Baltic Federal University, november, 2016

The theory of x-ray compound refractive lenses

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special site – http://xray-optics.ucoz.ru/main.htm

Interaction of x-ray radiation with matter

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2} = 1 - \frac{4\pi e^2}{m\omega^2} N, \quad n(\omega) = \varepsilon^{1/2} = 1 - \frac{\lambda^2 r_0}{2\pi} N, \quad r_0 = \frac{e^2}{mc^2}$$

$\varepsilon(\omega)$ is a dielectric function of electron gas, $n(\omega)$ is a refraction index,

ω_p is a plasmon frequency, e, m are a charge and a mass of electron,

λ is a wave length of x rays, r_0 is a classic electron radius,

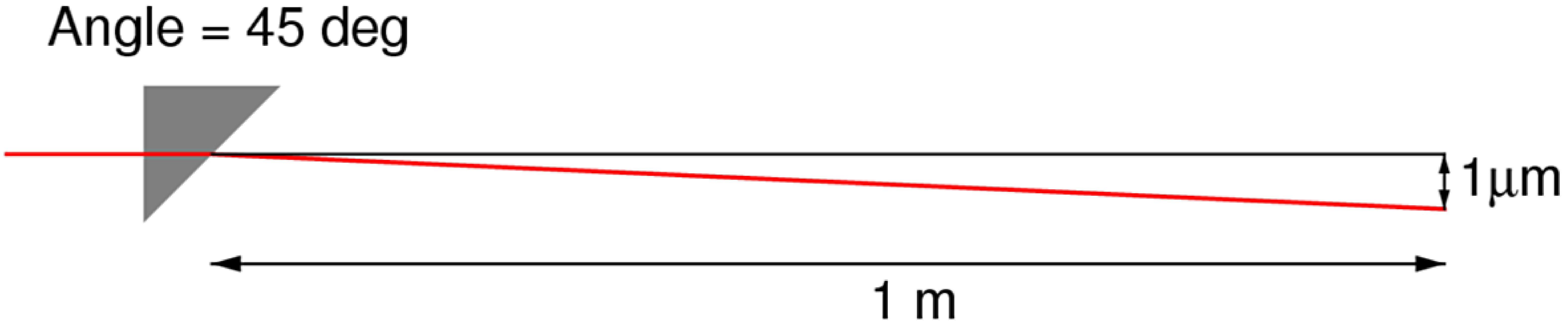
N is an electron density at the given point of space.

It is important that the phase shift is negative in matter, i.e. $n < 1$

In general case the refraction index $n = 1 - \delta + i\beta$, $\delta = (\lambda^2 r_0/2\pi)N + \delta_1$, where δ_1 and β are determined by photoelectric absorption of x rays by atoms, by compton scattering, scattering by phonons and so on. All processes of inelastic scattering have quantum mechanical nature and is very complicated. There are several programs to calculate accurately δ_1 and β which are based on the Henke's tables. One of them is the online Stepanov's program. My program is working both online and offline and it is described in the paper

V. G. Kohn, Crystallography Reports, 2006, Vol. 51, N. 6, p. 936-940

Example: PMMA, $C_5H_8O_2$, $\lambda = 0.1$ nm. We obtain $\delta = 1.61\times10^{-6}$, $\beta = 1.10\times10^{-9}$



X-ray refractive lens has been considered as not feasible for a long time
because
1. Refraction is small, 2. Absorption is importrant.
W. C. Roentgen has written "The are no refractive lens for x rays"
but
1. $n < 1$, i. e. a focusing lens is bi-concave and absorption is small on the optical axis
2. X-ray beams become narrow and long at the new Synchrotron radiation sources of third generation and X-ray free electron lasers



HISTORY. The first successful refractive lens consists of an array of 30 cylindrical holes of diameter 0.6 mm in an Al block which focus 14 keV x rays to 8 μm size

Nature, 1996, vol. 384, N. 6604, p. 49-51

Today is cited 880 (GA), 652 (WOS), 627 (RG)

A compound refractive lens for focusing high-energy X-rays

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THE development of techniques for focusing X-rays has occupied physicists for more than a century. Refractive lenses, which are used extensively in visible-light optics, are generally considered inappropriate for focusing X-rays, because refraction effects are extremely small and absorption is strong. This has lead to the development of alternative approaches[1,2] based on bent crystals and X-ray mirrors, Fresnel and Bragg–Fresnel zone plates, and capillary optics (Kumakhov lenses). Here we describe a simple procedure for fabricating refractive lenses that are effective for focusing of X-rays in the energy range 5–40 keV. The problems associated with absorption are minimized by fabricating the lenses from low-atomic-weight materials. Refraction of X-rays by one such lens is still extremely small, but a compound lens (consisting of tens or hundreds of individual lenses arranged in a

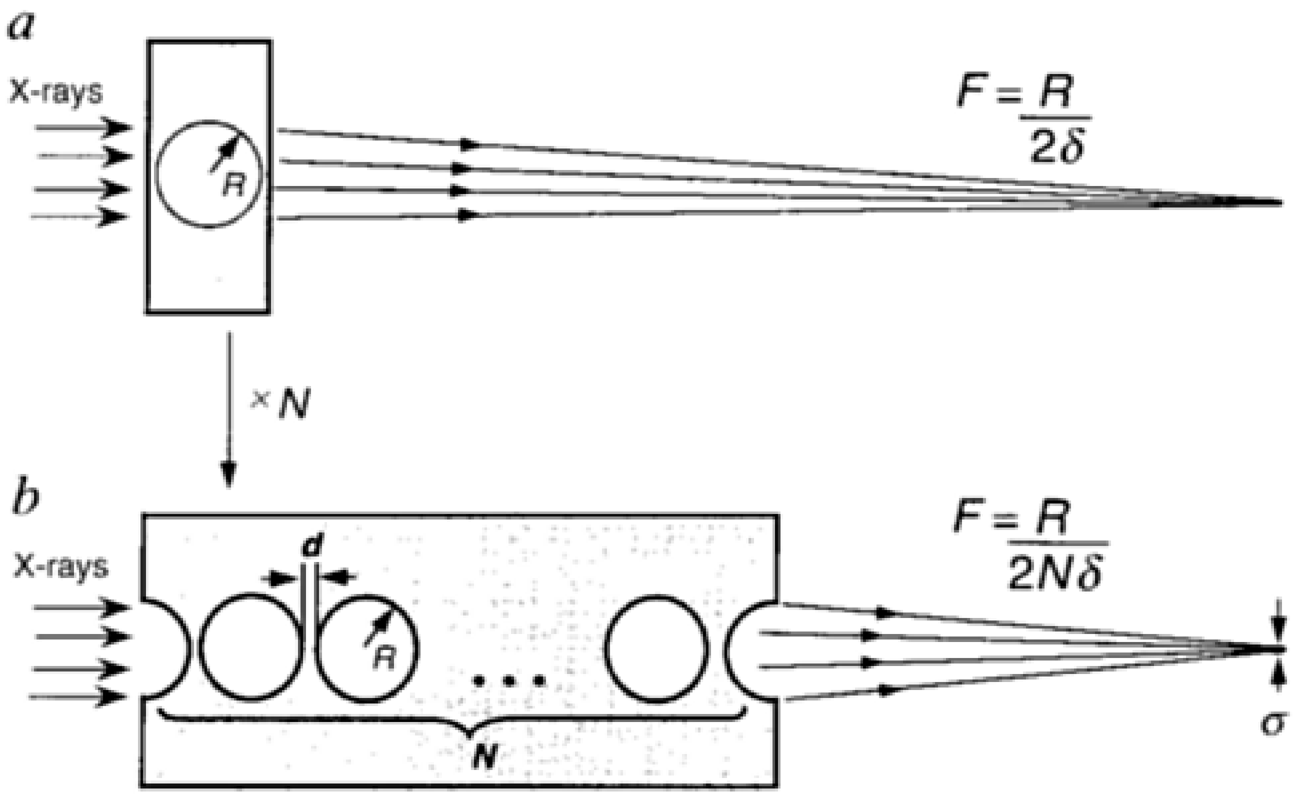
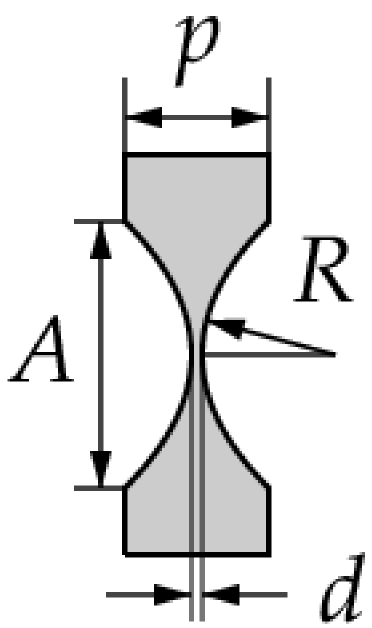


FIG. 1 Schematic diagram showing the principles of X-ray focusing by a compound refractive lens (CRL). As $(1-\delta)$ is smaller than 1 (where δ is the decrement of the refractive index), a collecting lens for X-rays must have a concave shape. *a*, A simple concave lens fabricated as a cylindrical hole in the material. *b*, A CRL consisting of a number (N) of cylindrical holes placed close together in a row along the optical axis, focuses the X-rays at a distance that is N times shorter compared to a single lens. R is the radius of the holes, d is the spacing between the holes, λ is the X-ray wavelength, and F is the focal distance for a parallel input beam.

PARABOLIC LENS. The basic parameters of parabolic lens are



R – a curvature radius of parabols shape,

A – a geometrical aperture of the lens,

p – a total length (thickness) of the lens,

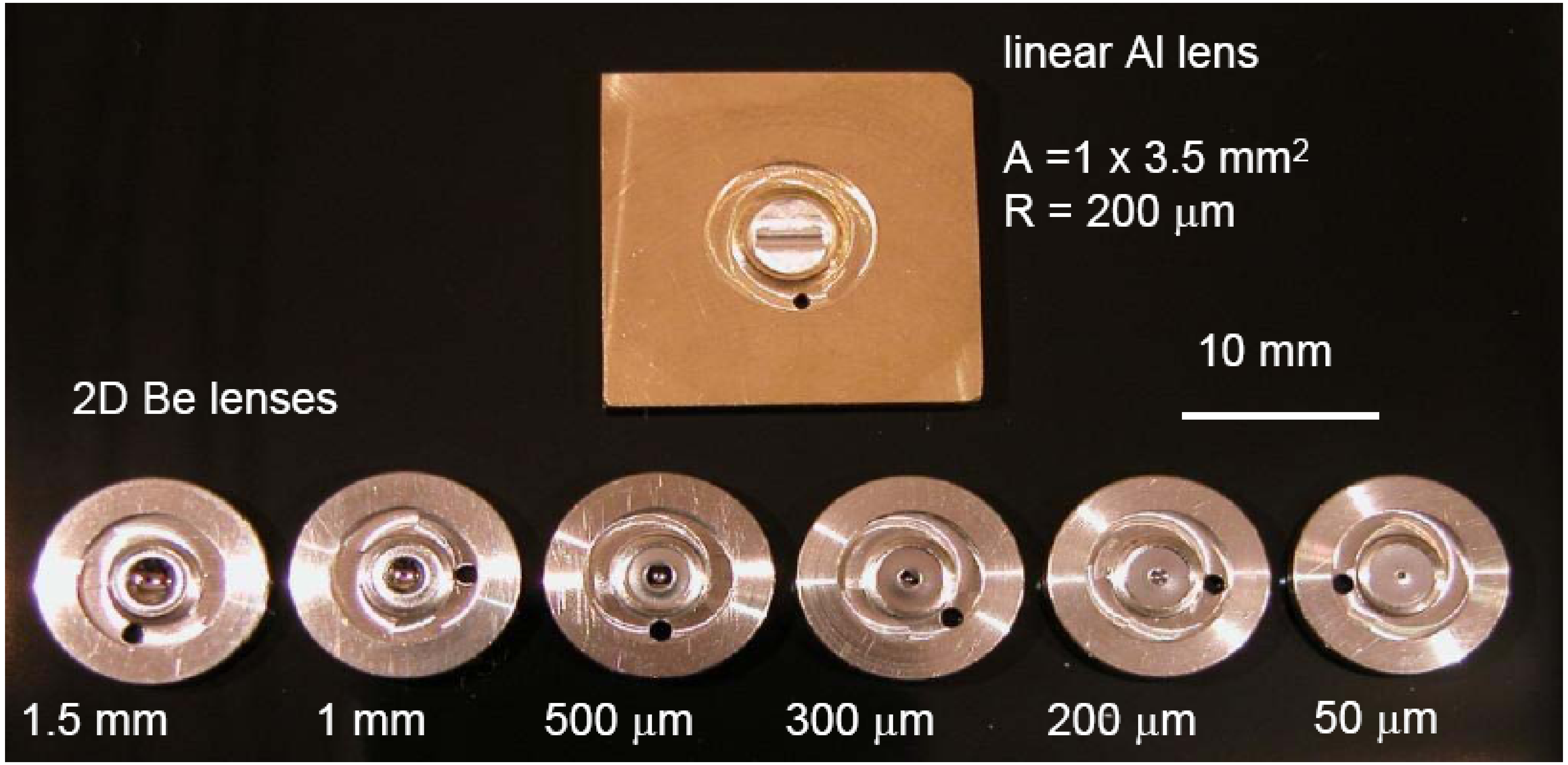
d – a web size between two neighboring surfaces

The paraxial approximation is valid for x rays with high accuracy. The focus distance is estimated as $F = R/2\delta >> p$. First parabolic lenses were made from Al with $R = 0.2$ mm. They have $F = 26$ m for x-ray photon energy $E = 12$ keV
A FWHM of the beam behined the lens is 341 μm due to absoption

The key idea to decrease the focus length is to use a compound refractive lens.

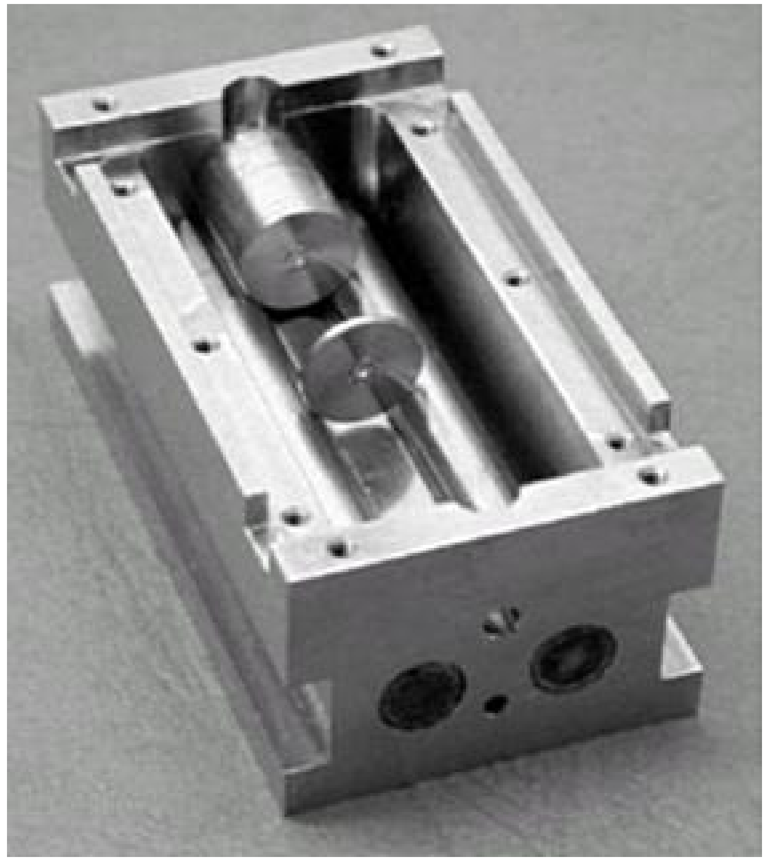
EXAMPLES OF MODERN LENSES.

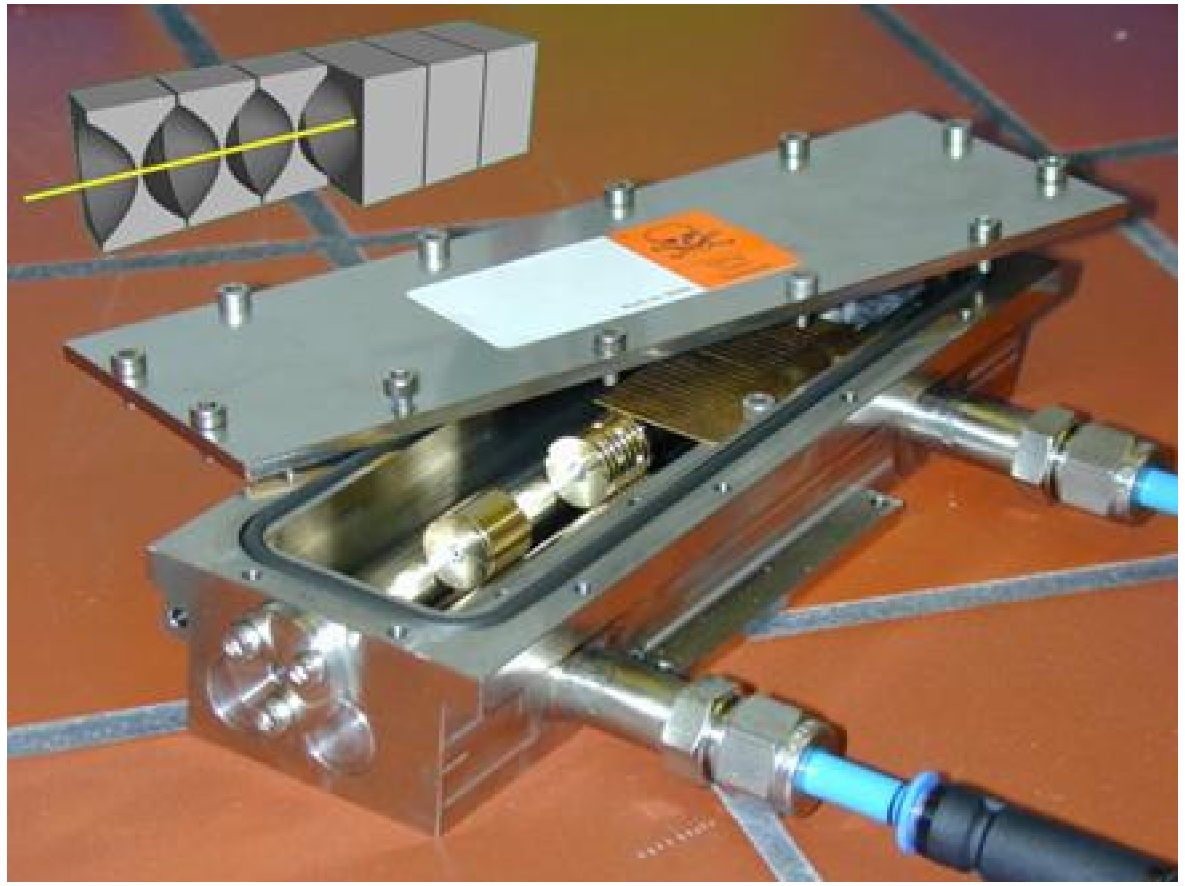
The best 2D (round) lenses are created by Bruno Lengeler in RWTH Aachen University (Germany) by pressing material with parabolic poincons. Now the 1D lenses becomes available with the same technique.
http://wwwo.physik.rwth-aachen.de/en/institutes/institute-iib/group-lengeler/



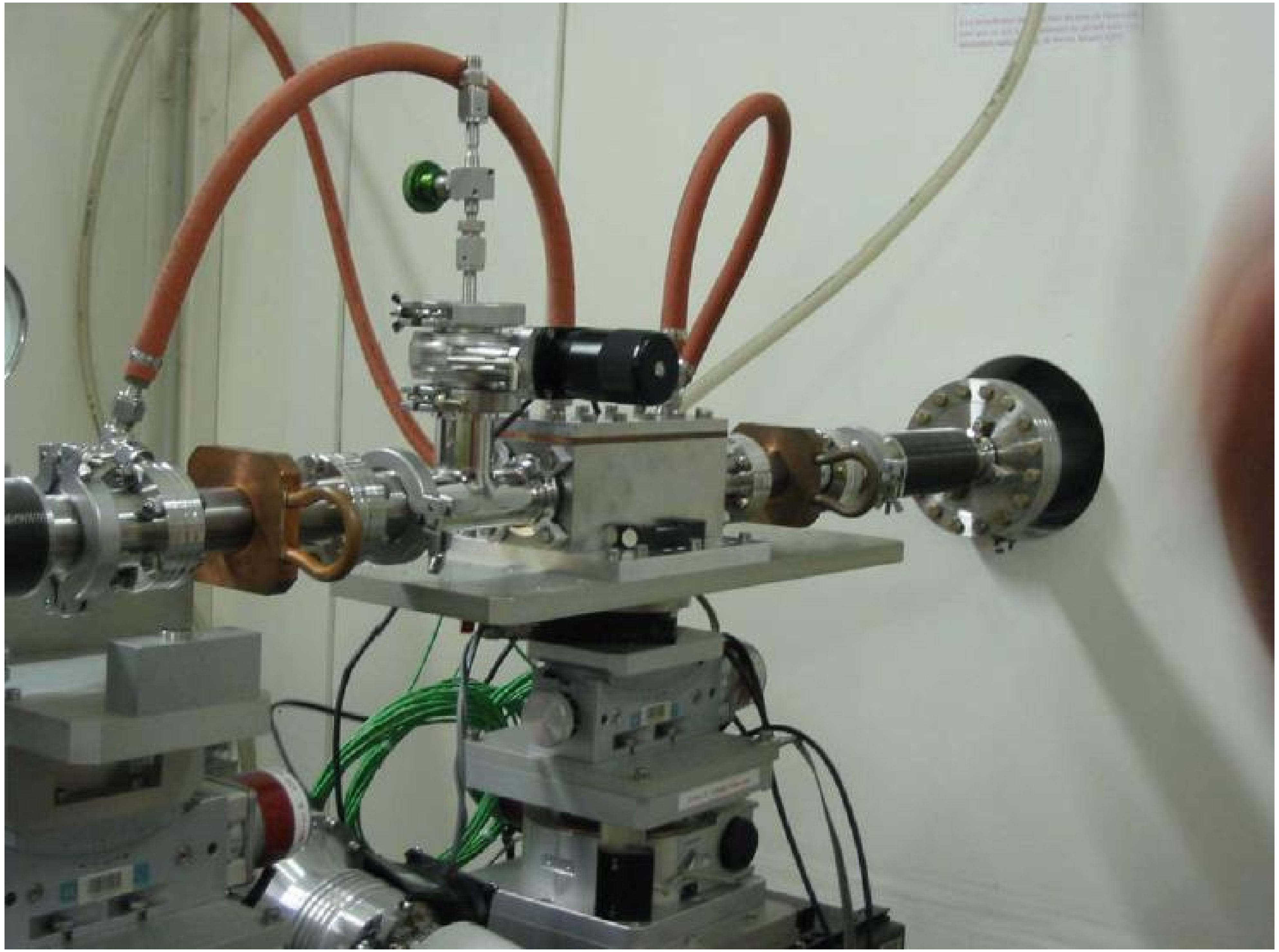
HOLDERS for parabolic CRL

top right -- Al in air (was first)
bottom right -- Be in vacuum
bottom left -- Modern holder

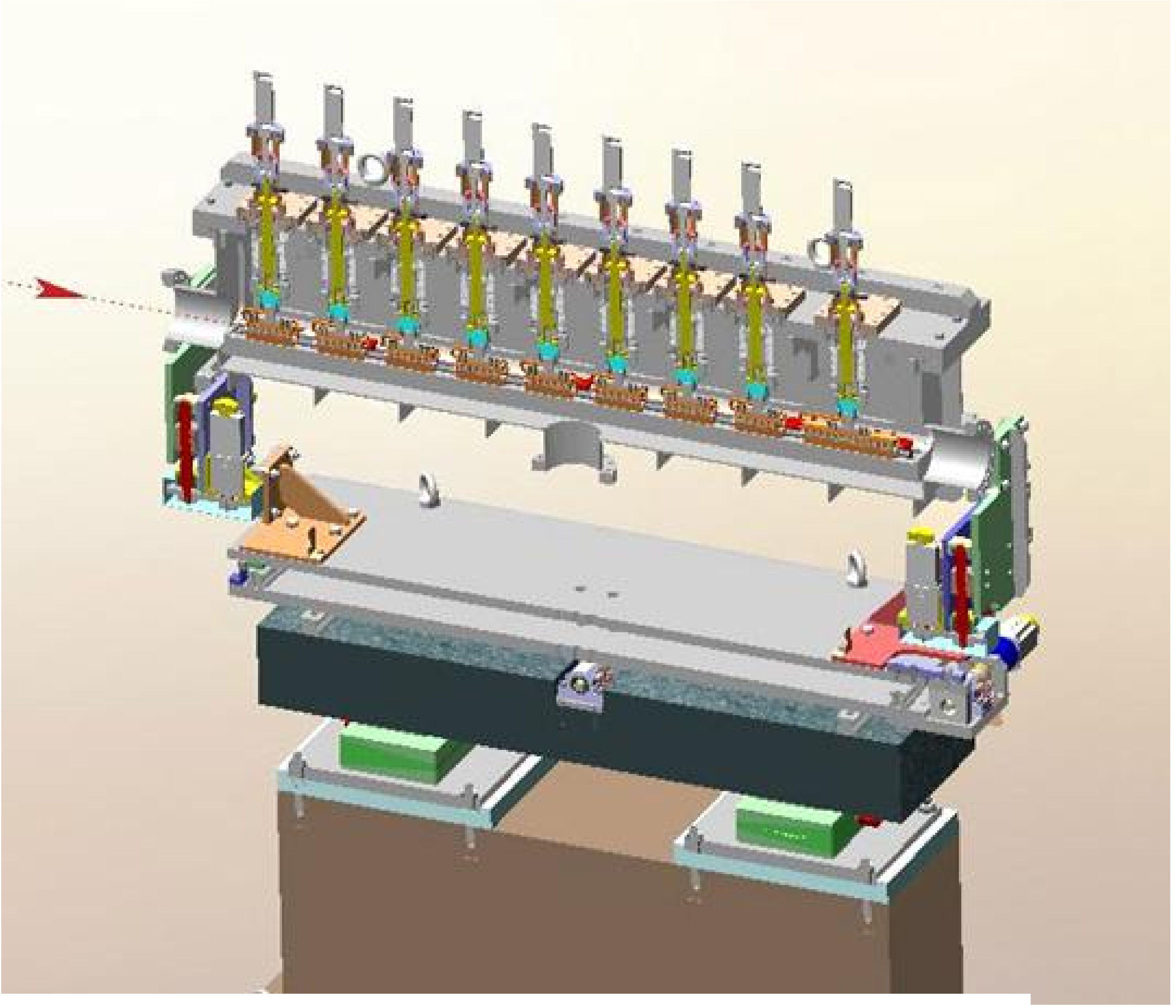


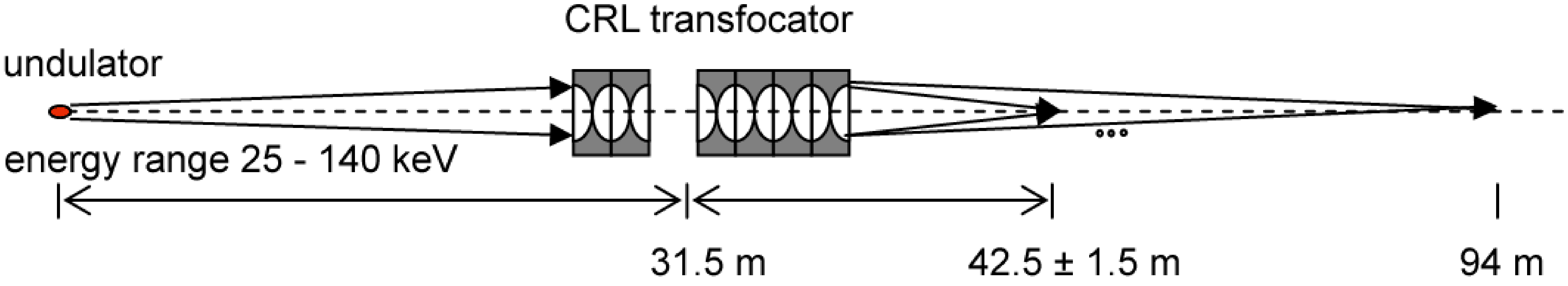


The useful property of 2D CRL is THERMAL STABILITY in the intense beam of x rays. Below the water cooled Be CRL is shown (ESRF, the station ID10).

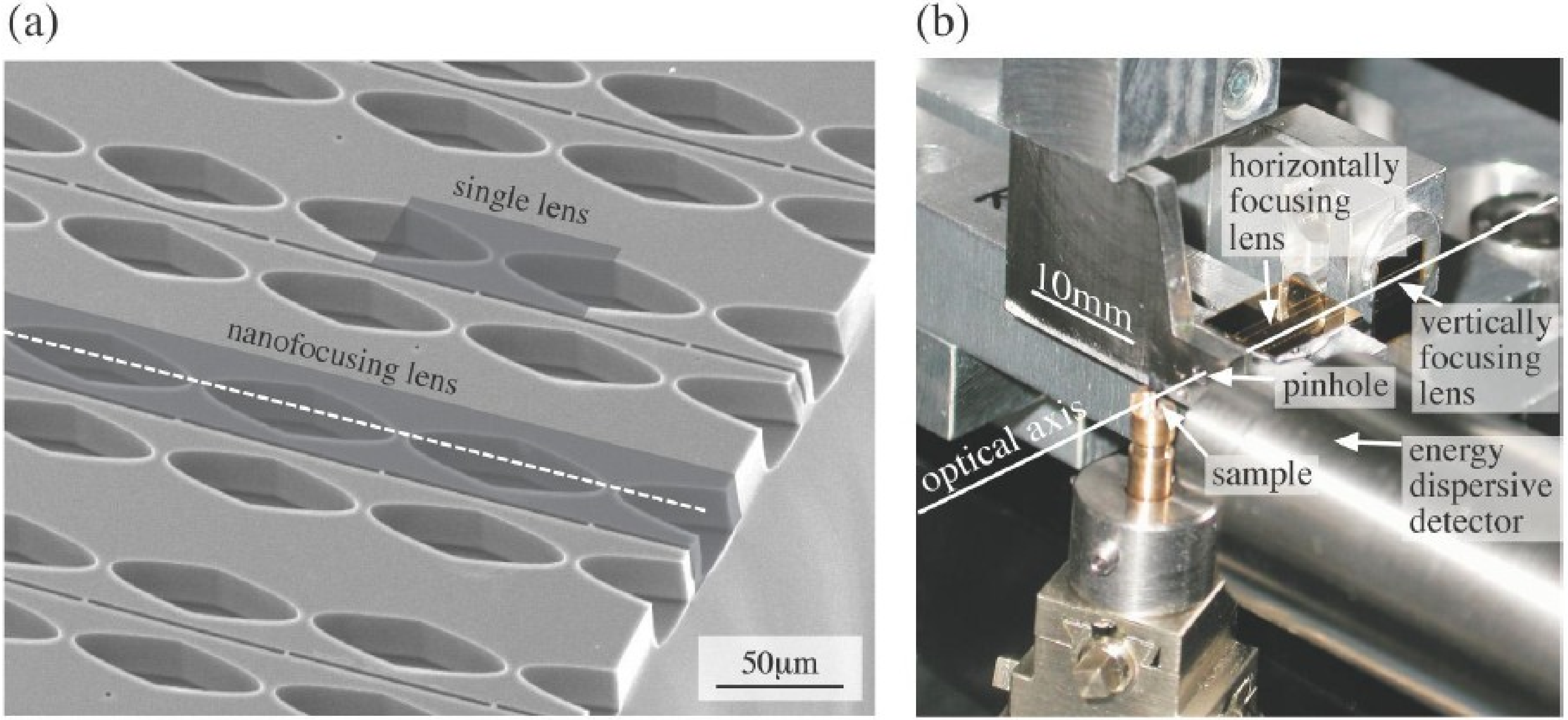


A TRANSFOCATOR as a new source of divergent beam of x rays closely to sample. It uses CRL. The position of source stays the same for all energies because elements of CRL can be inserted into or removed from the beam. It is cooled and it can be used as the first optical element of the experimental setup.

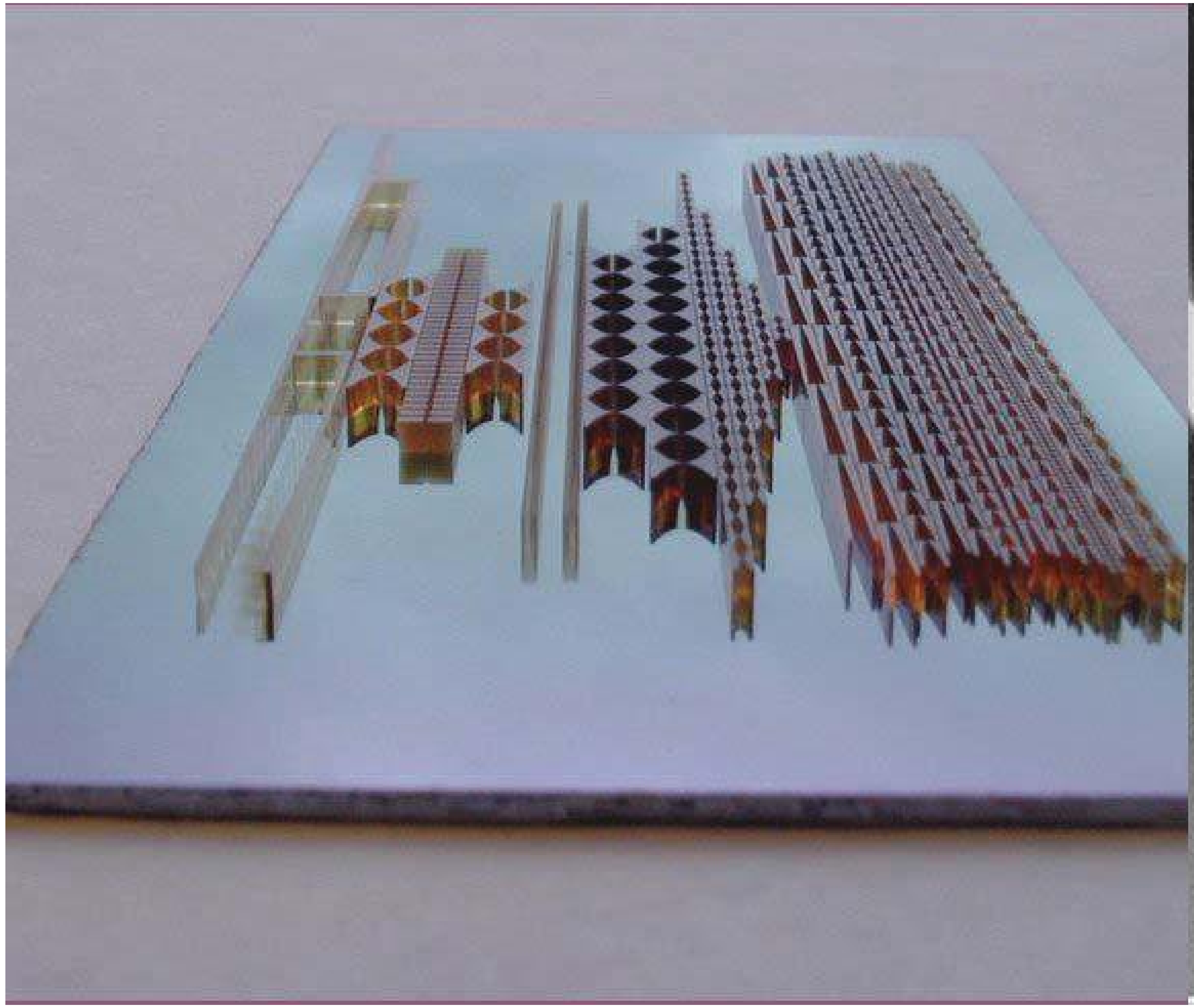


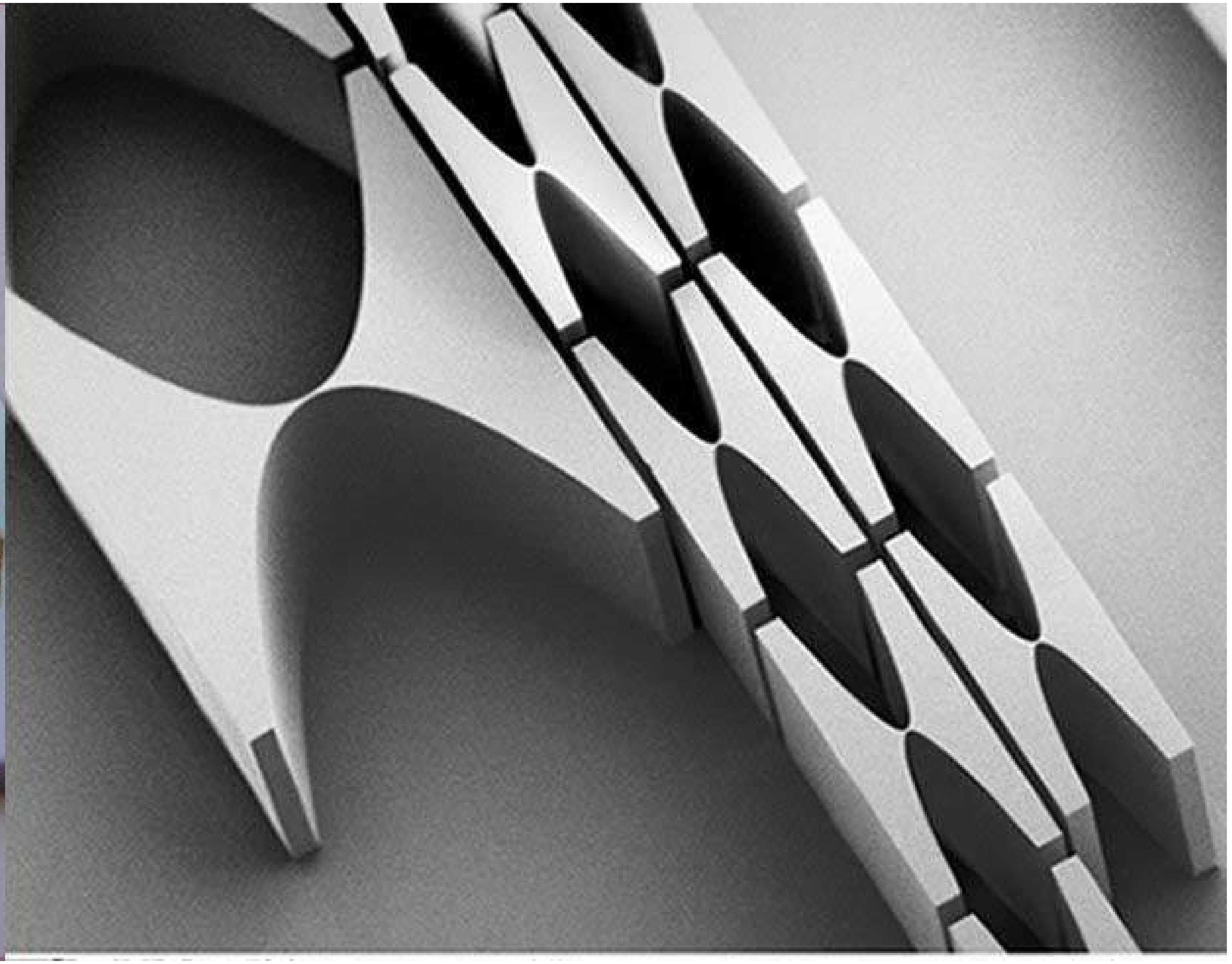


PLANAR SILICON parabolic lenses are made with microfabrication technique. The electron (e)-beam lithography and deep trench reactive ion etching are used. RWTH Aachen University, Shroer, . . ., Lengeler, APL, **82**, 1485 (2003)
One lens makes 1D focus, two lenses make 2D focus.

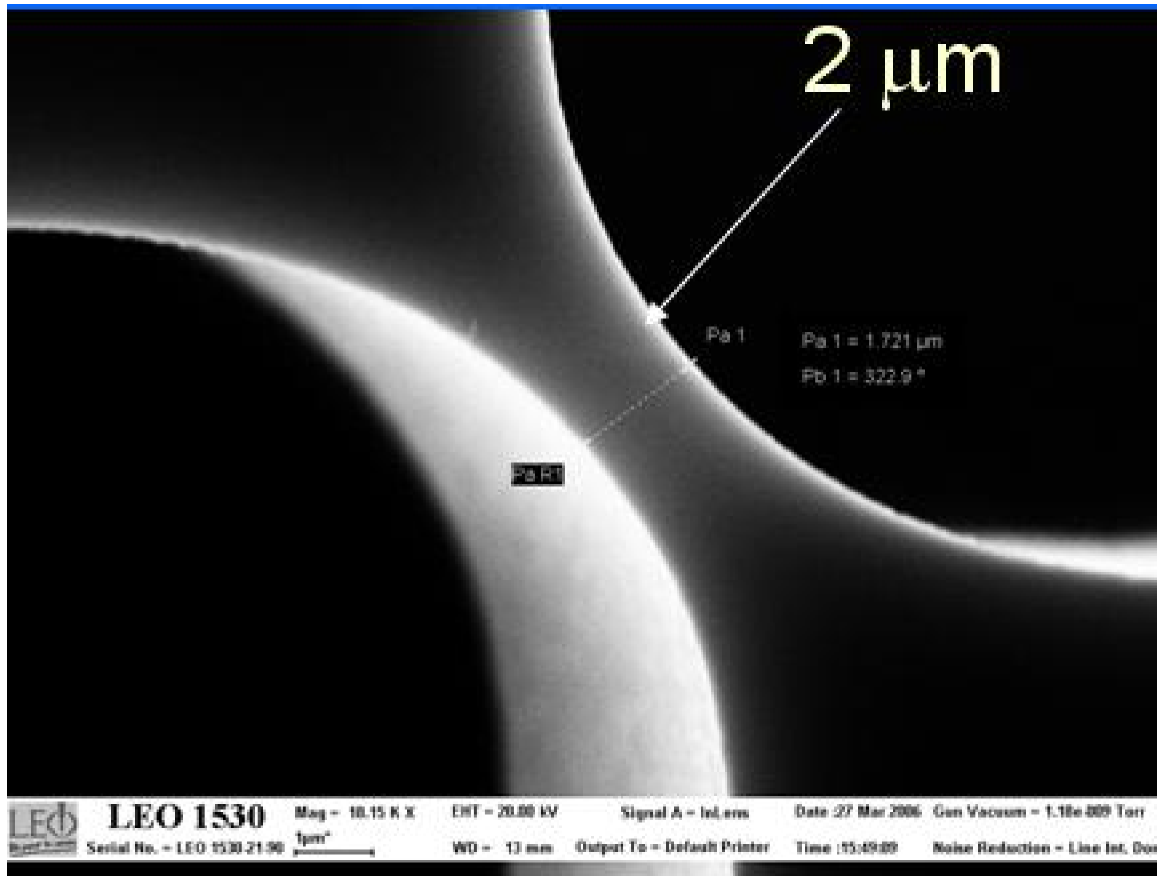


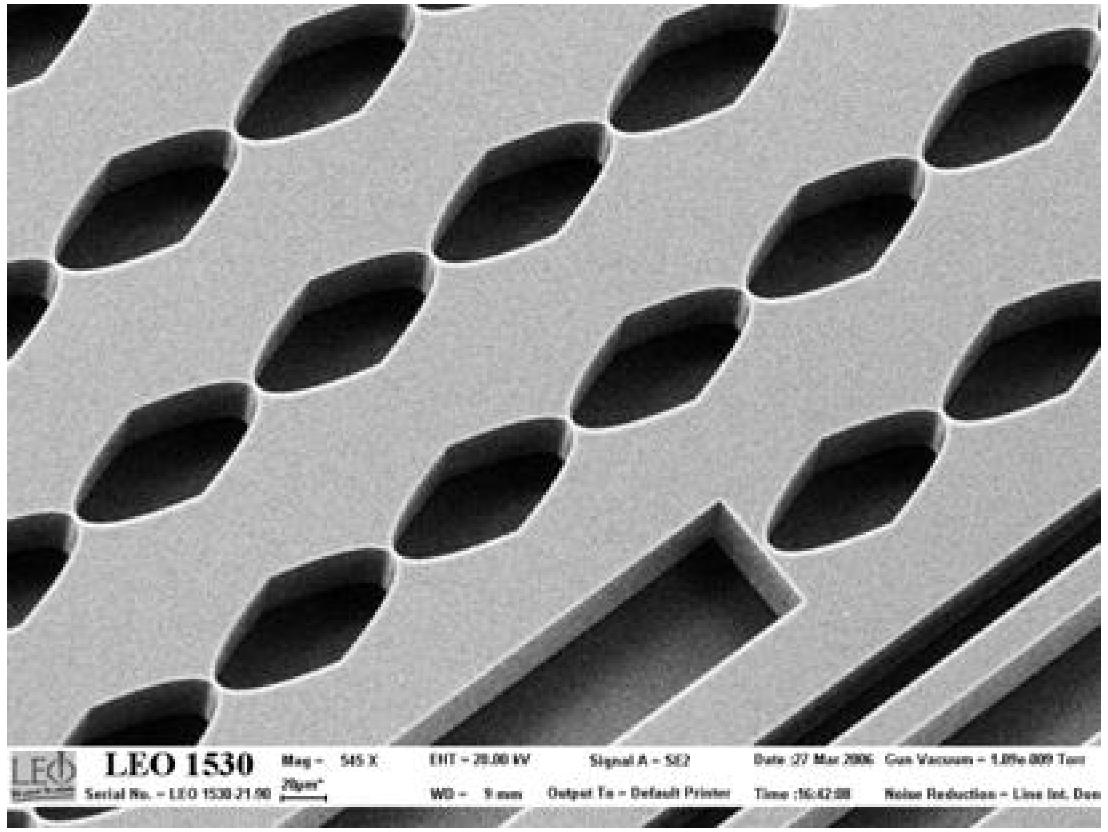
PLANAR SU-8 parabolic lenses made by LIGA technique (LItographie, Galvanoformung, Abformungelectron). ANKA source, LITHO-3 beamline, IMT/FZK Karlsruhe, Germany, SPIE, **5195**, 23 (2003), Nazmov

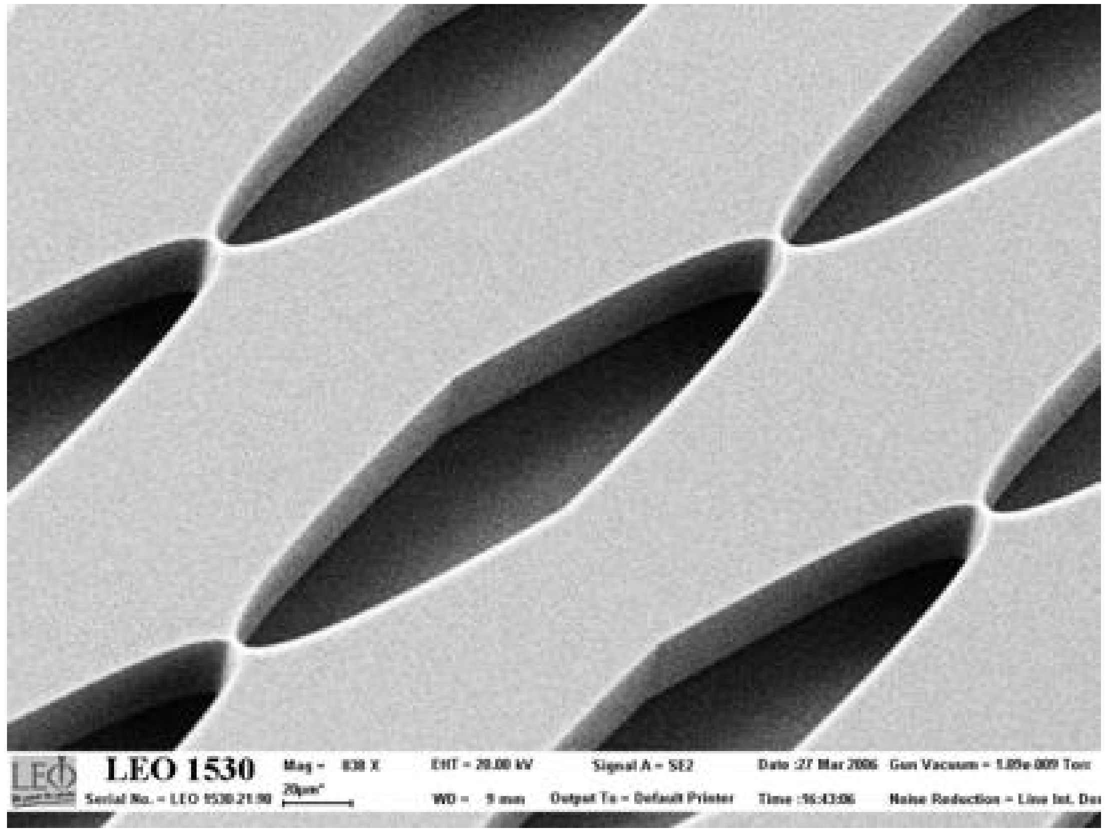




PLANAR SILICON parabolic lenses for nano-focusing and nano-interferometry. They are made by e-beam lithography and deep etching in Chernogolovka, Moscow district, Russia,
PRL, **103**, 06481 (2009), Yunkin et al.







Theory, 1D case for simplicity

Paraxial approximation for Maxwell's equation is valid very well

Polarization does not influence the results. Electric field is

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

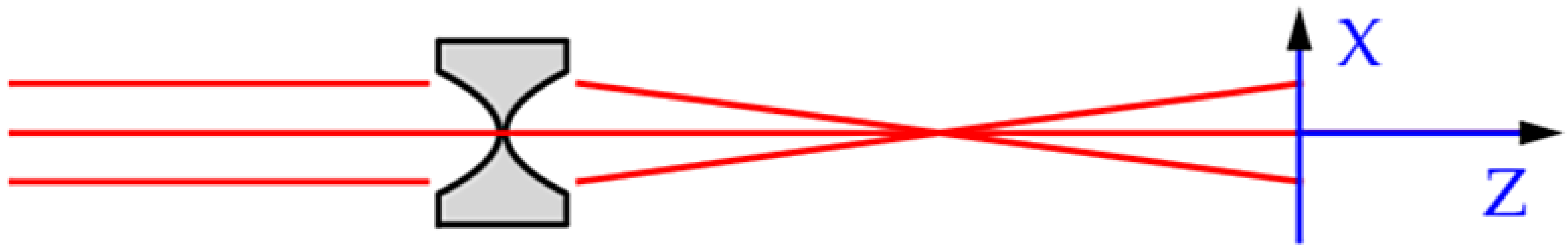
The main equation is a parabolic equation for $A(x,z)$

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

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

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

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



Solution for air (accurately)

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

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

The shifted wave function of radiation is calculated as a convolution which is a specific example of Huygens-Fresnel principle. Fresnel propagator $P(x,z)$ is a response on a point source. In general case the convolution can be calculated 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)

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

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

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

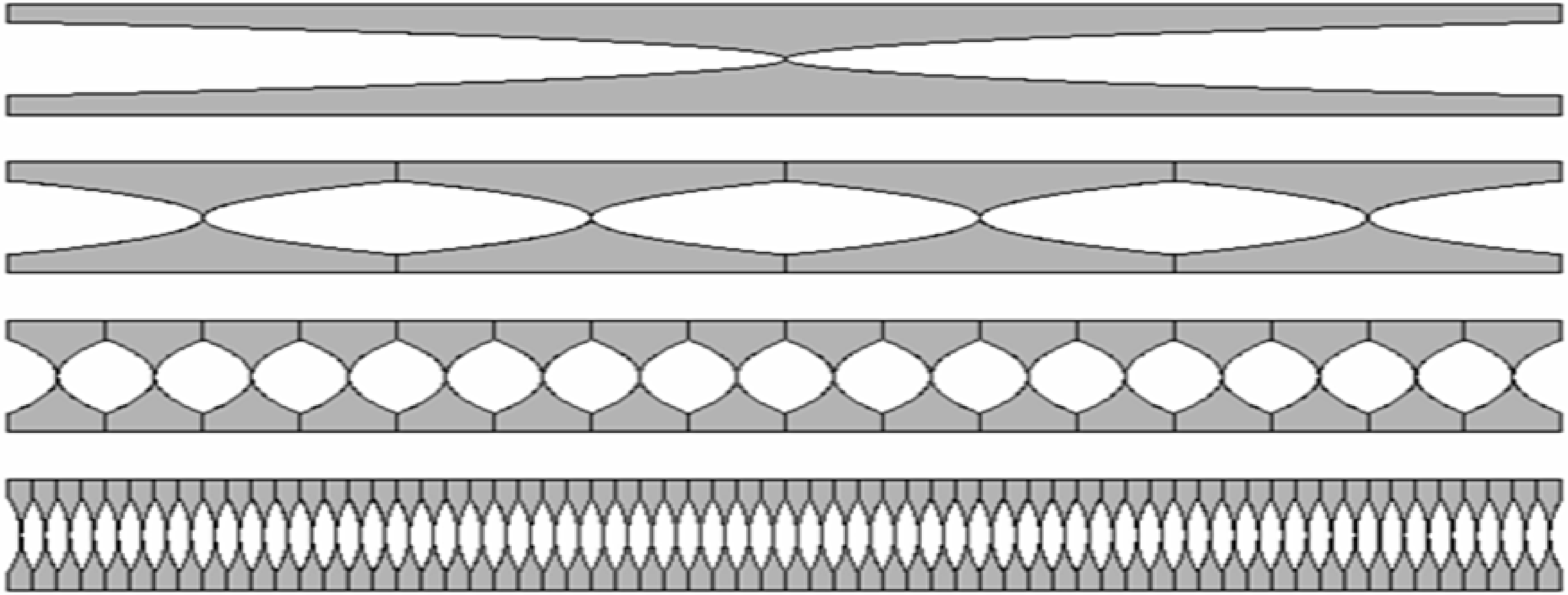
$$T(x,\Delta z) = \exp\left(-i\pi\frac{x^2}{\lambda F}[1-i\gamma]\right), \quad F = \frac{R}{2\delta}, \quad \gamma = \frac{\beta}{\delta}$$

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

Solution for long ideal CRL

In a thin lens approximation all lenses shown in the picture below 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, i.e. $s(x,z) \Rightarrow \overline{s(x)}$



Solution for long ideal CRL

For a parabolic refracting material the equation has a form

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

A propagator for this equation as a response on a point source is known Kohn, JETP, **97**, 204 (2003) therefore we can write a solution

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

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

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

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 in the limit of short CRL

We can formulate a condition for *thin lens approximation* as $\Delta z \ll z_c$. Then

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

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

It is more accurate than the transmission function. The latter can be obtained if we replace the Fresnel propagator by delta-function

$$P(x - x_1, \Delta z)\rfloor_{\Delta z \to 0} = \delta(x - x_1)$$

Then we arrive to the approximation of Phase Contrast

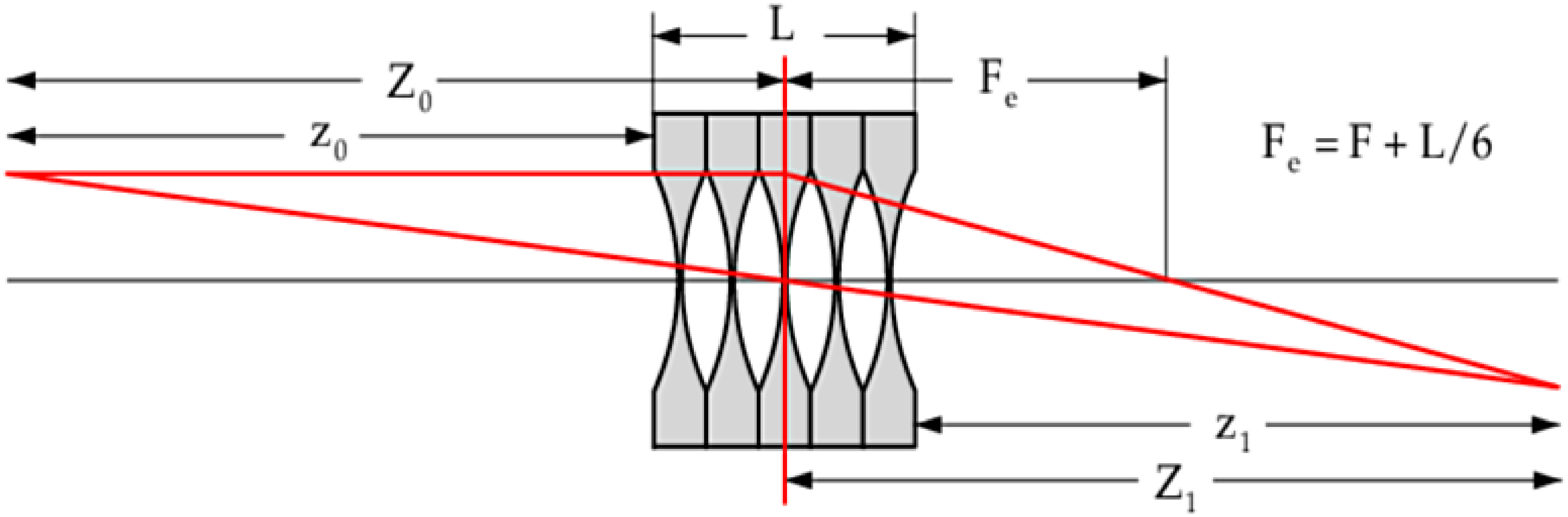
$$P_{pm}(x, x_1, \Delta z) = \exp\left(i\pi \frac{x^2}{\lambda F_c} \right) \delta(x - x_1)$$

Solution for short CRL focusing

Another sequence of accurate 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 me 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 described by

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

It was shown that if the wave function is $A(x,x_0,z_n) = T(x,a_n)P(x-x_0,b_n)T(x_0,c_n)$, where $T(x,a) = \exp(-i\pi x^2/\lambda a)$, $P(x,b)$ is the Fresnel propagator, then the integral operation does not change the form, and the reccurent relations exist

$$a_2 = d\frac{b_2}{b_1}, \quad b_2 = b_1 + \Delta z\left(1 - \frac{b_1}{d}\right), \quad c_2 = \frac{c_1}{1+\Delta z c_1/b_2 d}, \quad d = \frac{a_1}{1+a_1/F_c}$$

where $\Delta z = z_2 - z_1$. These recurrent relations can be used many times taking into account each lens in the complex lens system.

Kohn V.G., J. Surf. Invest., **3**, 358 (2009), J. Synchr. Rad., **19**, 84 (2012)

Semianalytical approach for Gaussian beams

Intensity as a function of distance z behind the last lens is defined by a, b, c as

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

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

$$M = B/(A-B), \quad A = -\mathrm{Im}\,a^{-1}, \quad B = -\mathrm{Im}\,b^{-1}, \quad C = -\mathrm{Im}\,c^{-1}$$

Some conclusions: σ_0 does not depend on z, integral intensity $\propto I_m(z)\sigma(z)$

and $G = |b|^2[A-B]$ does not depend on z, $M(z) = M_0 + M_1 z$, $b = B_0 + B_1 z$.

The focus distance is calculated from minimum $\sigma(z)$ as $z_f = -\mathrm{Re}(B_0 B_1^*)/|B_1|^2$

FWHM of the beam is equal to $w(z) = C\sigma(z), \quad C = (8\ln 2)^{1/2} = 2.355$

Semianalytical approach for Gaussian beams

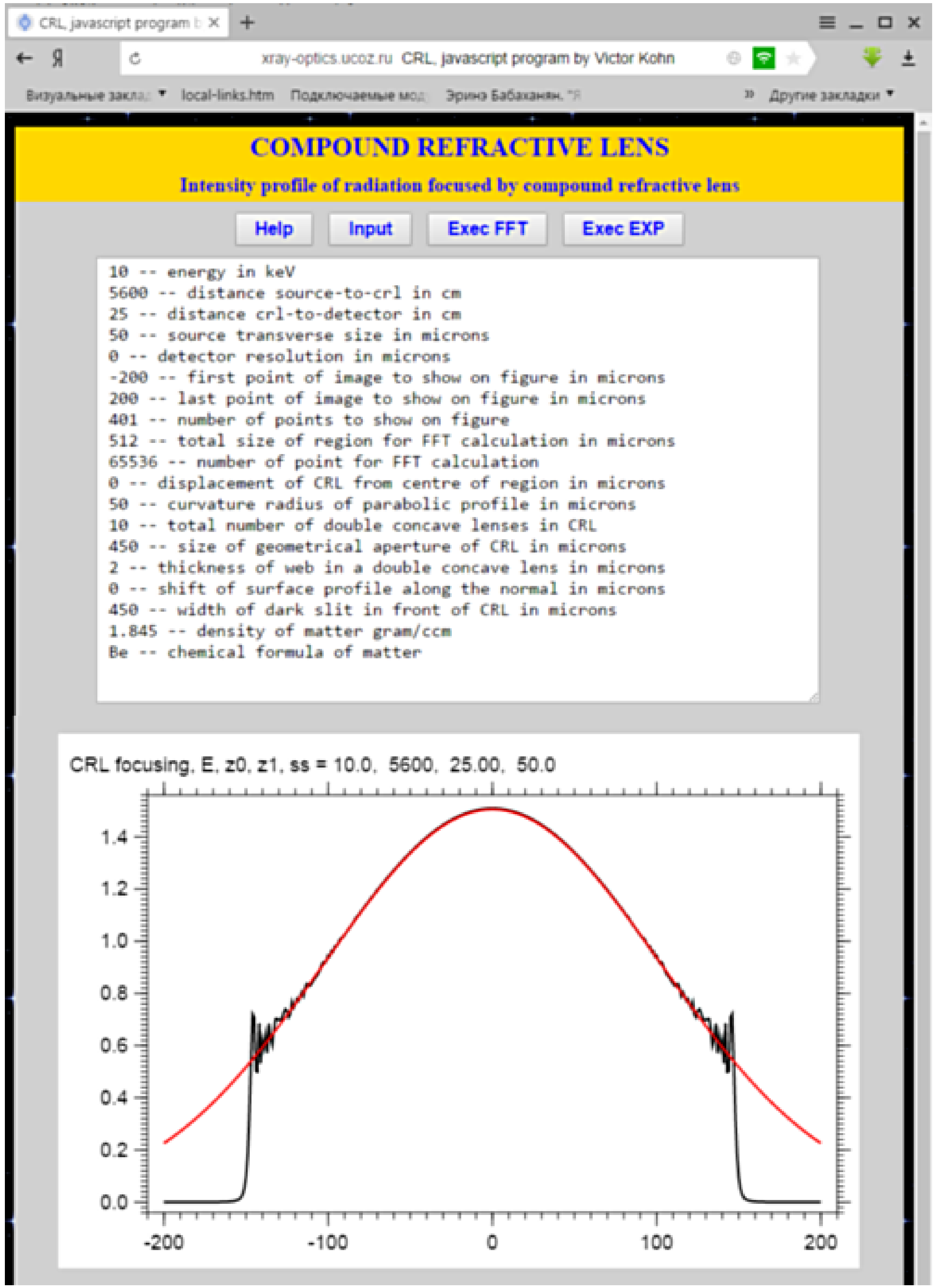
For one thin lens and $x_0 = 0$,

(1) Let $a_0 = \infty,\ b_0 = z_0$. Then $z_f = F/(C+\gamma^2/C),\ C = 1 - F/z_0,\ \gamma = \beta/\delta$. Due to an absorption the lens does not create completely a parallel beam because maximum $z_{fm} = F/2\gamma$ when $z_0 = F/(1-\gamma)$

(2) $a_0 = b_0 = \infty$: FWHM $w(z) = 0.66(\lambda F/\gamma)^{1/2}((1-z/F)^2 + \gamma^2(z/F)^2)^{1/2}$. This formula leads to the universal relation for the FWHM of the Gaussian beam: $w(F) = \gamma \bullet w(0) = 0.44\,\lambda F/w(0)$. The parameter γ allows estimation a power of focusing, the parameter $w(0)$ is an effective aperture, well known formula for a focus width has a multiplier 0.44.

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

Bergemann et all, PRL, **91**, 204801 (2003)



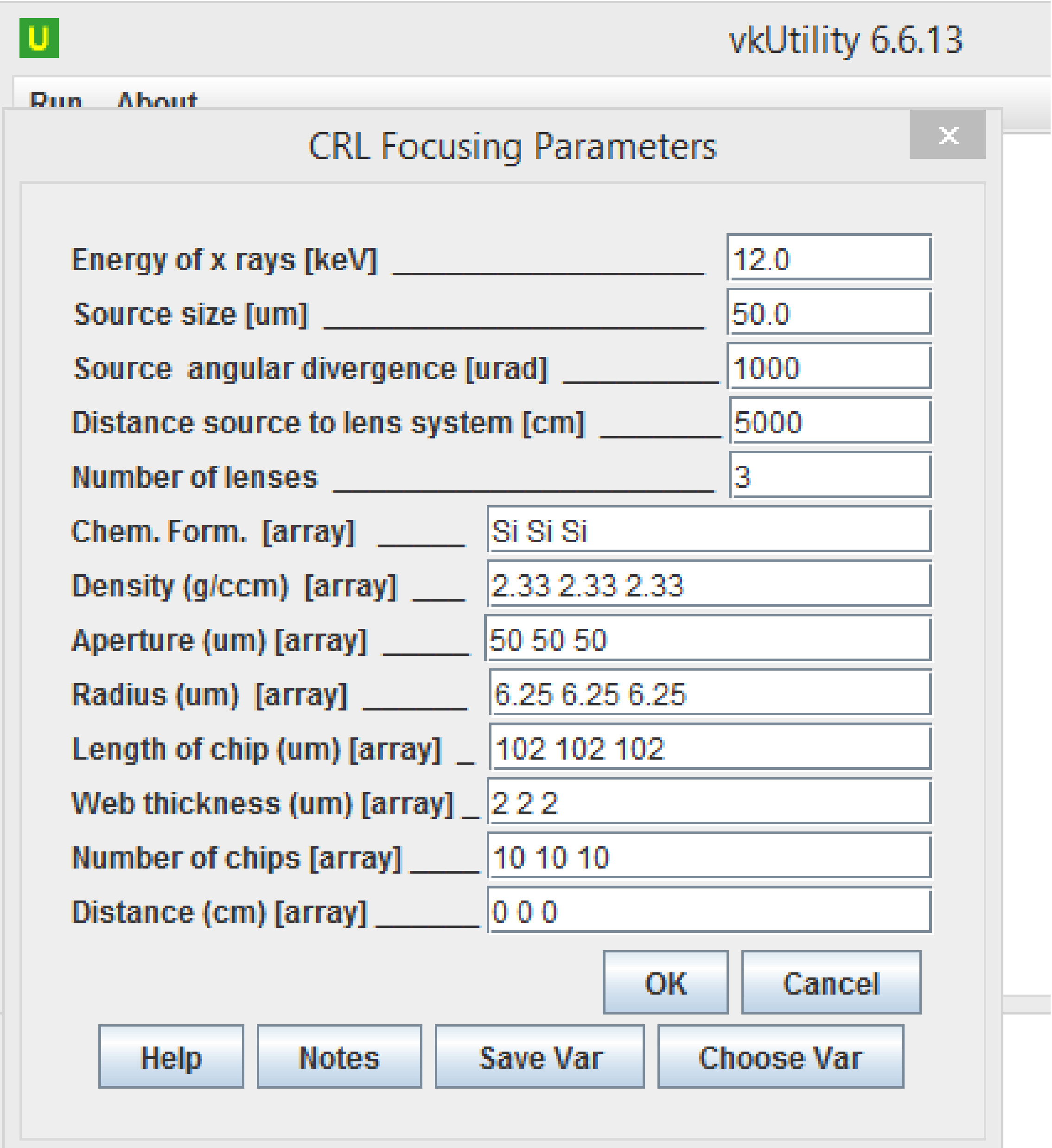
Computer simulations

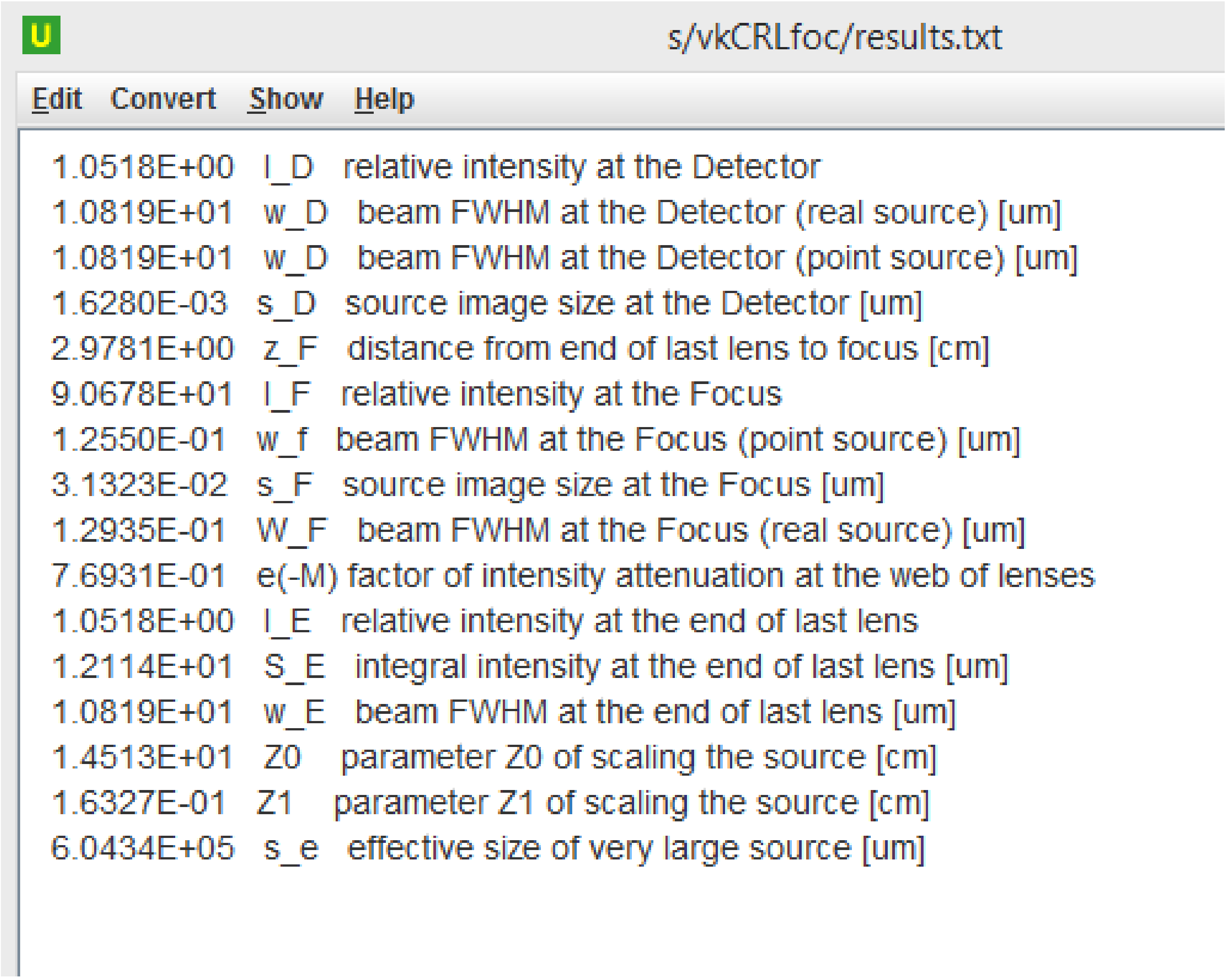
Various computer programs allow one to simulate properties of the intensity profile at the focus and any distance behind the CRL.

One internet program works online and in browser as js-application. At the left part of slide the site of program is shown. In the top window the user input the data for a calculation. The bottom window shows a figure with the intensity profiles in the semianalytic and accurate approaches. The numerical data are shown as well in the top window. The address of online program is http://xray-optics.ucoz.ru/js-pro/crl-pro.htm

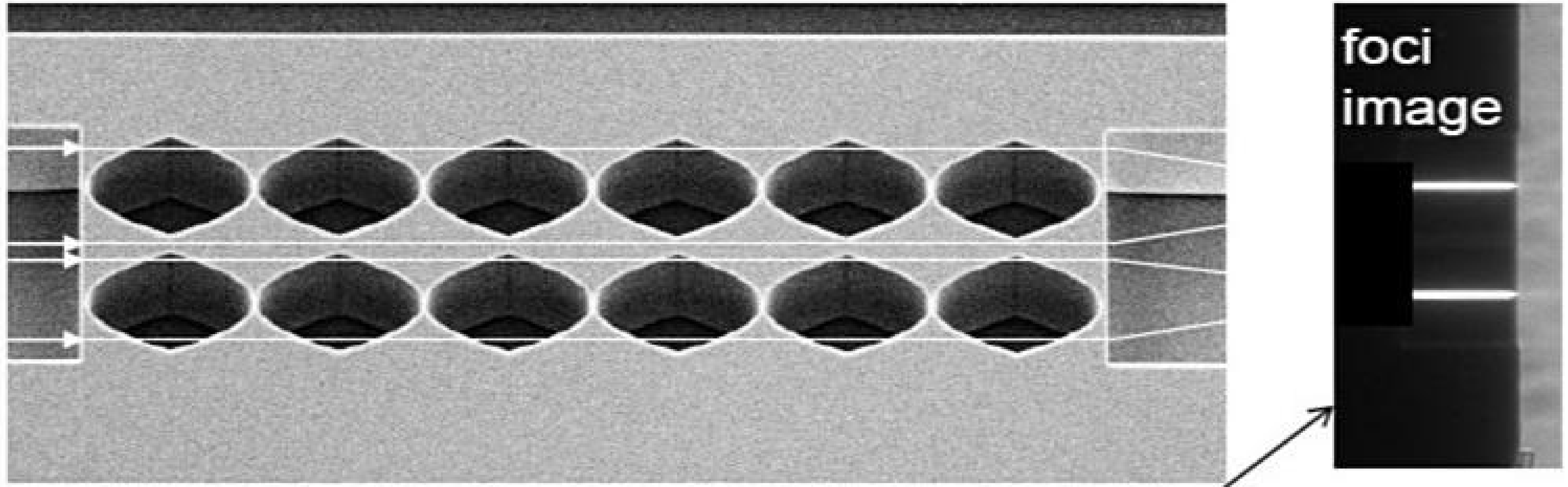
Computer simulations

One of many offline programs is written in Java. It can work in any operating system. It can be downloaded from my site as a part of the program vkUtility. It calculates the parameters oof semianalytical solution as a Gaussian beam for any combinations of CRLs with any distances between them.

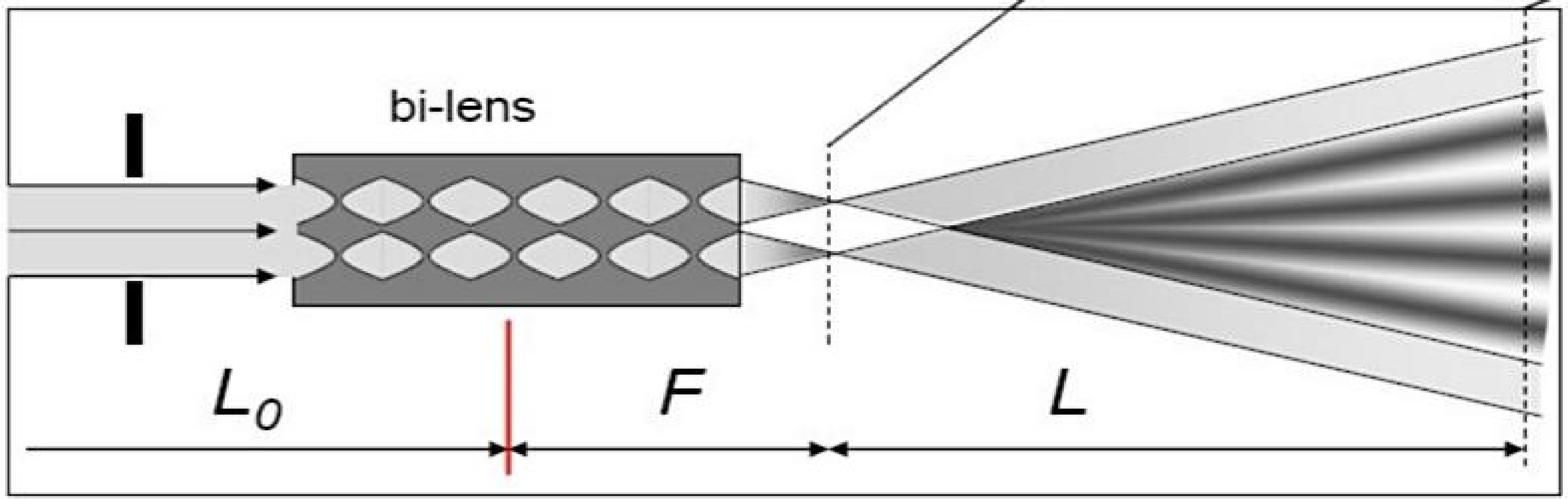




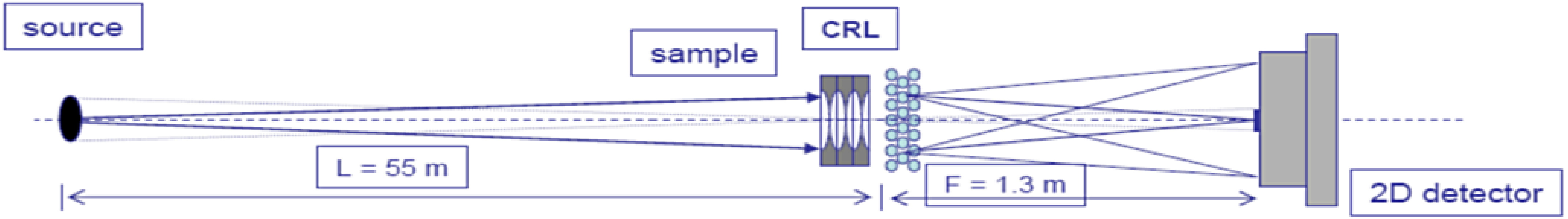
Silicon bilens (ESRF-Russia)



PRL-2009-103-064801



Some CRL applications. Fourier images APL-2005-86-014102
X-ray High Resolution Diffraction Using Refractive Lenses



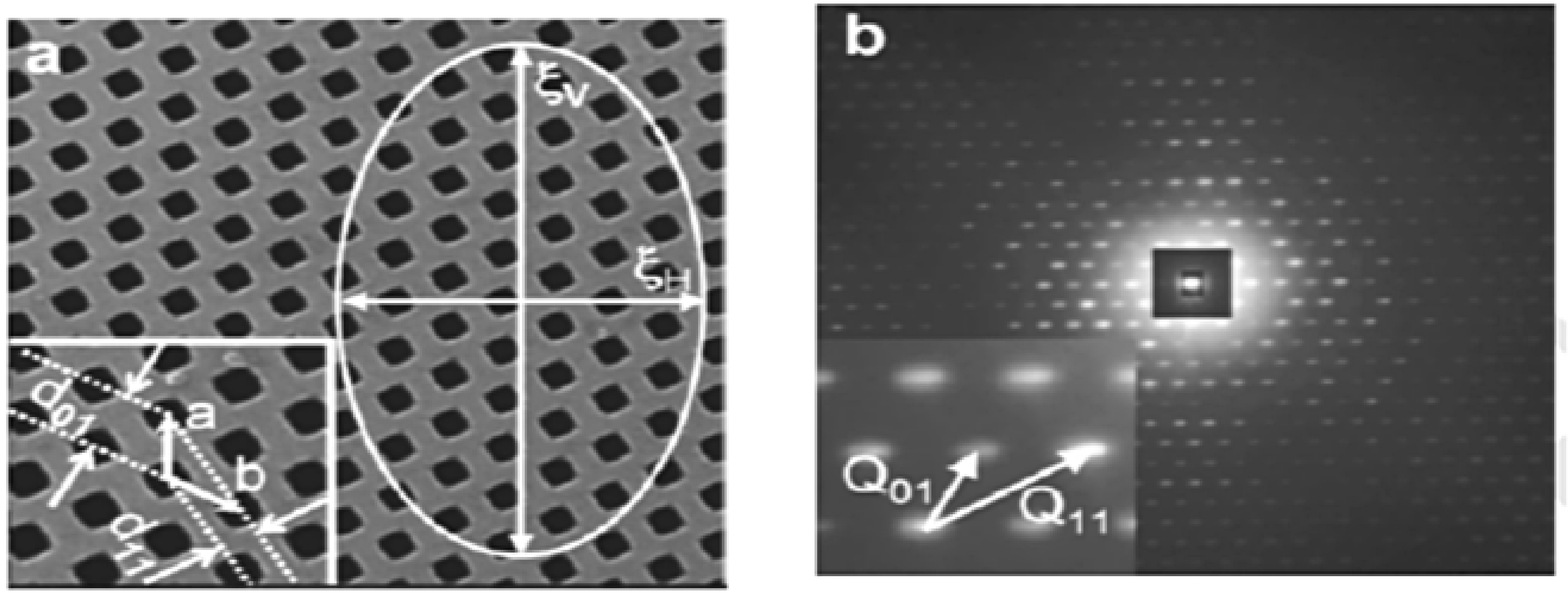
E = 28 keV
Al CRL, N = 112, F = 1.3 m

CCD resolution 2 μm
pixel / Θ = d

Resolution is limited
by angular source size:
s/L ~ 1 μrad

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

Si photonic crystal
$a=b=4.2$ μm $d_{01}=3.6$ μm $d_{11}=2.1$ μm



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

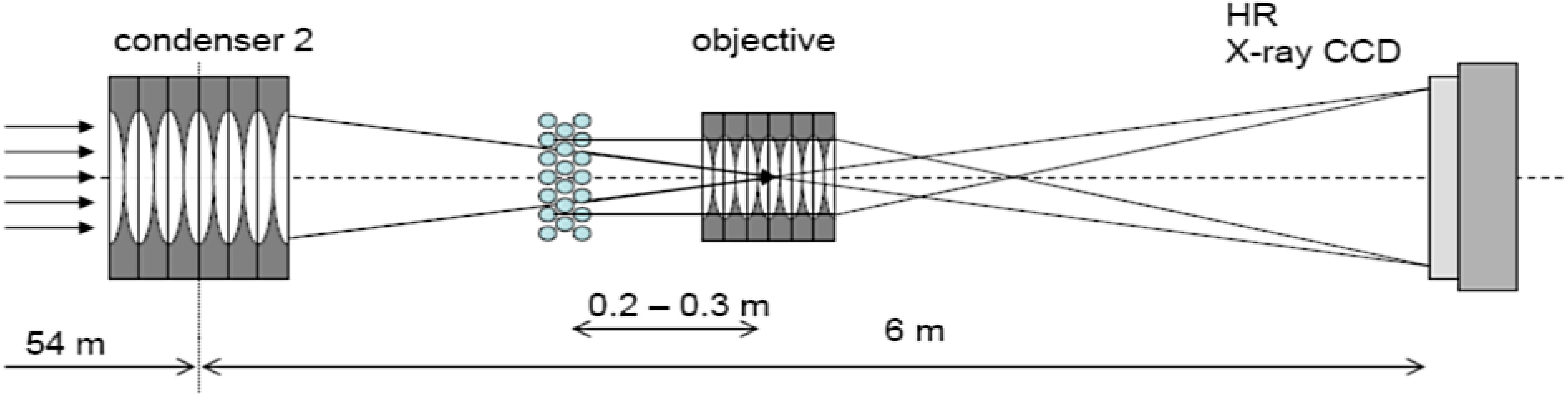
Theory allows one to account for an absorption in the CRL which influences high order peaks visibility Opt. Comm. 2003-216-247, JETP-2003-97-204

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 $1\ \mu m$)

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



MANY THANKS

FOR

ATTENTION