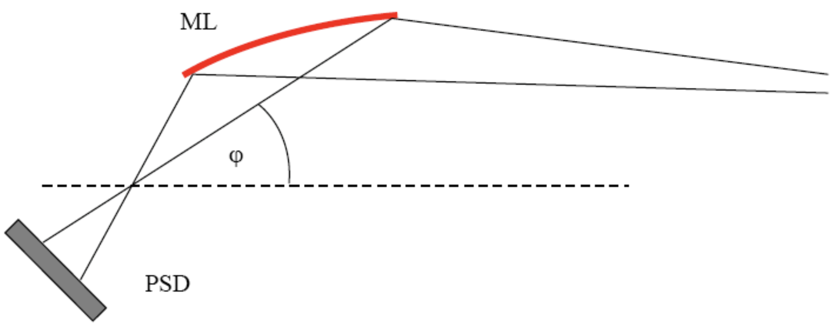
On the Focal plane



From semi-analytic and/or fully numerical solution we get amplitude and phase of the diffracted beam that is propagated along the focal plane

Asymmetric shape of the focal spot

Elliptically graded multilayer for EDXAS



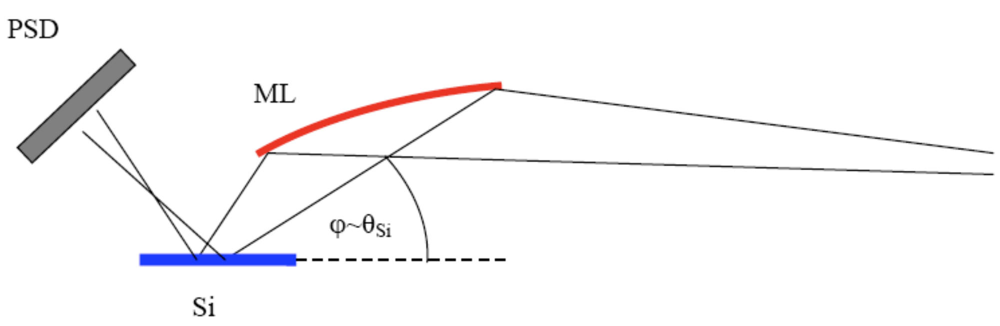
Advantages

Moderate curvature
Well established stable bending technology
Possible focal spot size <100 nm

Drawback

Limited energy resolution

Possible alternative

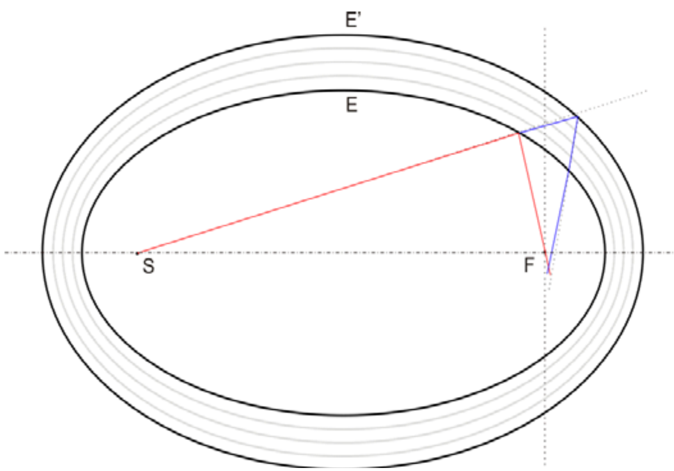


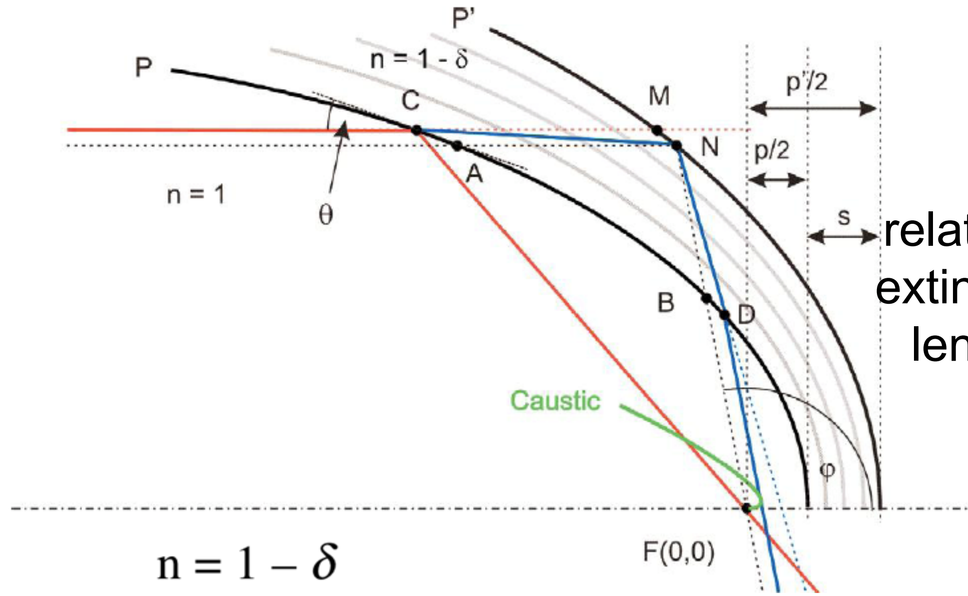
Drawback

Two optical elements

Aberration in focusing with curved Multilayer

a bi-layer refraction based analysis





related to extinction length

$$n = 1 - \delta$$
$$t = \tan(\varphi/2)$$

Parametric equations for the caustic curve

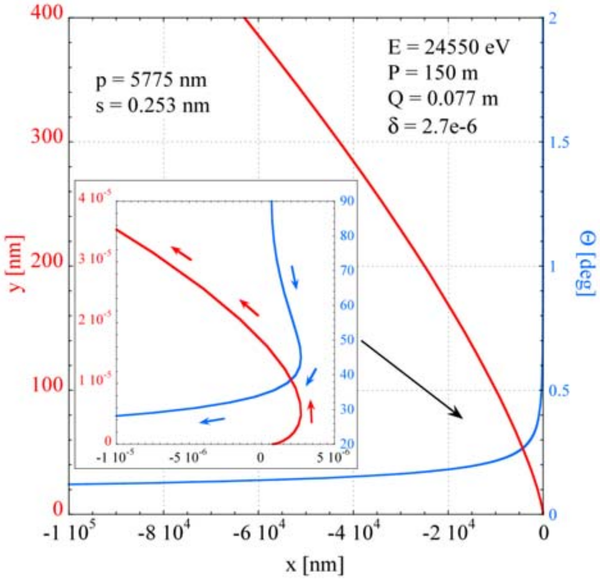
$$x(t) = \delta \cdot s \cdot (1 + s/p) \cdot (1 + 6 \cdot t^2 - 3 \cdot t^4)$$
$$y(t) = \delta \cdot s \cdot (1 + s/p) \cdot 8 \cdot t^3$$

Two fundamental aberrations :

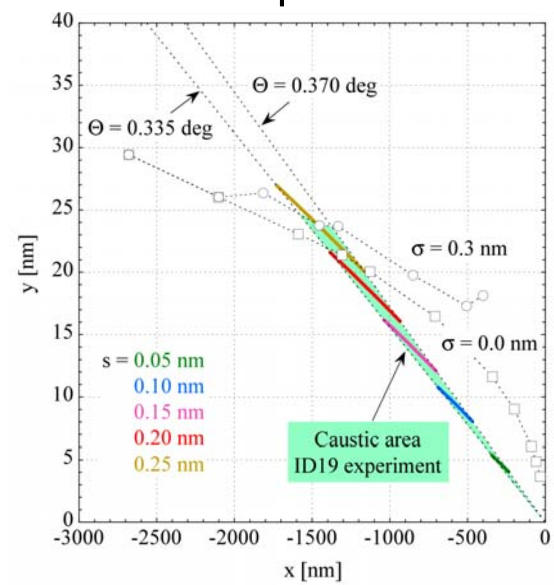
1. Aberrations due to a single interface illuminated at variable angles of incidence where δ = const and s = const, while t ranges from t_1 to t_2 , i.e. the mirror edges.
2. Aberrations originating from interfaces at variable penetration depths at a given angle of incidence where t = const, while s ranges from 0 (top surface) to s_{max} , given by the extinction depth z of the multilayer.

Considerations and limitations of geometric bi-layer refraction based analysis

Theory



Experiment



Assuming perfect ellipses or parabolas, the expected aberrations from the ideal focus are in the micrometer range along the optical axis and nanometric normal to it.

The analytical model described by such simplified approach, offers a general insight into the focusing performance of MLs in the hard x-ray range.

J.P Guigay, C. Morawe, V. Mocella, C. Ferrero, Opt Expr., 16, 12050, (2008)
C. Morawe, J.P Guigay, V. Mocella, C. Ferrero, Opt Expr., 16, 16138, (2008)

Optimum shapes of focusing RMLs are not perfect ellipses or parabolas, a better approach is assume that MLs have to fulfill Bragg's law locally, these modifications do not lead to simple mathematical expressions like a perfect ellipse or parabola .

Wave-optical models are required to carry out focusing experiments on the nanometer scale.

Beyond the geometrical approach: optical wave calculations for multilayers

First results of a full wave optical calculation for curved (or generally deformed) multilayers

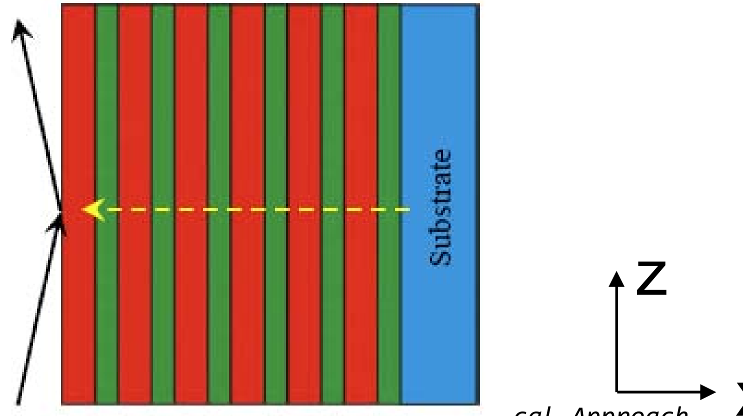
When a wave propagates along a waveguide for a large distance (larger compared with the wavelength), a rigorous numerical simulation (FDTD FEM) is difficult.

Solving propagation of light

$$\left(\nabla^2 + k_0^2 n^2 [x, z]\right)\psi = 0$$

for n slowly varying along z (the propagation direction).
the Parabolic Equation (PE) method is used, the same as in underwater acoustics

This is true for ML where Bragg angle is very small



Beyond the geometrical approach: optical wave calculations for multilayers

First results of a full wave optical calculation for curved multilayers

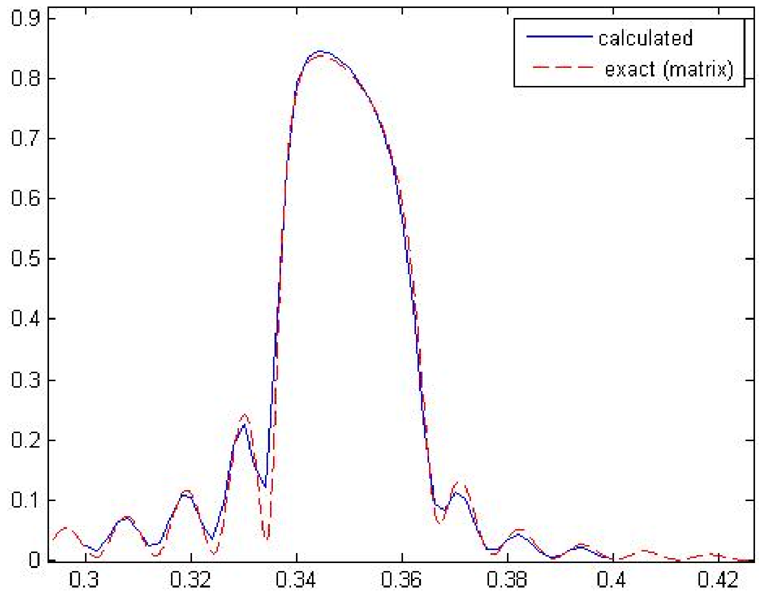
The approach is validated in the case of a flat ML,
where the exact solution can be calculated using matrix formalism (see Born & Wolf)

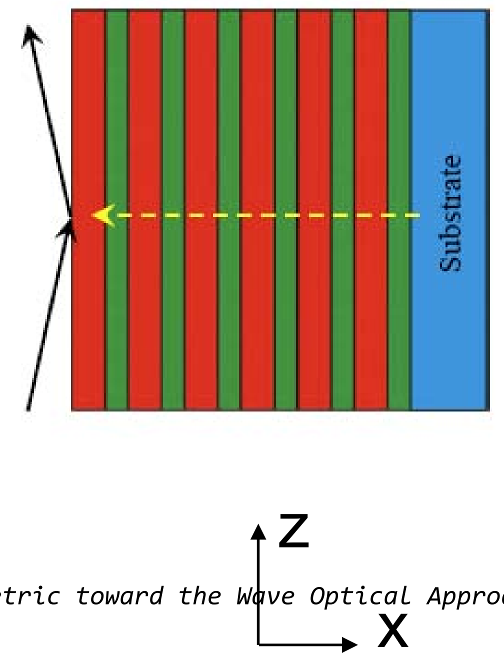
$W B_4 C$

$$E = 24.55 keV$$

$$\lambda = 0.05\, nm$$

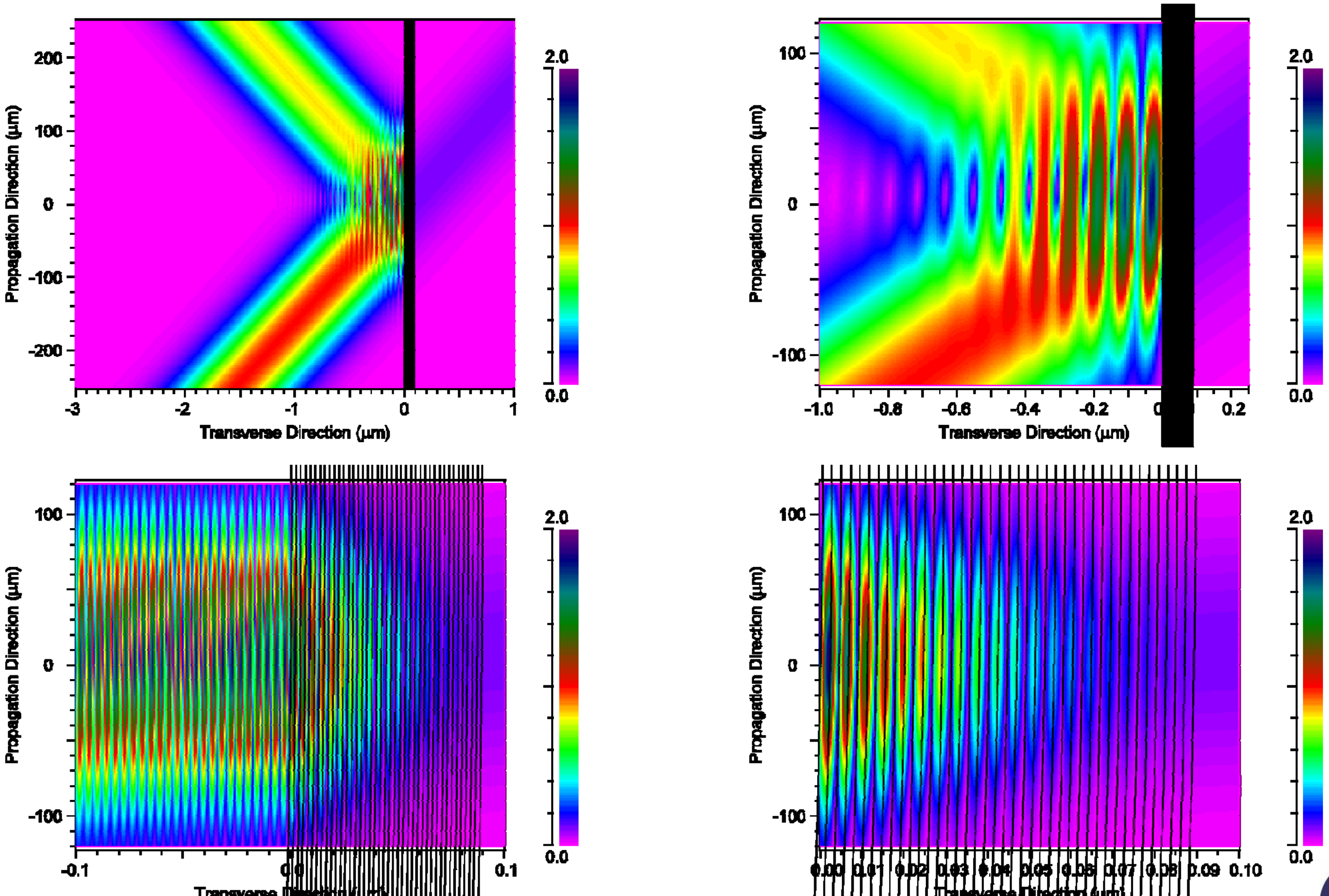
$$Period = 4.23\, nm$$



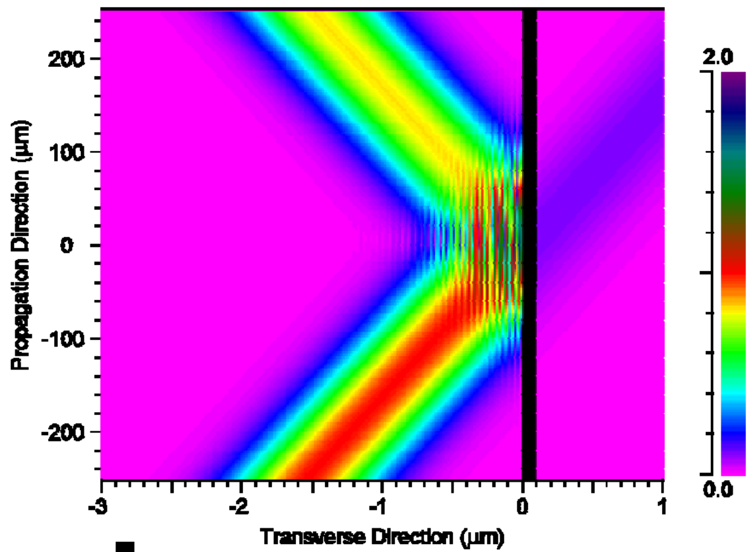


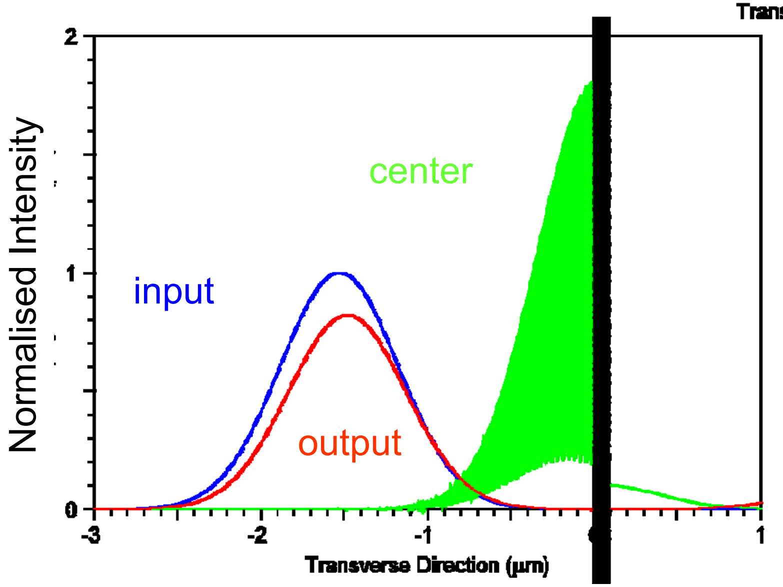
Optical wave calculations for elliptically curved Multilayers

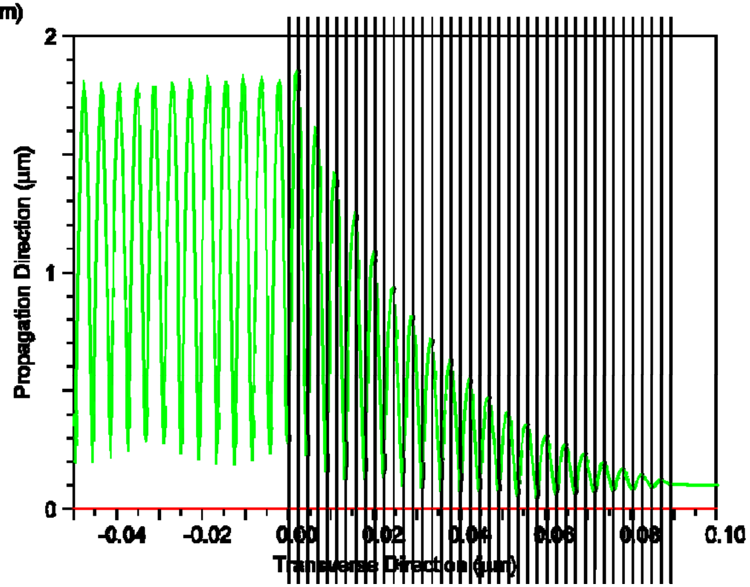
$$\theta_{inc} = 0.35^{\circ}$$



Optical wave calculations for elliptically curved multilayers



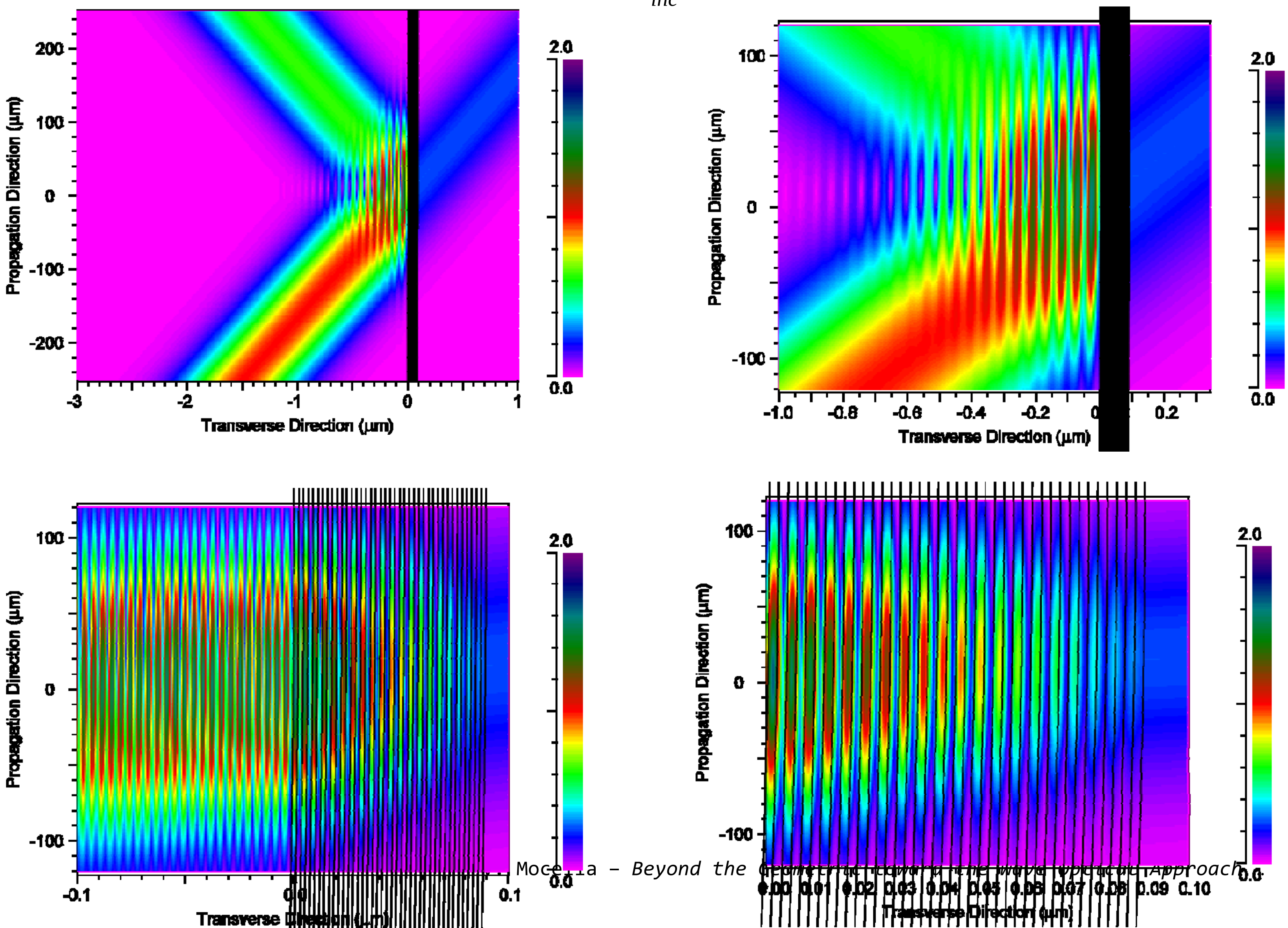




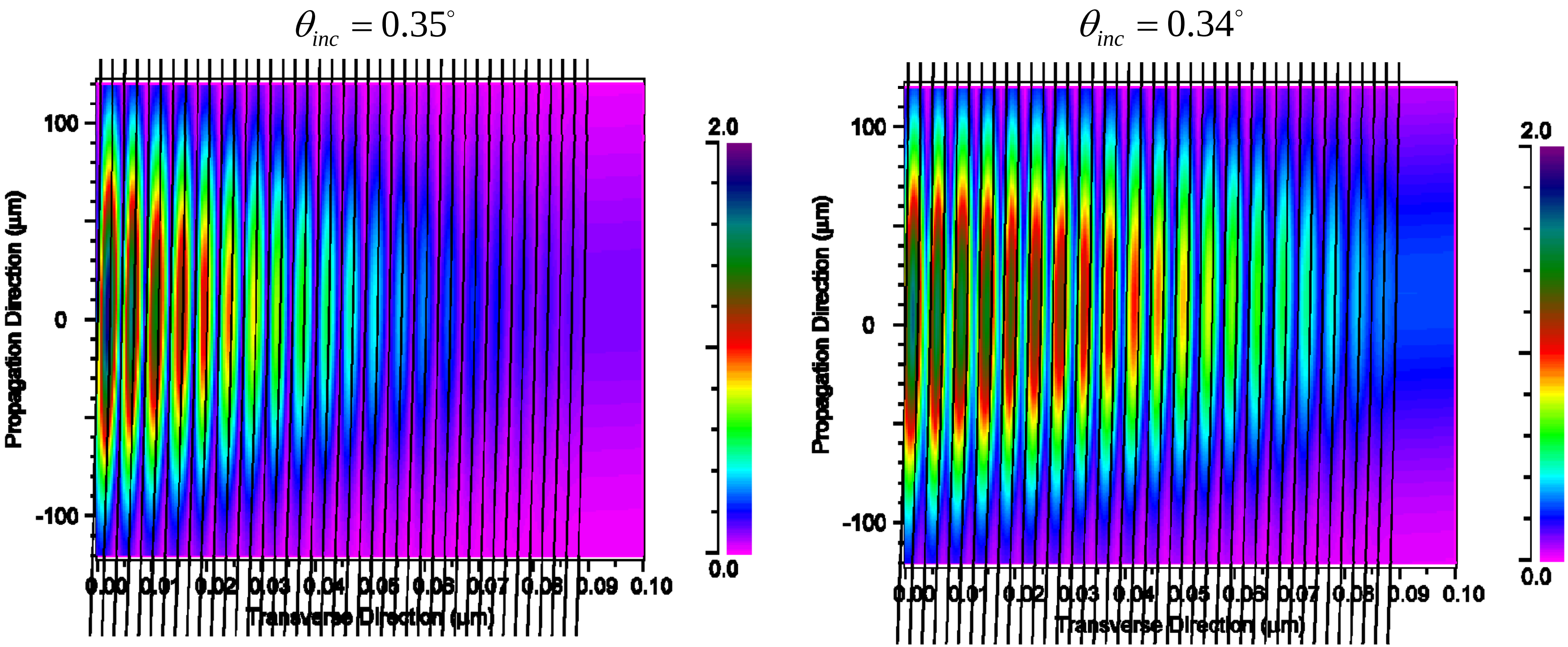
V. Mocella – *Beyond the Geometric toward the Wave Optical Approach …*

Optical wave calculations for elliptically curved Multilayers

$$\theta_{inc} = 0.34^{\circ}$$



Optical wave calculations for elliptically curved Multilayers



Comparison of extinction length (penetration depth)

Concluding…..

wave-optical calculations for elliptically curved Multilayers

- Extremely powerful and reliable calculations
- No limitation in geometry design, provided the paraxial approximation is satisfied
- Possible inclusion of surface roughness, fabrication imperfection, etc….

Conclusions

- **Wave optical** approaches are not simply useful but **unavoidable** if nanometric details are required.
- Analytic, semianalytic and numerical simulations from Takagi theory for crystals and multilayers are very useful for focusing optics design.
- A wave-optical approach has been successfully applied for the first time to a bent x-ray multilayer and should become a reference design technique for ML focusing purposes.