

*Theory of propagation
of hard x rays through
refractive optics.
Status and future directions*

V. G. Kohn

Russian-German kick-off workshop, 11-2010, Moscow

Introduction

X-ray refractive lenses has been considered as not feasible for a long time because $n = 1 - \delta + i\beta$ and

(1) refraction is small $\delta < 10^{-6}$

(2) absorption is important $\beta \propto 10^{-8}$

"There are no refractive lenses for x-rays" W.C.Roentgen

BUT

(1) $n < 1$ focusing lens is bi-concave,
therefore absorption is small on the optical axis

(2) X-ray beams become narrow and long
at SR sources and XFEL



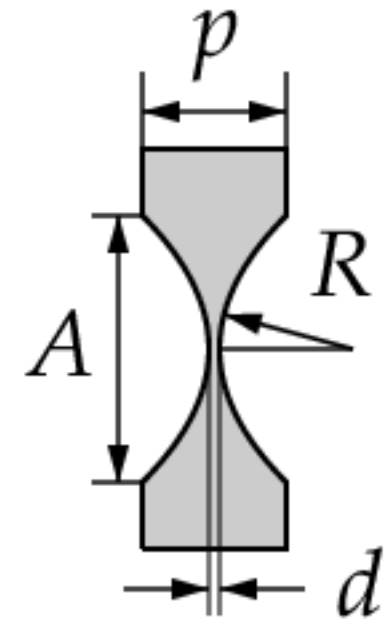
Basic Parameters

R – a curvature radius of parabola shape

A – a geometrical aperture

p – total length of the lens

d – web size between two surfaces



Paraxial approximation is satisfied very well

Thin lens formula for the focal length

$$F = \frac{R}{2\delta}, \quad p \ll F$$

For **Al** lens with $R = 0.2$ mm and $E = 12$ keV we obtain

$$\delta = 3.78 \cdot 10^{-6}, \quad F = 26 \text{ m},$$

half-width of the beam behind lens is **341** microns

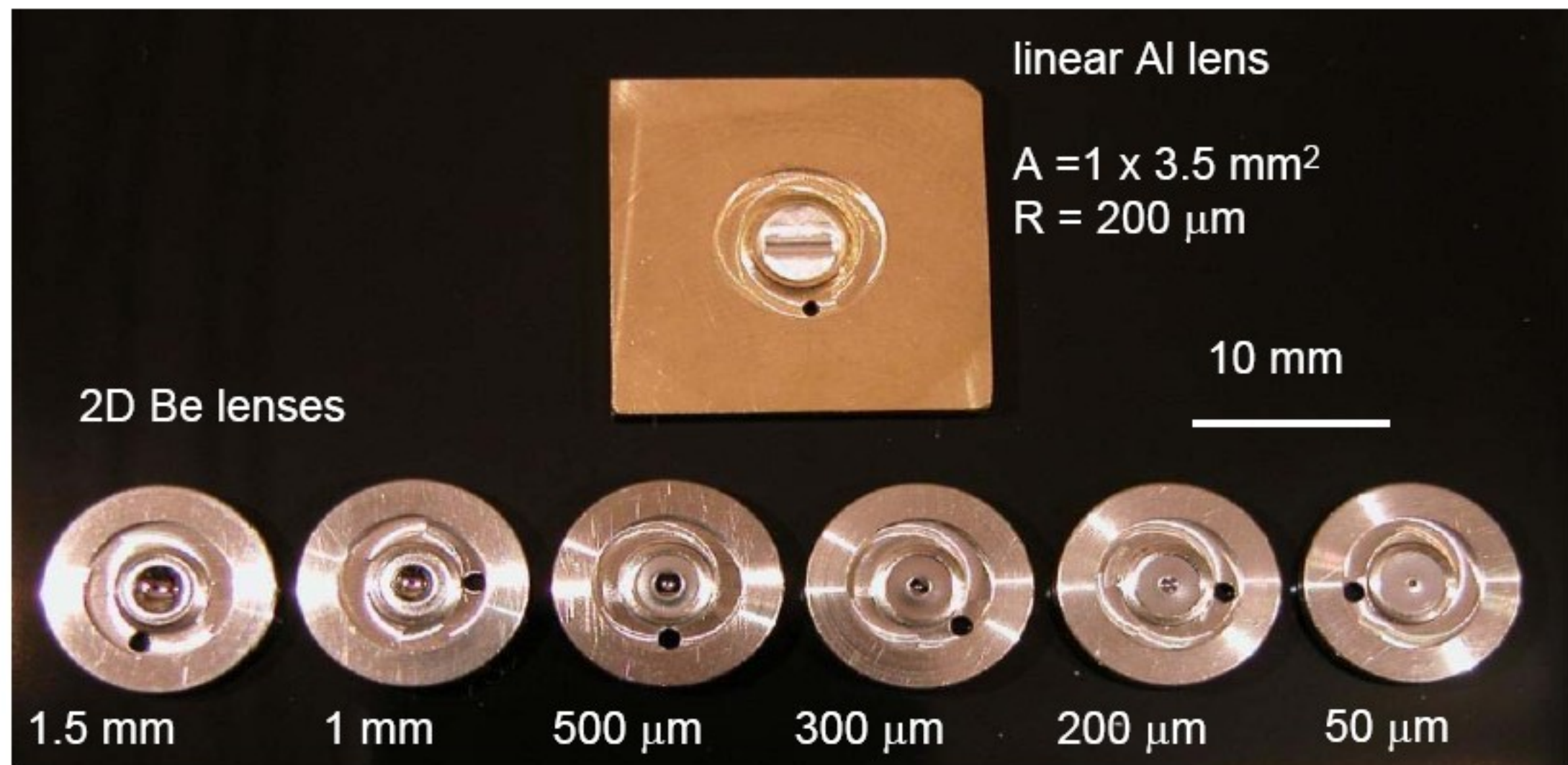
Key idea was to use a compound refractive lens

Snigirev, Kohn, Snigireva, Lengeler, Nature, 1996

Examples of real lenses

The best 2D lenses are created by Bruno Lengeler
in RWTH Aachen University (Germany) by pressing materials
Recently 1D lenses becomes available (the same technology)

<http://www.physik.rwth-aachen.de/en/institutes/institute-iib/group-lengeler>

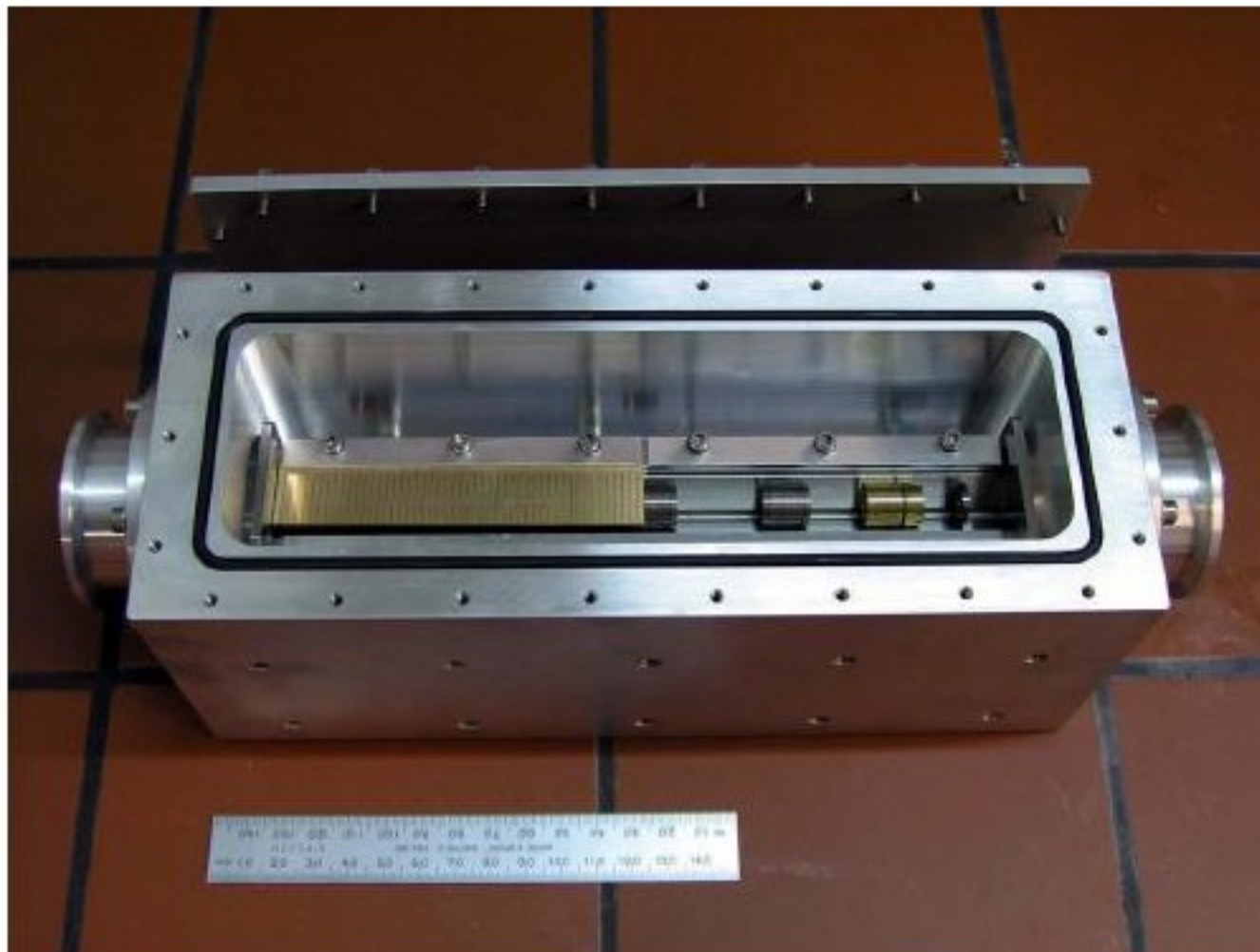
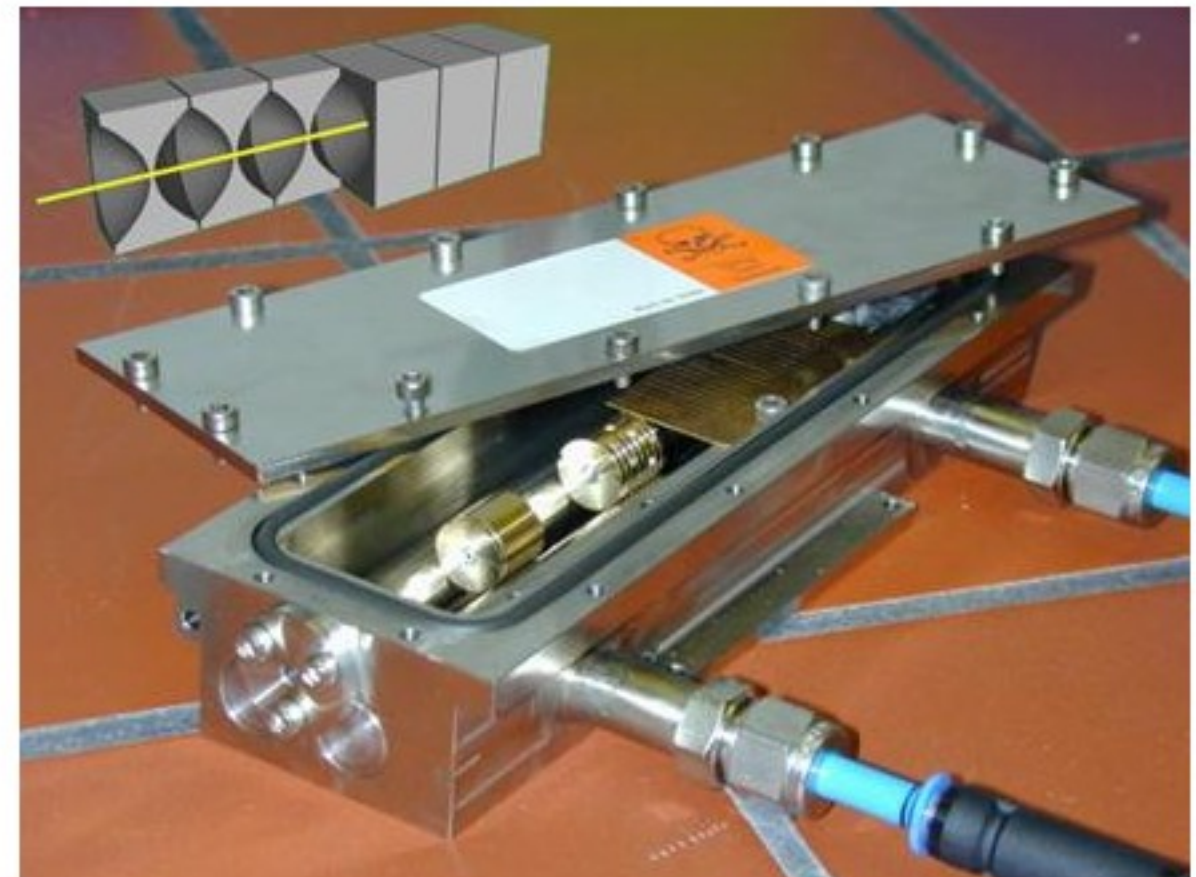
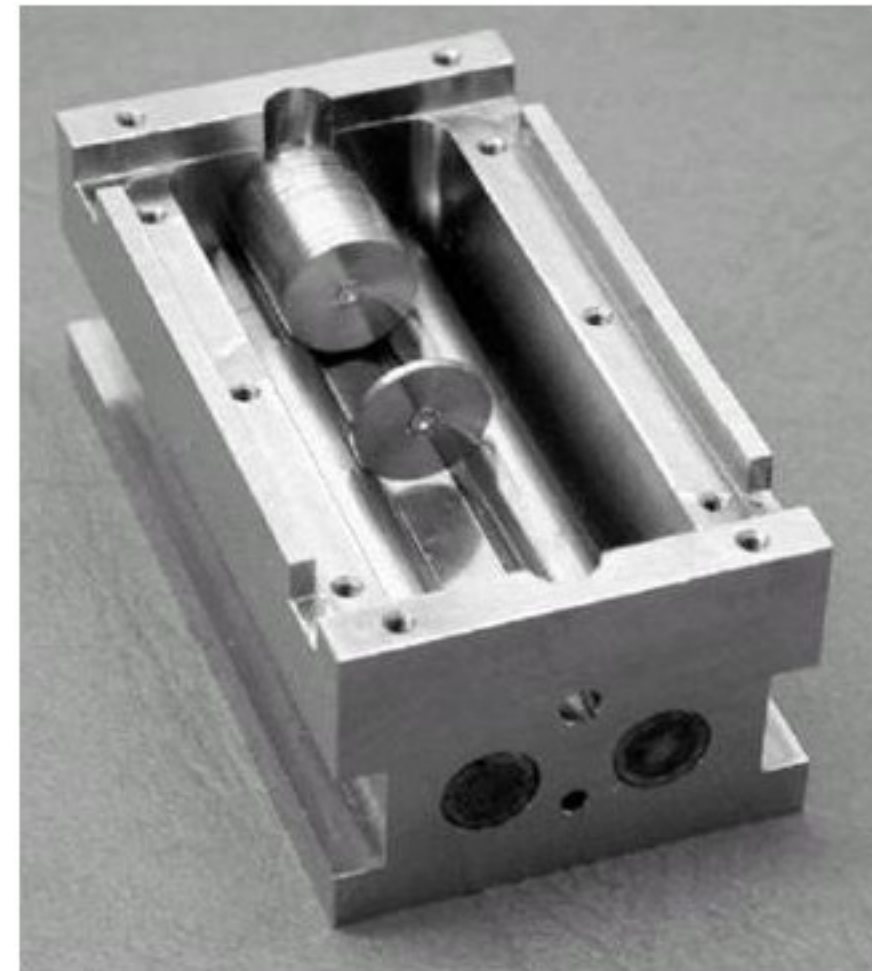


Holders for Compound refractive lenses (CRL)

top right – Al (air) old

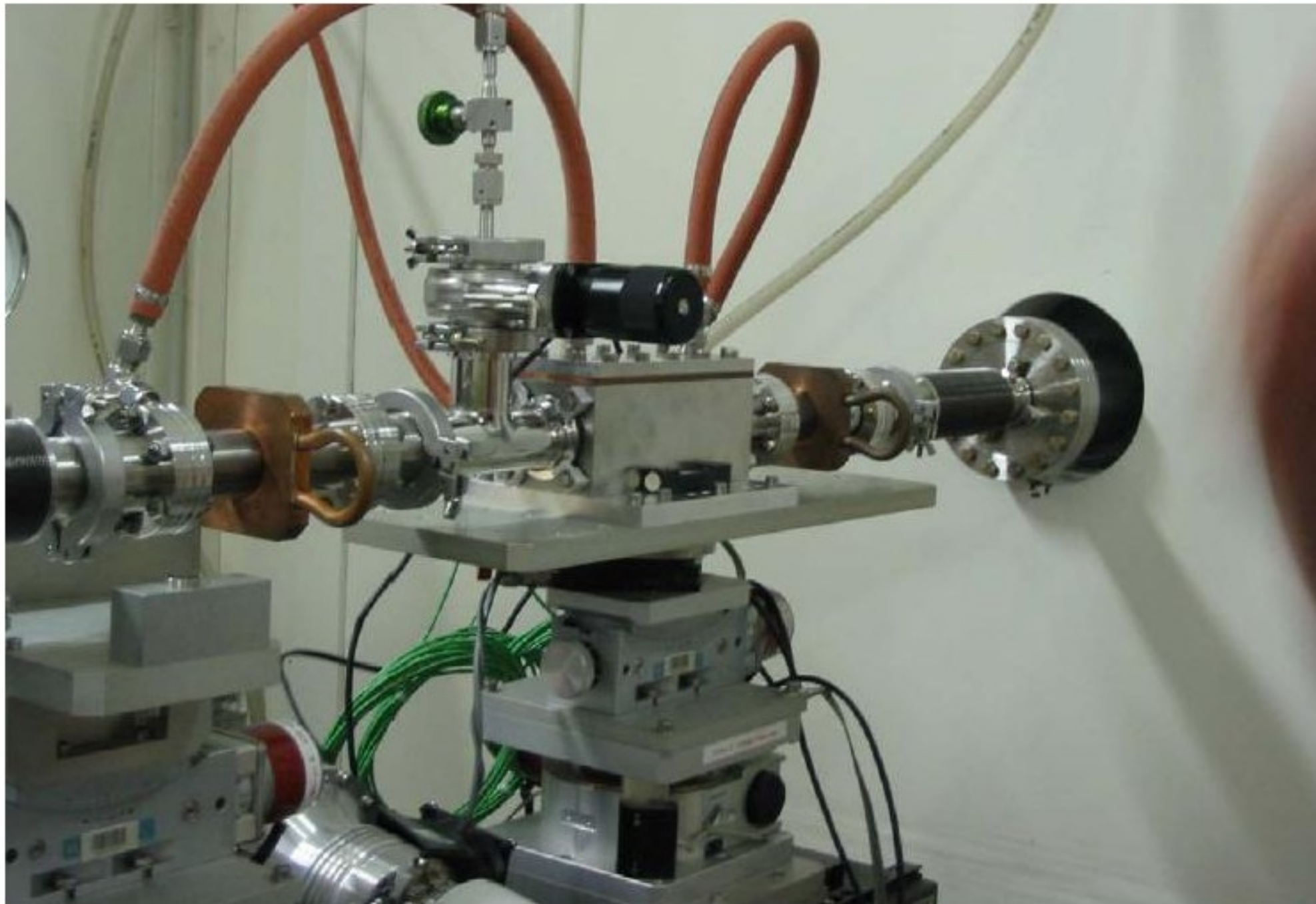
bottom right – Be (vacuum)

bottom left – New holder

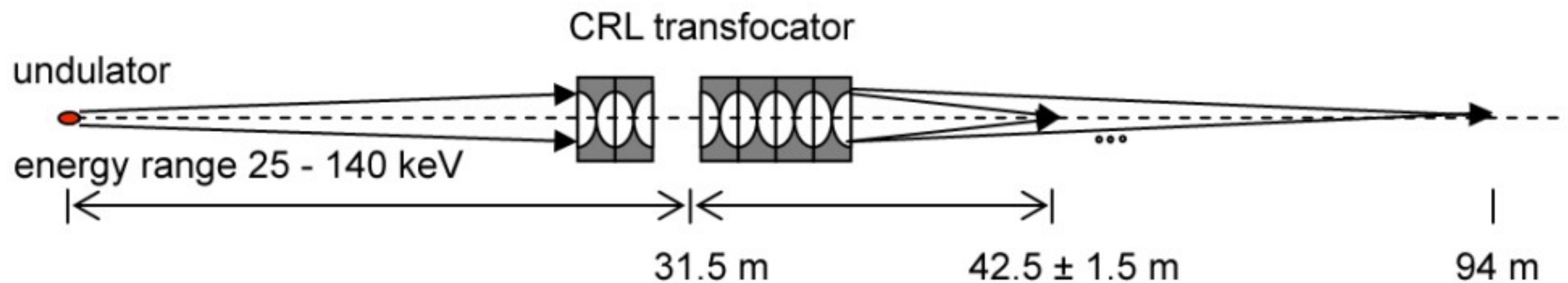
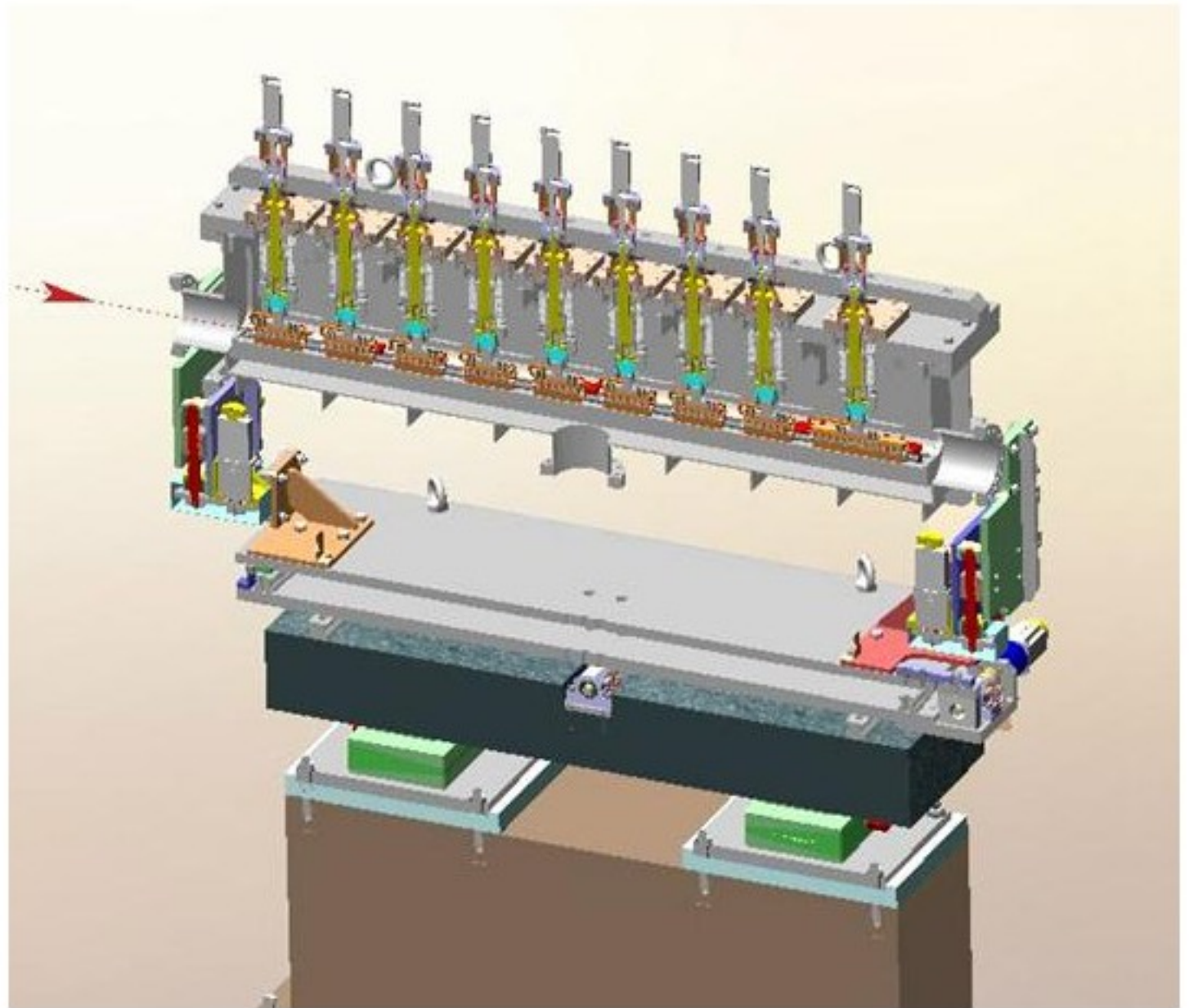


Thermal stability in the intense beam

Water cooled beryllium CRL at the ESRF (ID 10)



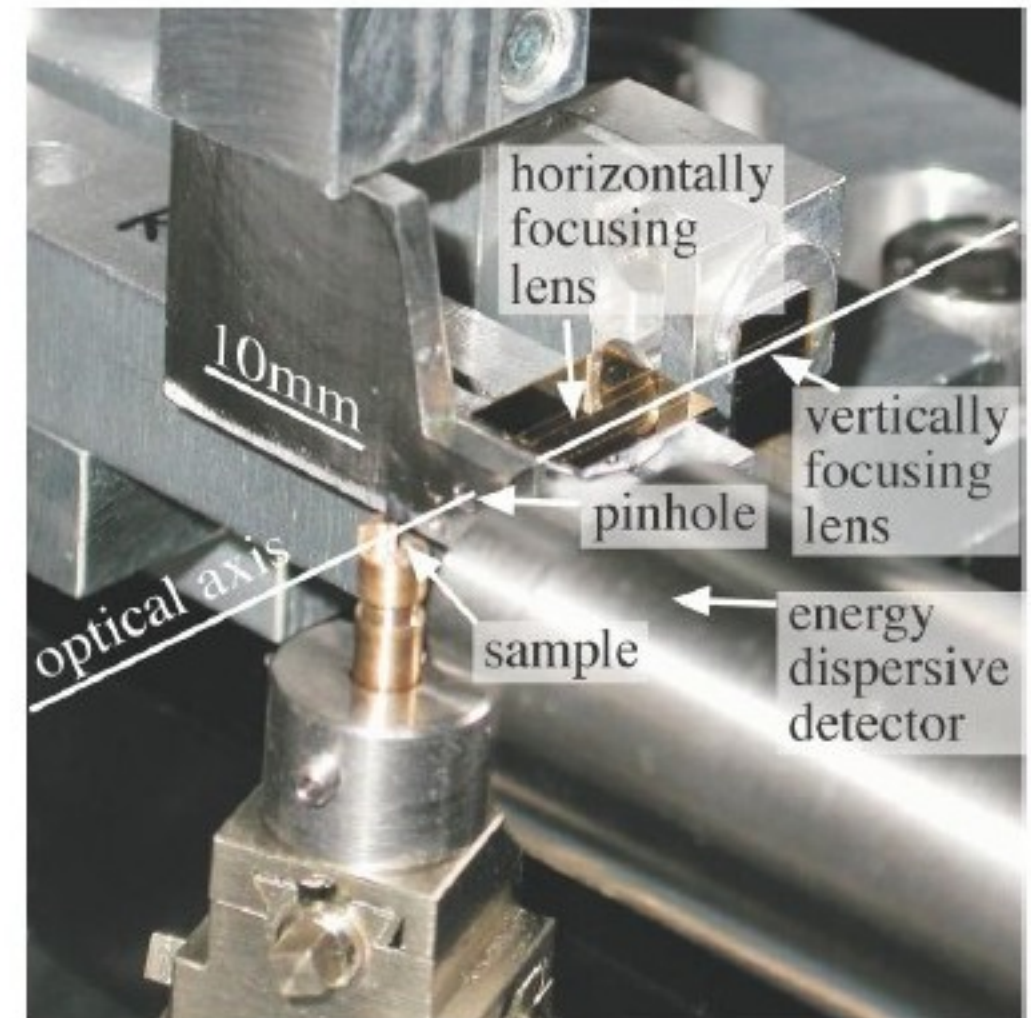
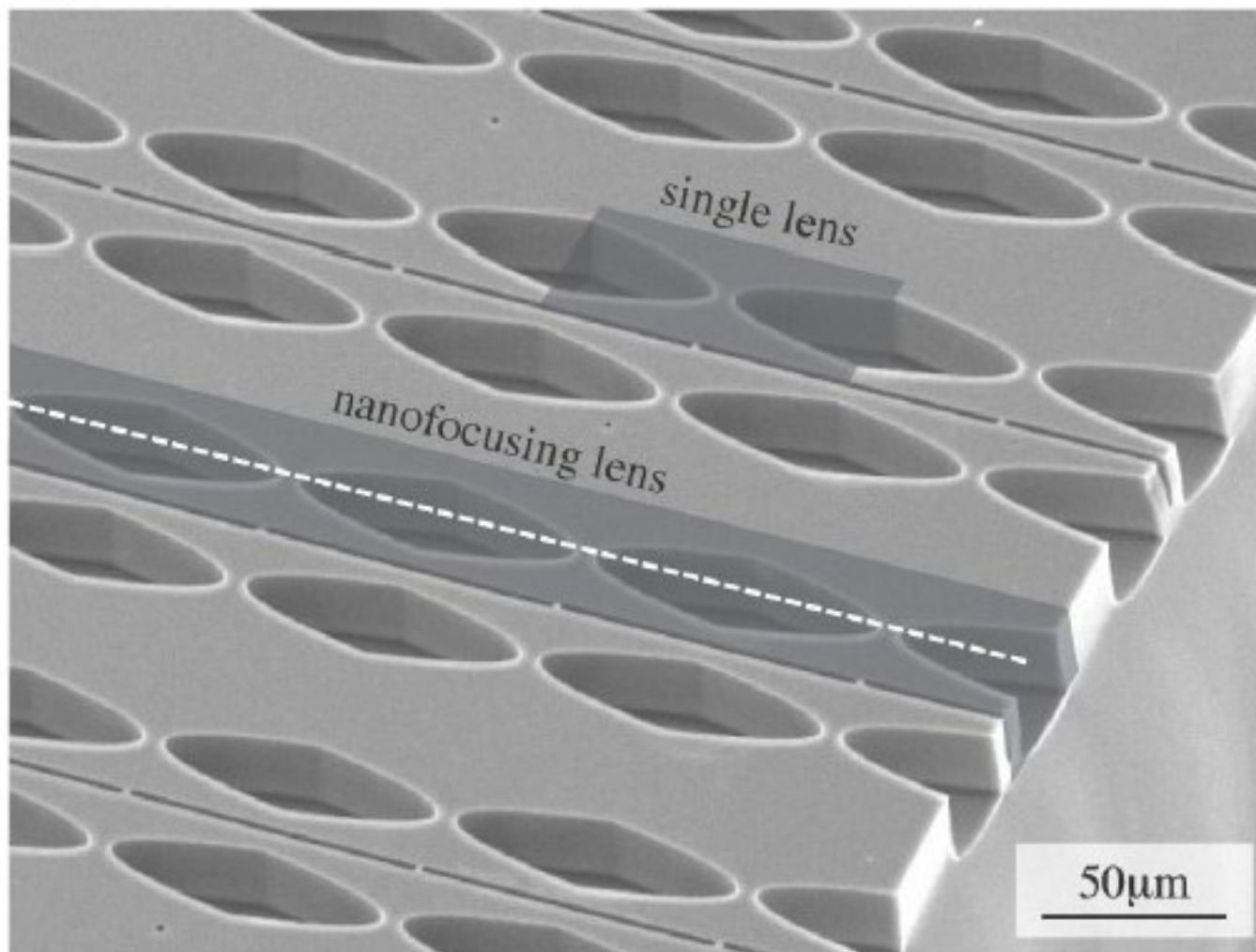
Transfocator
as compound CRL
is a new possibility to create
source of divergent beam
closely to sample. The
position of source is the
same for all energies. It is
cooled and is placed as first
optical element.



Planar silicon parabolic lenses made by microfabrication techniques

The lenses are fabricated using electron (e)-beam lithography and deep trench reactive ion etching. APL-2003-82-1485
RWTH Aachen University, Shroer, , Lengeler

One lens makes 1D focus, two lenses make 2D focus

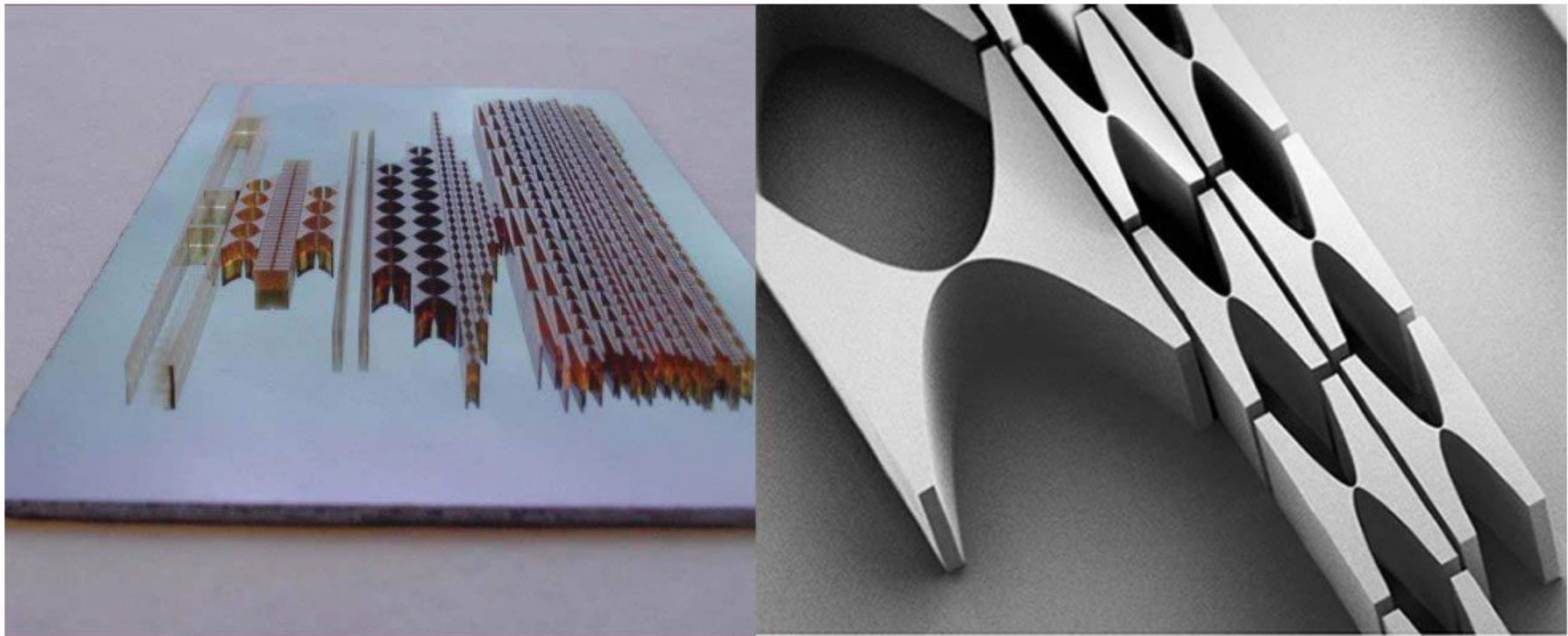


Planar SU-8 parabolic lenses made by LIGA techniques

The lenses are fabricated from SU-8 resist using LIGA
(Litographie, Galvanoformung u Abformungelectron)

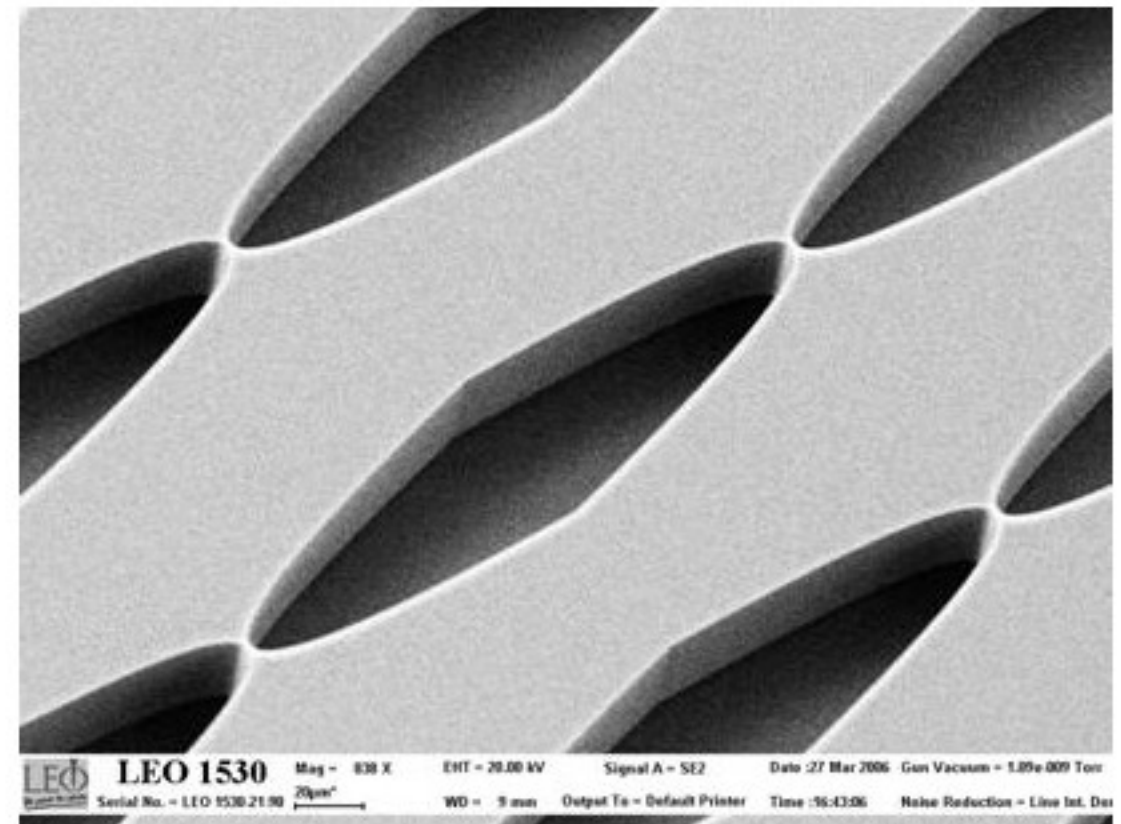
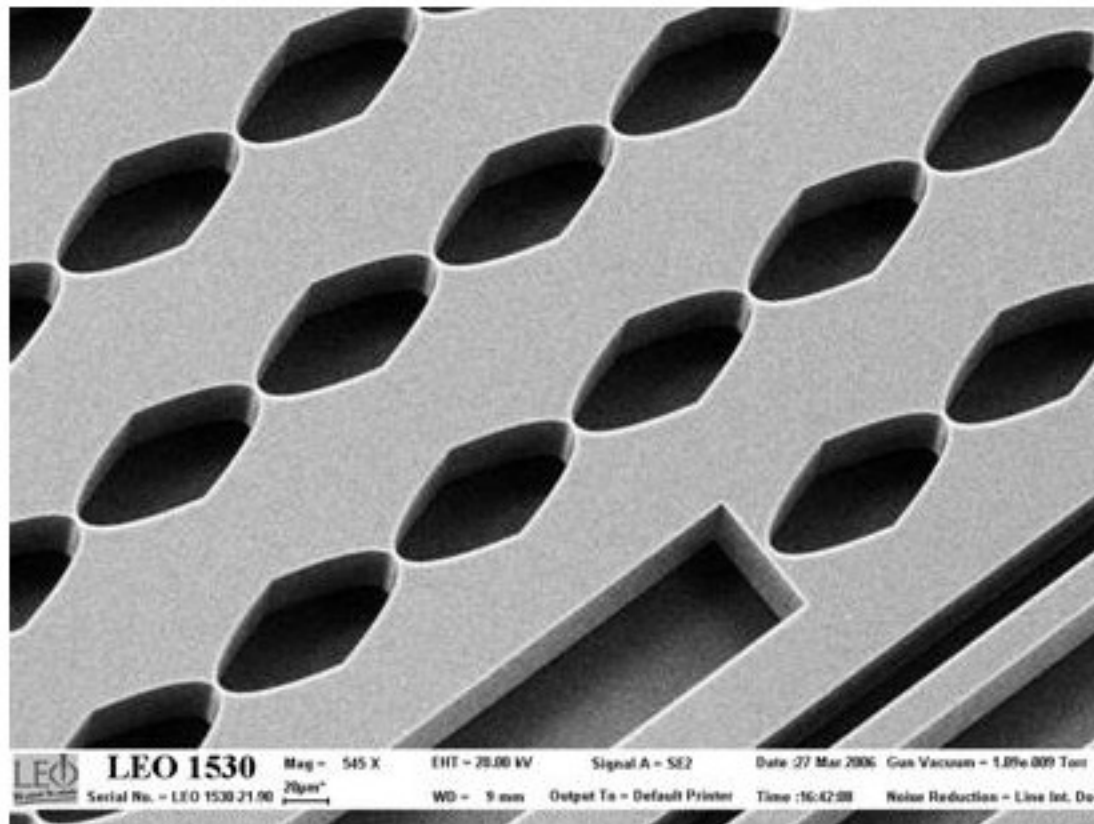
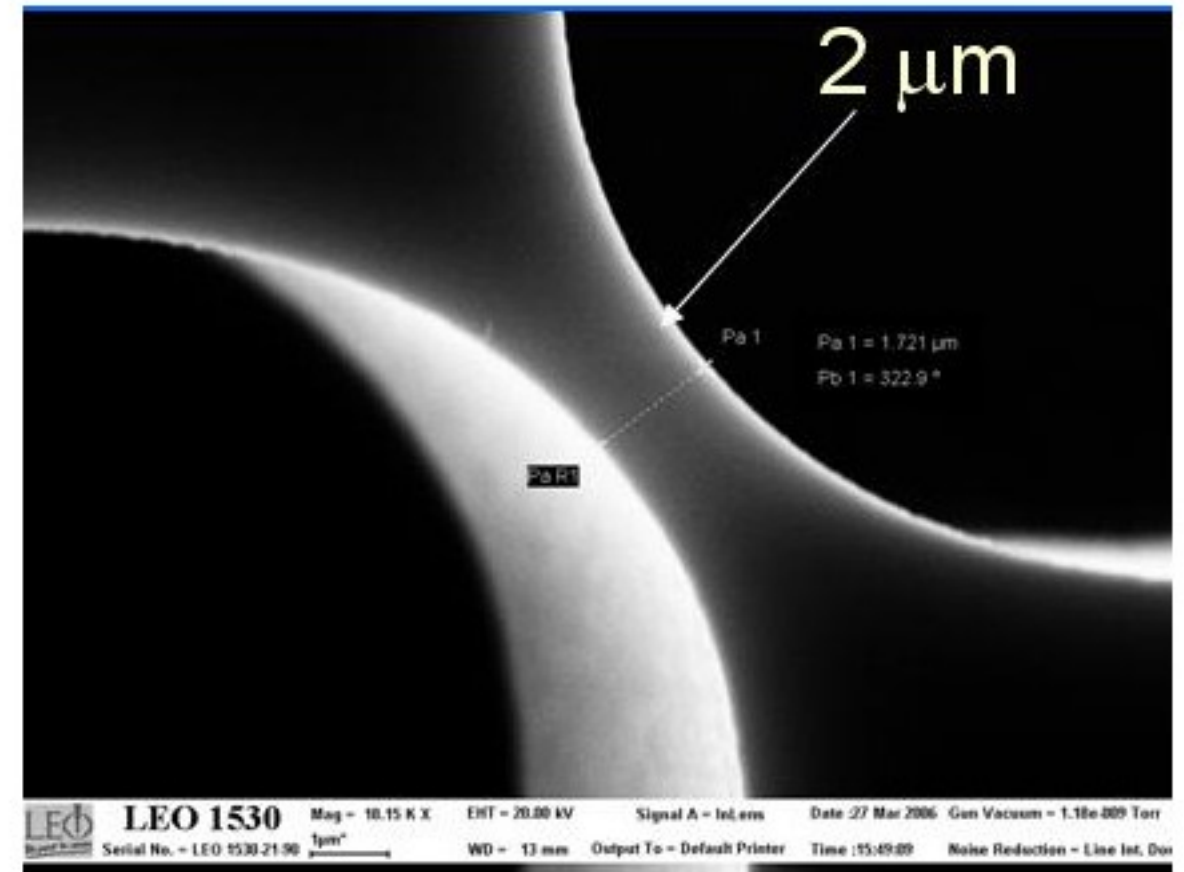
LITHO-3 ANKA beamline, SPIE-2003-5195-21

IMT/FZK Karlsruhe, Germany, Nazmov, Reznikova



Planar Si lenses nano-focusing and nano-interferometry

Developed e-beam lithography and
deep etching. PRL-2009-103-064801
Chernogolovka, Russia, Yunkin



Theory, 1D case for simplicity

Paraxial approximation for Maxwell's equation is valid very well

Polarization does not influence the results. Electric field is

$$E(x, z) = A(x, z) \exp(ikz), \quad k = 2\pi/\lambda, \quad I(x, z) = |A(x, z)|^2$$

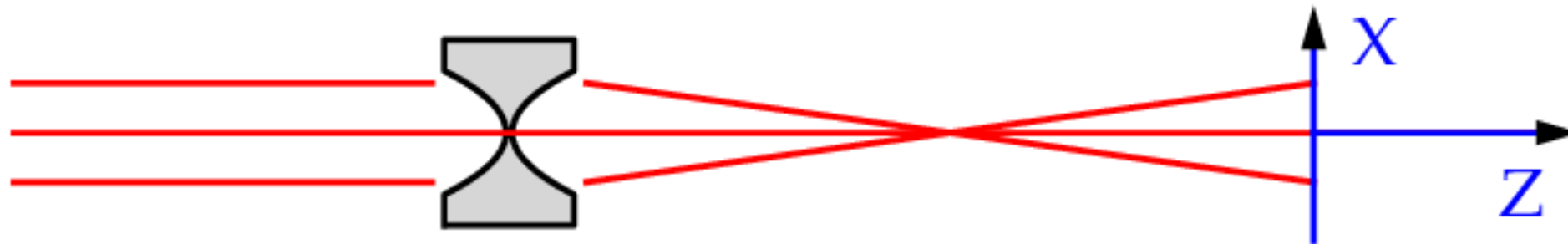
The main equation is a parabolic equation for $A(x, z)$

$$\frac{dA(x, z)}{dz} = -ik\eta s(x, z)A(x, z) + \frac{i}{2k} \frac{d^2 A(x, z)}{dx^2}, \quad \eta = \delta - i\beta$$

refraction index $n = 1 - \delta + i\beta$, $s(x, z) = 1$ (matter) = 0 (air)

Si, $E = 12$ keV: $k\delta = 2000 \text{ cm}^{-1}$, is very large

$1/(2kx^2) = 0.001 \text{ cm}^{-1}$, for $x = 10 \text{ }\mu\text{m}$, is very small



Solution for air (exactly)

$$\frac{dA(x, z)}{dz} = \frac{i}{2k} \frac{d^2 A(x, z)}{dx^2}, \quad P(x, z) = \frac{1}{(i\lambda z)^{1/2}} \exp(i\pi \frac{x^2}{\lambda z})$$

$$A(x, z_2) = \int dx' P(x - x', z_2 - z_1) A(x', z_1)$$

The operation is known as a convolution.

It is a specific case of Kirchhoff-Fresnel principle,

Propagator $P(x, z)$ is a reaction on a point source.

In general case the convolution can be calculated only numerically. It is convenient to use double FFT.

$$A(x, z_1) \Rightarrow A(q, z_1), \quad A(q, z_1) P(q, \Delta z) \Rightarrow A(x, z_2)$$

Applying many points (65536) one can obtain the result quickly and exactly.

Solution for CRL (thin lens approximation)

$$\frac{dA(x, z)}{dz} = -ik\eta s(x, z)A(x, z), \quad A(x, z_2) = T(x, \Delta z)A(x, z_1)$$

$$T(x, \Delta z) = \exp\left(-ik\eta \int_{z_1}^{z_2} dz' s(x, z')\right)$$

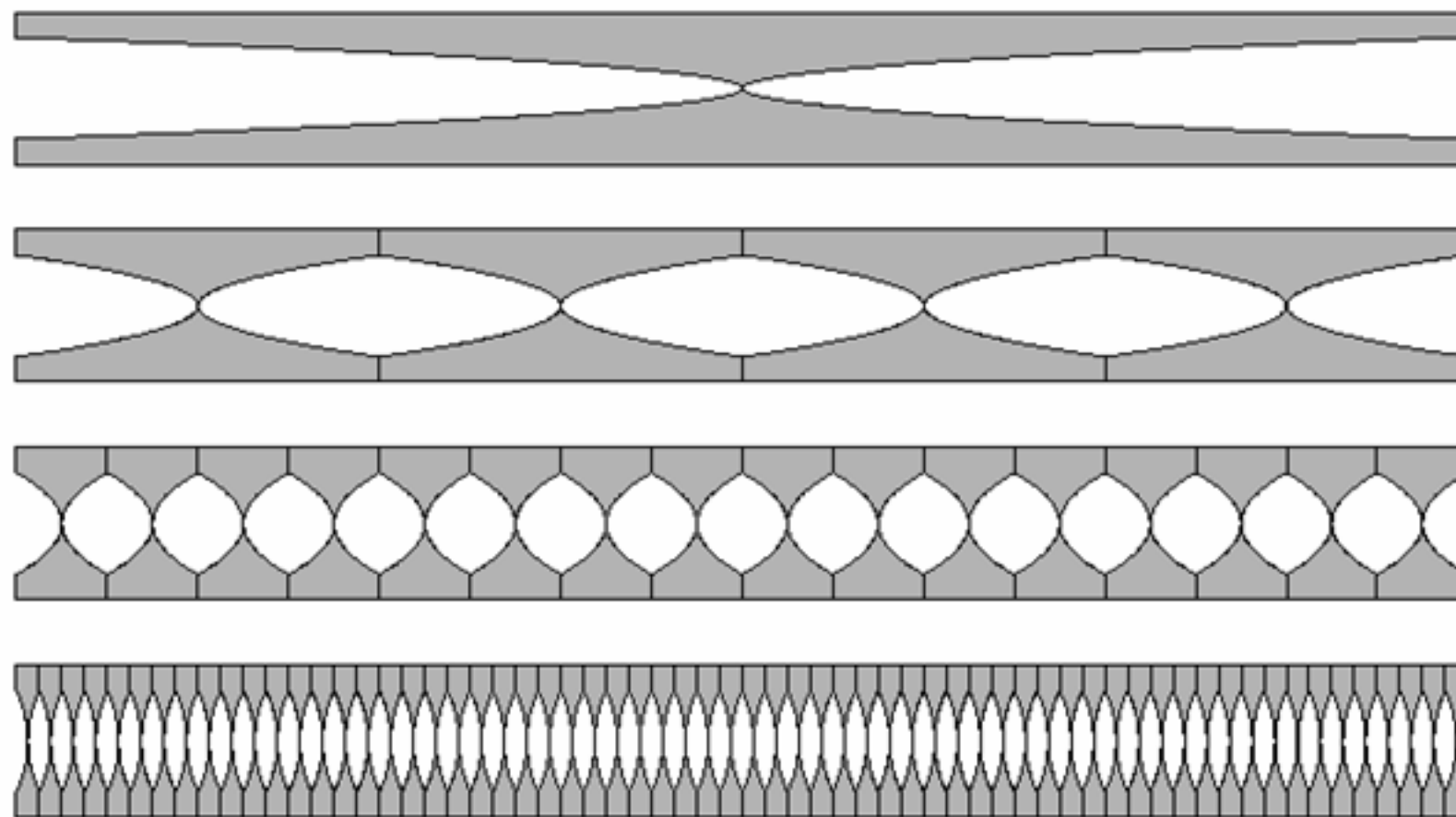
$T(x, \Delta z)$ is known as the transmission function. In the case of parabolic profile the function is simple, BUT there may be various distortions of the parabolic profile. In any case this task is not convenient. For the wide parabolic profile the real aperture can be neglected and

$$T(x, \Delta z) = \exp\left(-i\pi \frac{x^2}{\lambda F} [1 - i\gamma]\right), \quad F = \frac{R}{2\delta}, \quad \gamma = \frac{\beta}{\delta}$$

Here F is the focal length of the CRL. Many lenses (N) works as one with $R = R_0/N$ so CRL is equivalent to one lens.

Solution for long CRL (exactly parabolic)

In a thin lens approximation all lenses shown in the picture are equivalent because only an integral over z is important. However, the bottom lens has periodical z -dependence with a small period. We consider a limit case of very small period and average over it, eliminating z -dependence $s(x, z) \Rightarrow \overline{s(x)}$



Solution for long CRL (exactly parabolic)

So we obtain a parabolic refracting material and the equation

$$\frac{dA(x, z)}{dz} = -ik \frac{x^2}{2z_c^2} A(x, z) + \frac{i}{2k} \frac{d^2 A(x, z)}{dx^2}, \quad z_c = \left(\frac{pR}{2\eta} \right)^{1/2}$$

A propagator for this equation as a reaction on a point source is now known as well as it's imaging properties (Kohn, JETP, 2003-97-204) therefore we can write

$$A(x, z_2) = \int dx_1 P_{pm}(x, x_1, \Delta z) A(x_1, z_1),$$

$$P_{pm}(x, x_1, \Delta z) = \frac{1}{(i\lambda z_c S_z)^{1/2}} \exp \left(i\pi \frac{(x^2 + x_1^2) C_z - 2xx_1}{2z_c S_z} \right),$$

$$S_z = \sin \left(\frac{\Delta z}{z_c} \right), \quad C_z = \cos \left(\frac{\Delta z}{z_c} \right)$$

The integral is not a convolution, therefore numerical calculation is more complicated in this case. However, for Gaussian beam there is analytical solution as a Gaussian beam again.

Exact Solution for short CRL

Exact solution allows one to formulate a condition for *thin lens approximation* as $\Delta z \ll z_c$. Under this condition we have

$$P_{pm}(x, x_1, \Delta z) = \exp\left(i\pi \frac{x^2 + x_1^2 + xx_1}{3\lambda F_c}\right) P(x - x_1, \Delta z)$$

$$F_c = \frac{F}{1 - i\gamma} = \frac{z_c^2}{\Delta z} = \frac{R}{2\eta N}, \quad N = \frac{\Delta z}{p}$$

It is more correct than the transmission function. The latter can be obtained replacing Kirchhoff propagator by delta-function

$$P(x - x_1, \Delta z) \Big|_{\Delta z \rightarrow 0} = \delta(x - x_1)$$

Only then we obtain

$$P_{pm}(x, x_1, \Delta z) = \exp\left(i\pi \frac{x^2}{\lambda F_c}\right) \delta(x - x_1)$$

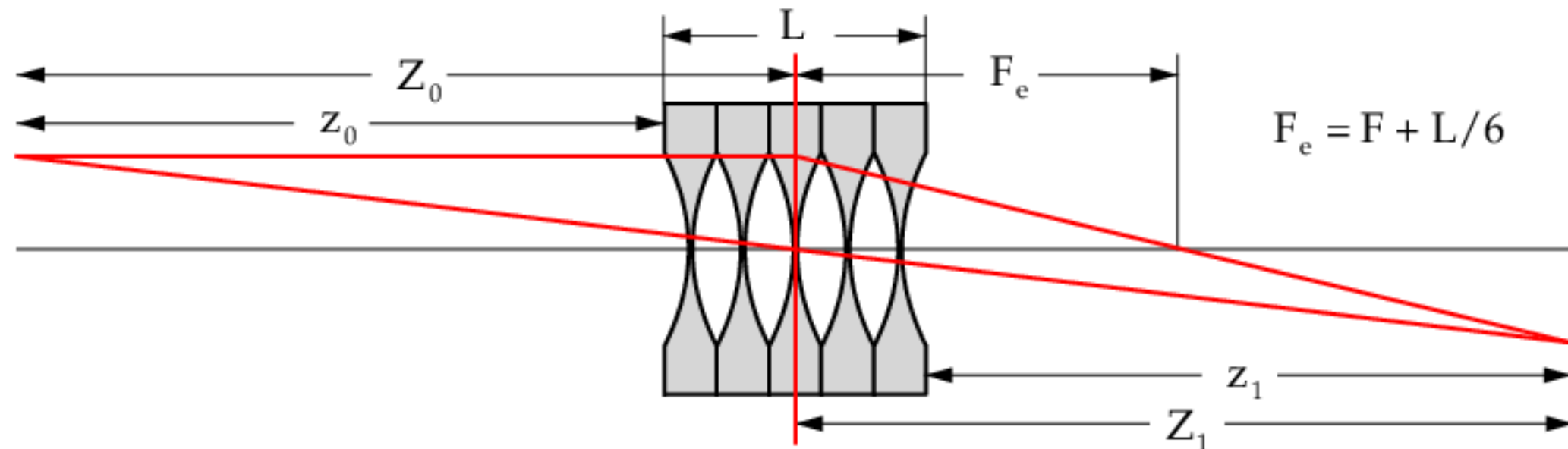
This is more strong approximation of the Phase Contrast Imaging

Exact Solution for short CRL focusing

Another sequence of exact solution for short CRL is an improvement of the lens formula for focusing. If $L = \Delta z$ is the lens length, z_0 and z_1 are distances in front and behind the lens, then

$$Z_0^{-1} + Z_1^{-1} = F_e^{-1}, \quad Z_0 = z_0 + L/2 \quad Z_1 = z_1 + L/2 \quad F_e = F_c + L/6$$

This means that the lens can be considered as having no thickness and is placed at its middle point, but focal length is longer by $L/6$



Semianalytical approach for Gaussian beams

Propagation through a thin lens and some distance in air is defined by

$$A(x, x_0, z_2) = \int dx_1 P(x - x_1, \Delta z) \exp\left(i\pi \frac{x_1^2}{\lambda F_c}\right) A(x_1, x_0, z_1)$$

There is a theorem (Kohn, J. Surface Invest., 2009-3-358). If

$$A(x, x_0, z_1) = T(x, a_0)P(x - x_0, b_0)T(x_0, c_0), \quad T(x, a) = \exp\left(i\pi \frac{x^2}{\lambda a}\right)$$

then the integral is calculated analytically and

$$A(x, x_0, z_2) = T(x, a)P(x - x_0, b)T(x_0, c)$$

There are recurrent relations for three complex parameters a, b, c

$$a = d \frac{b}{b_0}, \quad b = b_0 + \Delta z \left(1 - \frac{b_0}{d}\right), \quad c = \frac{c_0}{1 + \Delta z c_0 / b d}, \quad d = \frac{a_0}{1 + a_0 / F_c}$$

These recurrent relations can be used many times with various lenses, placed disorderedly and made from various materials. The method was used for a calculation of translocator properties.

Semianalytical approach for Gaussian beams

Intensity as a function of distance behind the last lens is defined by

$$I(x, x_0, z) = I_m(x_0, z) \exp\left(-\frac{(x - x_m(z))^2}{2\sigma^2(z)}\right), \quad I_m(x_0, z) = \frac{Z}{|b|} \exp\left(-\frac{x_0^2}{2\sigma_0^2}\right)$$

$$\sigma(z) = (2k[A - B])^{-1/2}, \quad \sigma_0 = (2k[C - AM])^{-1/2}, \quad x_m(z) = -M(z)x_0,$$

$$M = \frac{B}{A - B}, \quad A = -\text{Im}\left(\frac{1}{a}\right), \quad B = -\text{Im}\left(\frac{1}{b}\right), \quad C = -\text{Im}\left(\frac{1}{c}\right)$$

Some conclusions:

σ_0 does not depend on z , numerically it is right, but analytically ??.

Integral intensity $\propto I_m(z)\sigma(z)$ does not depend on z , from this we have

$G = |b|^2[A - B]$ does not depend on z , numerically it is right, but ...

We have as well $M(z) = M_0 + M_1z$, and $b = B_0 + B_1z$. Focus distance is calculated from minimum $\sigma(z)$ as $z_f = -\text{Re}(B_0B_1^*)/|B_1|^2$

Half-width (FWHM) is equal to $w(z) = C\sigma(z)$, $C = (8\ln 2)^{1/2} = 2.355$

Semianalytical approach for Gaussian beams

Sequence for one thin lens

$$(1) \quad a_0 = \infty, \quad b_0 = z_0 : \quad z_f = \frac{F}{1 - F/z_0 + \gamma^2(1 - F/z_0)^{-1}}, \quad \gamma = \frac{\beta}{\delta}$$

so, due to absorption the lens is not suitable *as a collimator*,

$$(2) \quad a_0 = b_0 = \infty : \quad w(z) = 0.66 \left(\frac{\lambda F}{\gamma} \right)^{1/2} \left(\left(1 - \frac{z}{F} \right)^2 + \gamma^2 \left(\frac{z}{F} \right)^2 \right)^{1/2},$$

so, there is universal relation for the half-width of the Gaussian beam:

$$w(F) = \gamma \cdot w(0) = 0.44 \frac{\lambda F}{w(0)}$$

the parameter γ can be called as power of focusing,

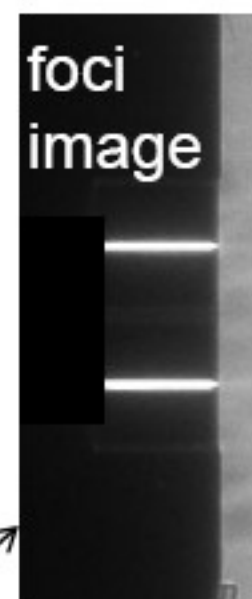
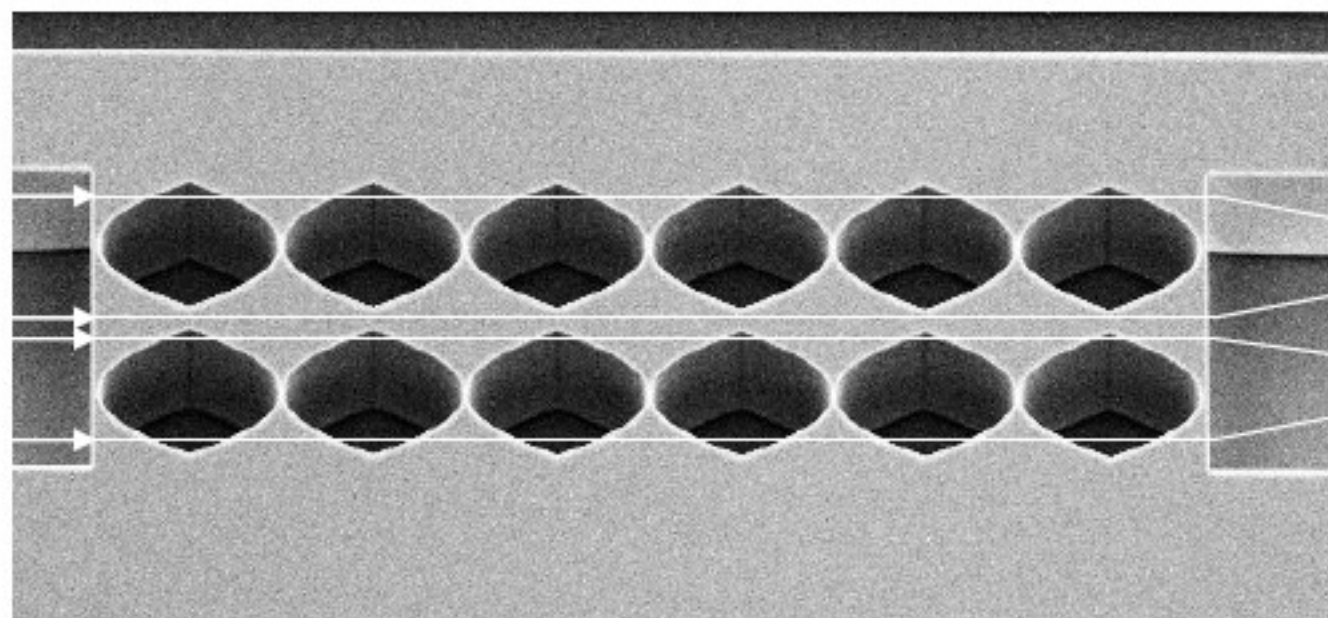
the parameter $w(0)$ can be called as effective aperture,

well known formula for a focus width has a multiplier 0.44.

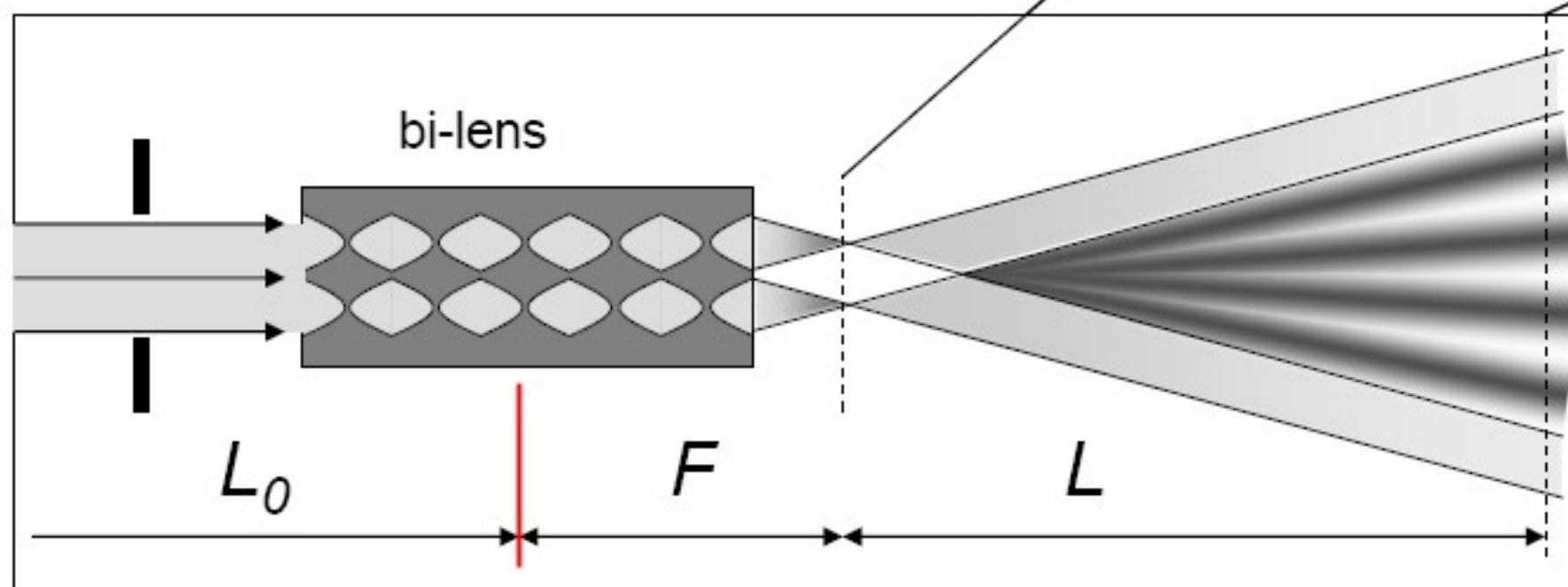
A minimum focus width can be estimated as $w_{\min}(F) = (\lambda/(8\delta))^{1/2}$.

Bergemann et al, PRL-2003-91-204801

Silicon bilens (ESRF-Russia)



PRL-2009-103-064801



Computer simulations

Various computer programs allow one to simulate properties of the intensity profile at the focus and any distance behind the CRL

Some programs even works in *Internet* as java-applets

ACL (V.Kohn) v.0.8.26 applet

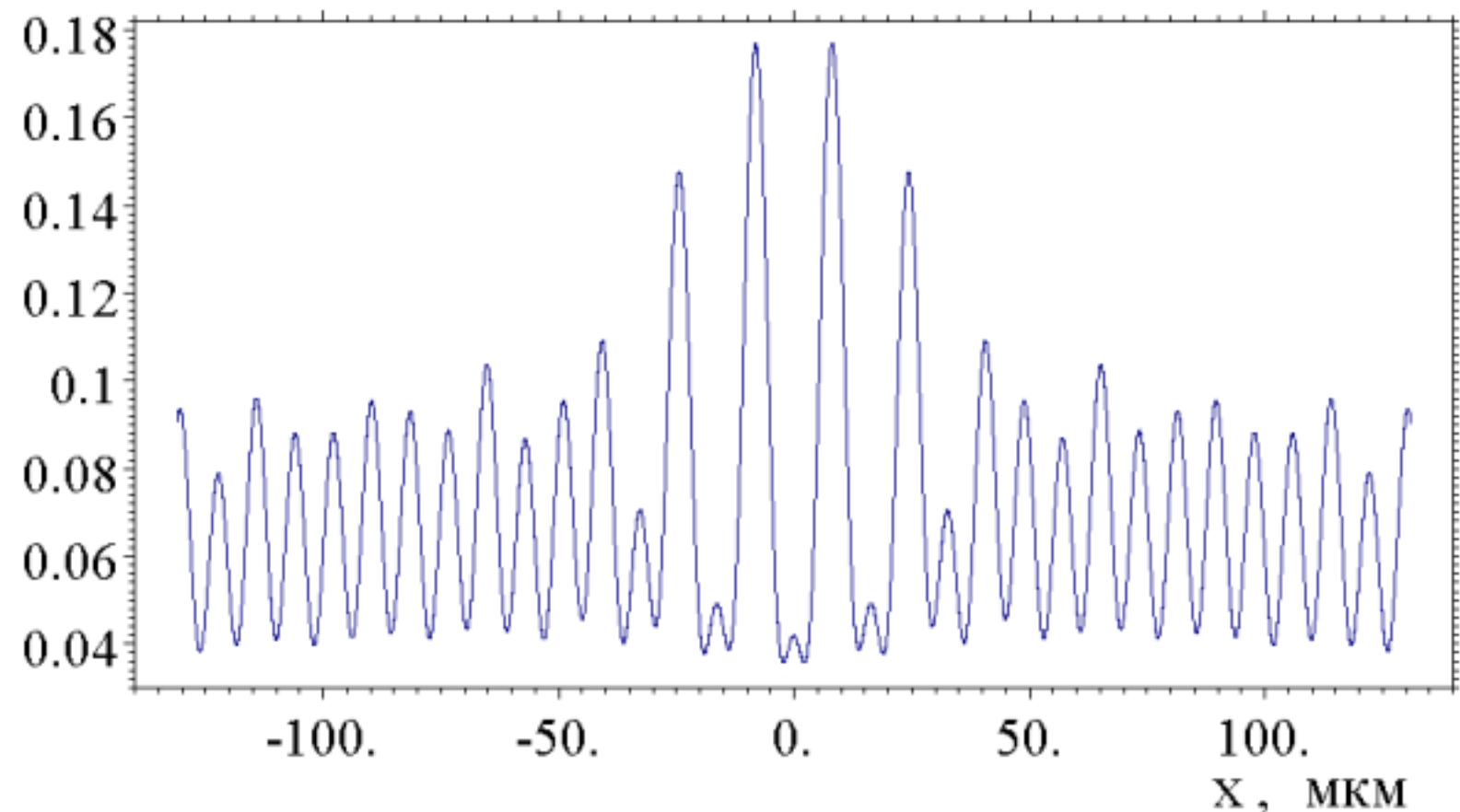
Prog Exec Run View Help

Diffraction of x rays by Bilens

| | |
|--|--------|
| Energy of x rays in [keV] | 12 |
| Distance source-bilens in [cm] | 5760 |
| Distance bilens-detector in [cm] | 273 |
| Source size in [um] | 50 |
| Aperture of the lenses in [um] | 50 |
| Curvature radius of parabola in [um] | 0.2404 |
| Distance between the lenses in [um] | 60 |
| Width of the slit in [um] | 110 |
| Shift of slit center in [um] from the middle | 0 |
| Size of the pixel for a FFT grid in [um] | 0.02 |
| Size of Region to Figure [%] | 50 |
| Shift of Region to Figure [%] | 0 |

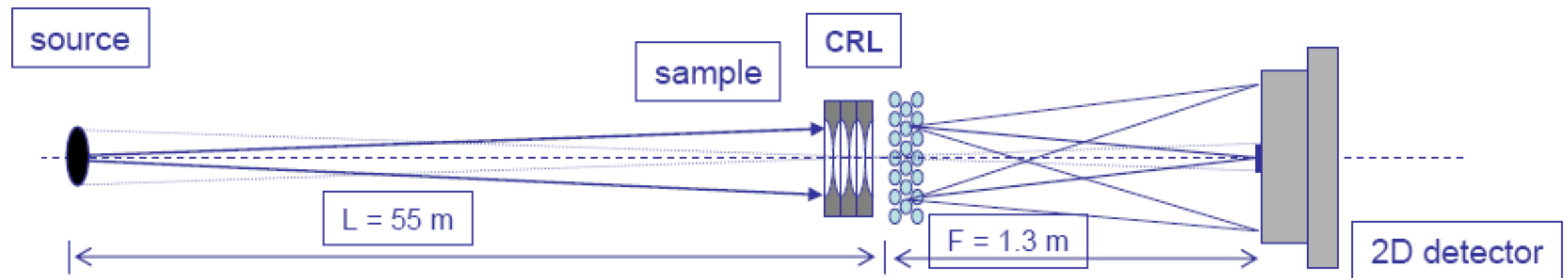
OK Cancel

12-6-490



Some CRL applications. Fourier images APL-2005-86-014102

X-ray High Resolution Diffraction Using Refractive Lenses



$E = 28 \text{ keV}$

Al CRL, $N = 112$, $F = 1.3 \text{ m}$

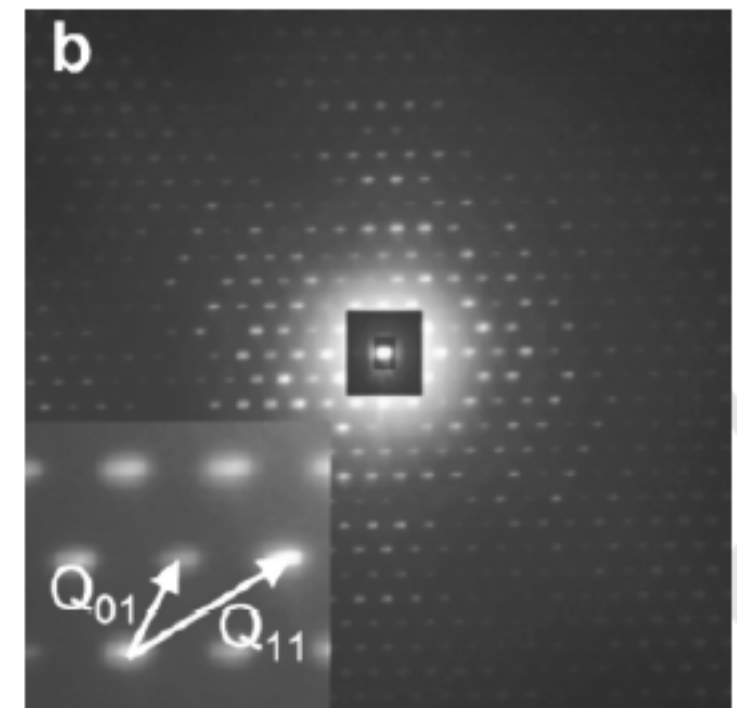
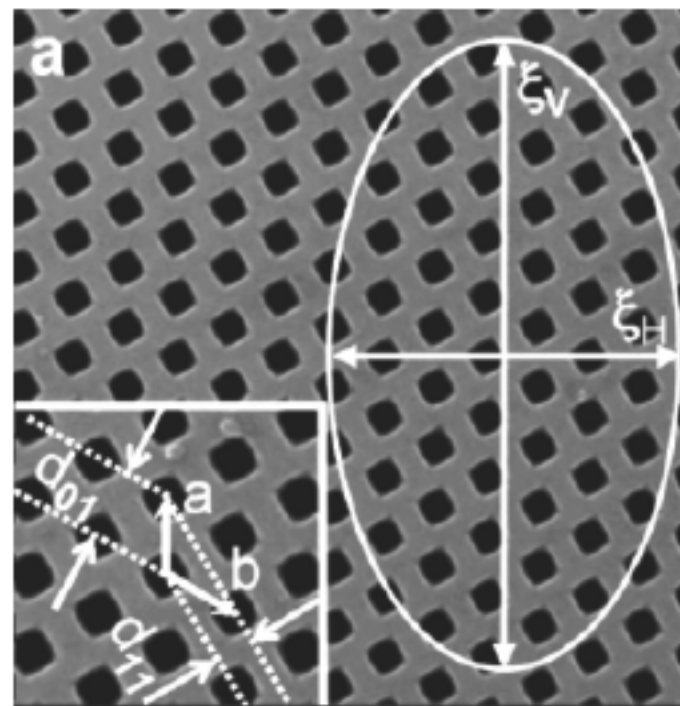
Si photonic crystal

$a=b=4.2 \text{ }\mu\text{m}$ $d_{01}=3.6 \text{ }\mu\text{m}$ $d_{11}=2.1 \text{ }\mu\text{m}$

CCD resolution $2 \text{ }\mu\text{m}$
pixel / $\Theta = d$

Resolution is limited
by angular source size:
 $s/L \sim 1 \text{ }\mu\text{rad}$

Momentum transfer
Resolution: 10^{-4} nm^{-1}



Lattice vectors $g_{01} = 1.75 \cdot 10^{-3} \text{ nm}^{-1}$ $g_{11} = 3 \cdot 10^{-3} \text{ nm}^{-1}$

Theory allows one to account for an absorption in the CRL which influences high order peaks visibility Opt. Comm. 2003-216-247, JETP-2003-97-204

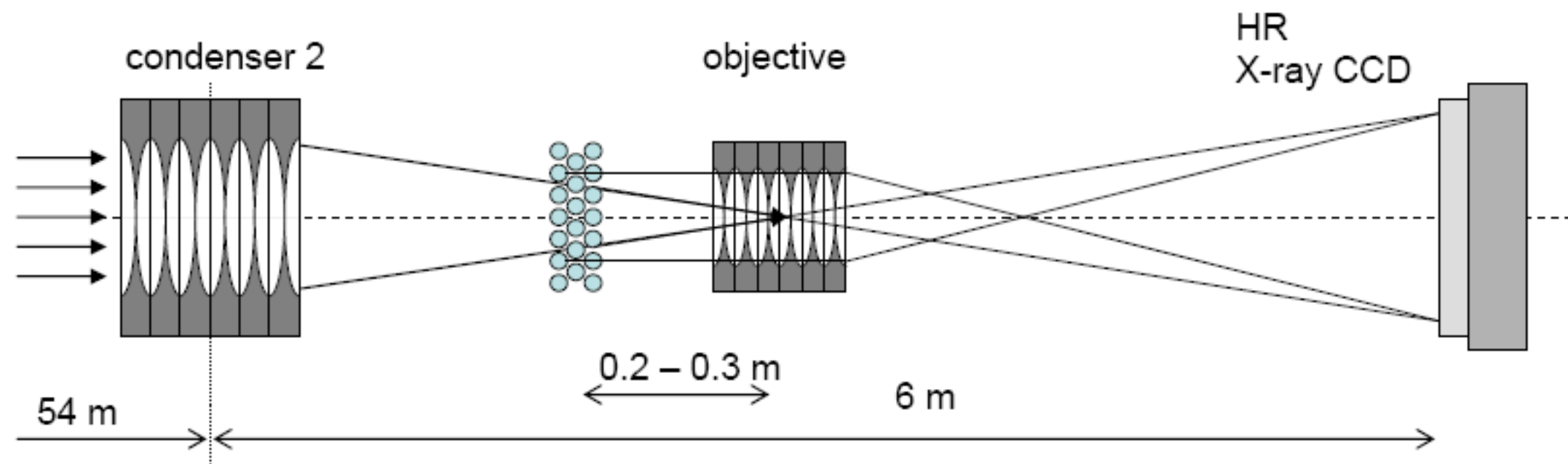
Some CRL applications. **High resolution x-ray 2D microscopy.**

Snigirev et al. with Lengeler's CRLs

(1) – The object is illuminated through a CRL with a large aperture to condense the beam at the object area under illumination (condenser 2)

(2) – Objective CRL (objective) has a short focus length and it works as a microscop. Large magnification is necessary to adjust CCD detector resolution (about $1\ \mu\text{m}$)

This technique allows one to see a real structure of opal crystals and photon crystals. The theory is not developed



The theory is developed for a monochromatic radiation.
It is assumed that a monochromator is used.

What happens with a short pulse of radiation?

The answer will be done in the future topics (next workshops)

MANY THANKS

FOR

ATTENTION