Baltic Federal University, november, 2016

# The theory and applications of x-ray phase contrast imaging

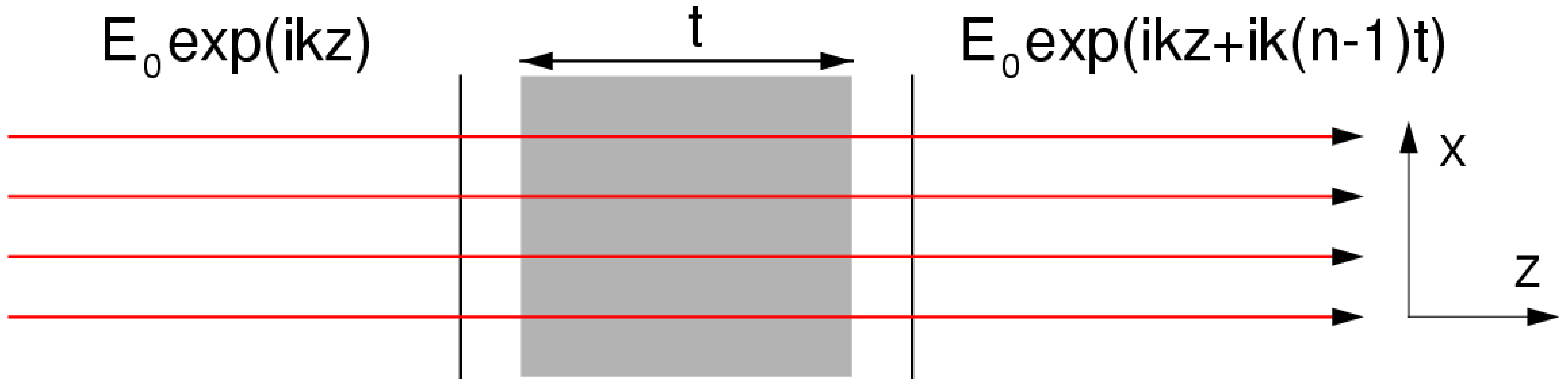
by Victor Kohn

National Research Centre "Kurchatov Institute"

personal site – http://kohnvict.ucoz.ru/main.htm

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

# plane wave, constant thickness



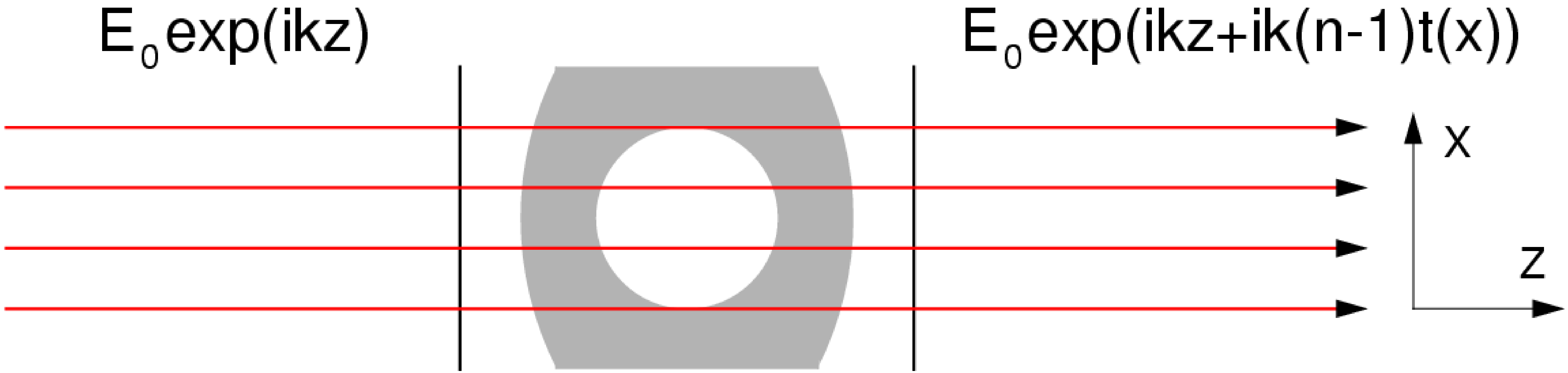

$k = 2\pi/\lambda$ is a wave number, $\lambda$ is a wavelength,

$n = \varepsilon^{1/2} = 1 - \delta + i\beta$ is a refraction index,

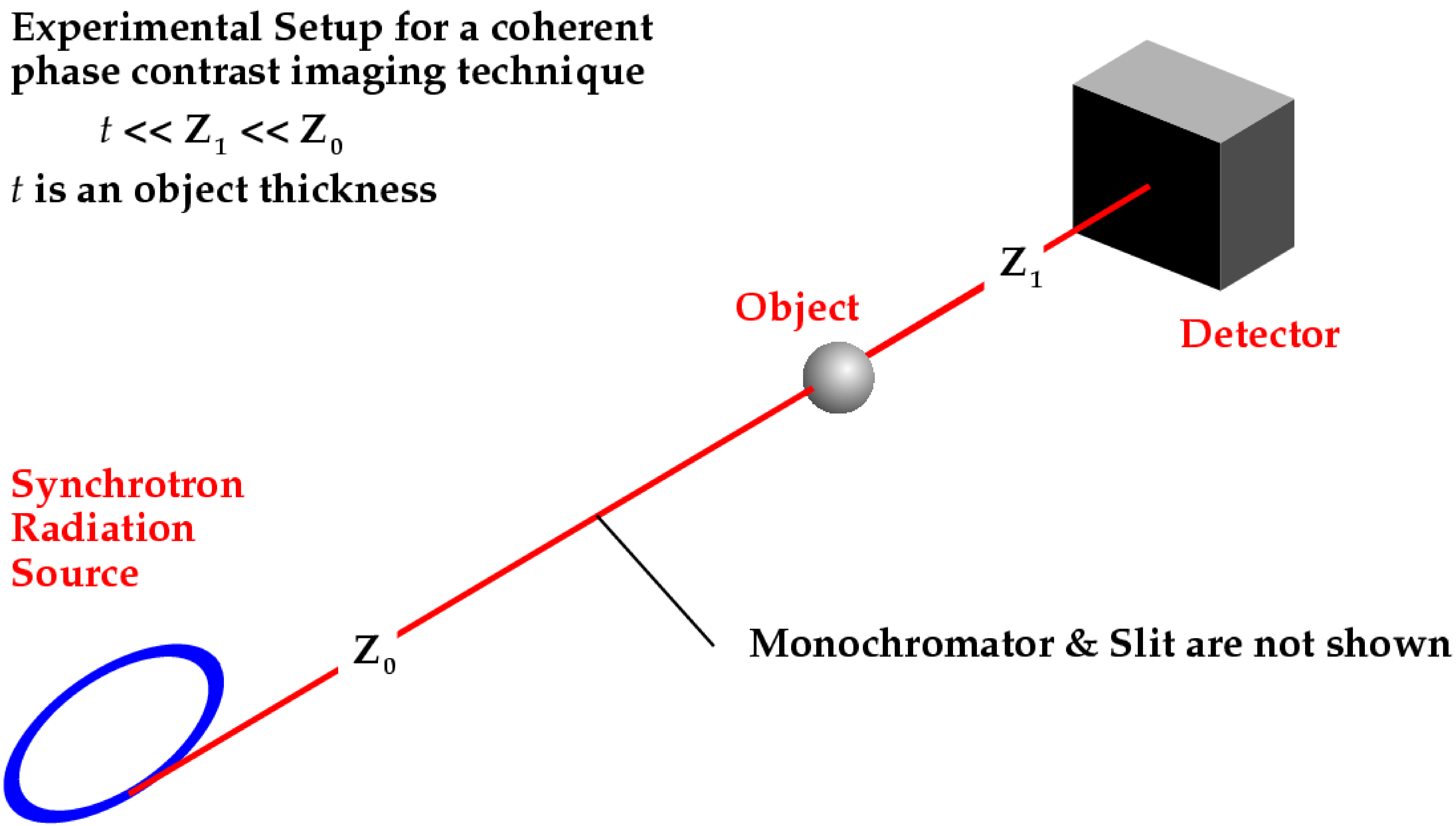
For hard x rays $\delta \approx 10^{-6}$, $\gamma = \beta/\delta < 10^{-2}$

A radiation wave field amplitude has an additional complex phase, $k(n-1)t$, but it is independent of x. A contrast is absent.

# plane wave, variable thickness




Now an additional complex phase $k(n-1)t(x)$ depends on x because object has a variable thickness. We can neglect a deviation of ray trajectories inside the object because a refraction is very small, but we need to take into account a variable phase shift. It is the basics of phase contrast.


Experimental Setup for a coherent
phase contrast imaging technique
t << Z1 << Z0
t is an object thickness
Object
Z1
Detector
Synchrotron
Radiation
Source
Z0
Monochromator & Slit are not shown

# The formulae for computer simulations
(the case of point source)

$$E(x,y,Z_t) = \int dx_1 dy_1 P_2(x - x_1, y - y_1, Z_1) T(x_1, y_1) P_2(x_1, y_1, Z_0)$$

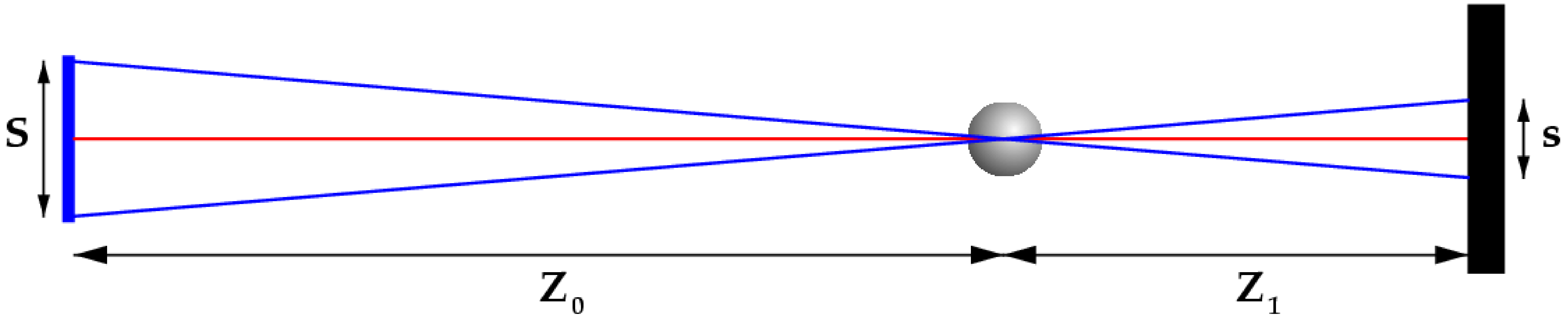
$$P_2(x,y,Z) = P(x,Z)P(y,Z), \quad P(x,Z) = (i\lambda Z)^{-1/2} \exp(i\pi x^2/\lambda Z)$$

$$E(x,y,Z_t) = P_2(x,y,Z_t) \int dx_1 dy_1 P_2(x_r - x_1, y_r - y_1, Z_r) T(x_1, y_1)$$

$$x_r = x Z_0/Z_t, \quad y_r = y Z_0/Z_t, \quad Z_r = Z_1 Z_0/Z_t, \quad Z_t = Z_0 + Z_1$$

$T(x,y) = \exp(\pm ik[\delta - i\beta] t(x,y))$ is a transmission function,
the sign $+$ is for a void in matter, the sign $-$ is for an object in air.
$P(x,Z)$ is a Fresnel propagator (spherical wave at long distance).

# The problem of spatial coherence due to the source size

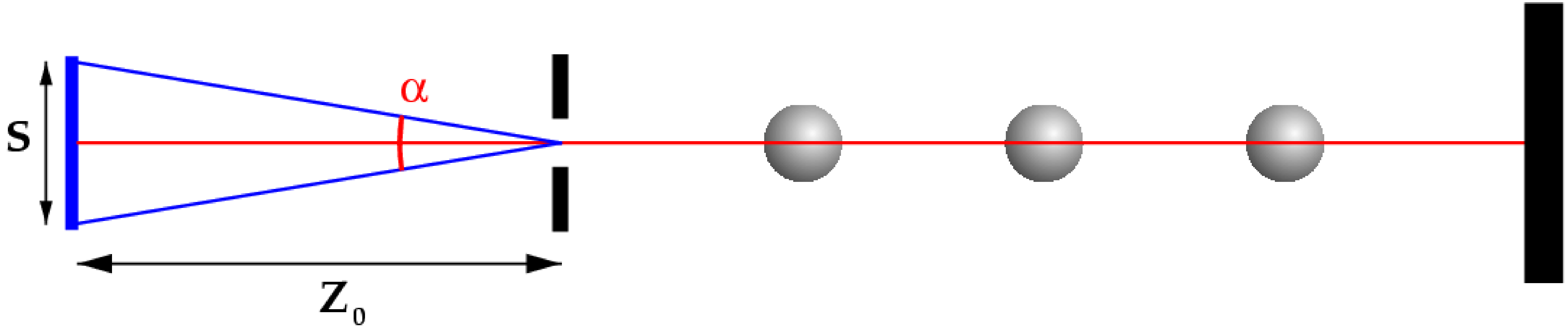



S is the source transverse size,  s is the source projection.

$s = S\, Z_1/Z_0$ – this relation follows from geometry

Each point source has an own optical axis. Each point source creats the same image of the object which is shifted from the main optical axis. A convolution of image over a source projection can kill the contrast because a mean intensity is not changed.

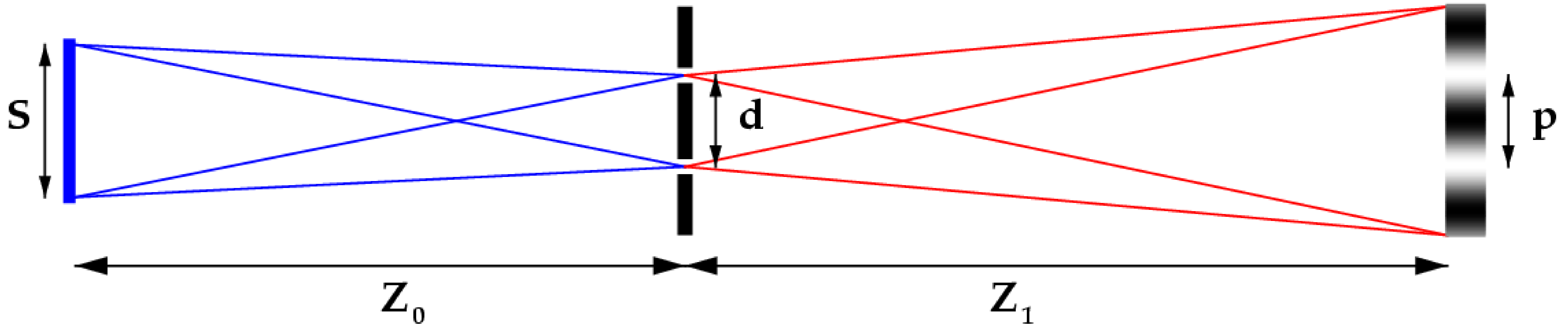
# Transverse Coherence Length




A very useful parameter is a transverse coherent length $L_{tc} = \lambda/\alpha$, where $\lambda$ is a wave length, $\alpha = S/Z_0$ is an angle of source. If a transverse size of object $d < L_{tc}$, then a radiation diffracted by object is coherent.

If the object is a slit then it plays a role of secondary coherent source for all subsequent objects. The 2D slit or a pinhole is a standard way to obtain a coherent source.

# How to understand Coherence




A simple example with a two slits interference (Young's experiment). It is followed from Fresnel propagator that period of fringes $p = \lambda Z_1/d$. The source projection is $s = SZ_1/Z_0$. A convolution of fringes over the distance $s$ does not kill the contrast if $s < p$ or $d < L_{tc} = \lambda Z_0/S$.

**Coherence is a condition to observe interference.**

It is necessary for the phase contrast because a phase does not change the integral intensity.

5486 Rev. Sci. Instrum. 66 (12), December 1995

# On the possibilities of x-ray phase contrast microimaging by coherent high-energy synchrotron radiation

A. Snigirev and I. Snigireva
*ESRF, B.P. 220, 38043 Grenoble Cedex, France*

Today is cited 1211 (GA), 917 (WOS), 767 (RG)

V. Kohn
*Russian Research Centre, "Kurchatov Institute," 123182 Moscow, Russia*

S. Kuznetsov and I. Schelokov
*Institute of Microelectronics Technology RAS, 142432 Chernogolovka, Moscow region, Russia*

(Received 26 April 1995; accepted for publication 5 September 1995)

Coherent properties of the x-ray beam delivered at the ESRF allow the observation of very weak perturbations of the wave front, resulting in the phase contrast. A straightforward experimental setup for phase contrast imaging is proposed and used to record holographic images from organic samples of 10–100 $\mu$m at energy 10–50 keV with the contrast up to 50%–100%. The theory of phase contrast imaging is considered and some theoretical estimations are made to reveal the performance of the proposed technique in terms of resolution, sensitivity, geometrical requirements, and energy range applicability. It is found that for carbon-based fibers a detectable size with 2% contrast is 0.1 $\mu$m for 10 keV and $-1$ $\mu$m for 100 keV. It is demonstrated that the fine interference structure of the image is very sensitive to the shape, density variation, and internal structure of the sample. Some prospects for the practical use and future development of the new coherent techniques such as phase contrast microscopy, microtomography, holography, and interferometry at high energies are also discussed. 

APPLIED PHYSICS LETTERS **91**, 171901 (2007)

# Study of micropipe structure in SiC by x-ray phase contrast imaging

V. G. Kohn
*Russian Research Center, "Kurchatov Institute", 123182 Moscow, Russia*

T. S. Argunova
*Ioffe Physico-Technical Institute, RAS, Polytekhnicheskaya St. 26, 194021 St. Petersburg, Russia and X-ray Imaging Center, Department of Materials Science and Engineering, Pohang University of Science and Technology, San 31 Hyoja-dong, Namku, Pohang 790-784, Republic of Korea*

Jung Ho Je[a)]
*X-ray Imaging Center, Department of Materials Science and Engineering, Pohang University of Science and Technology, San 31 Hyoja-dong, Namku, Pohang 790-784, Republic of Korea*

(Received 10 July 2007; accepted 2 October 2007; published online 22 October 2007)

Phase contrast images of dislocation micropipe in SiC crystal are experimentally studied at various distances from the sample using synchrotron white beam. Computer simulation of these images enabled us to understand the peculiarities of image formation and measure the diameter of the micropipe. The phase contrast imaging of micropipes without monochromator is explained by the absorption of x rays in a thick (490 $\mu$m) SiC crystal, effectively forming a high brilliance radiation spectrum with a pronounced maximum at 16 keV. 

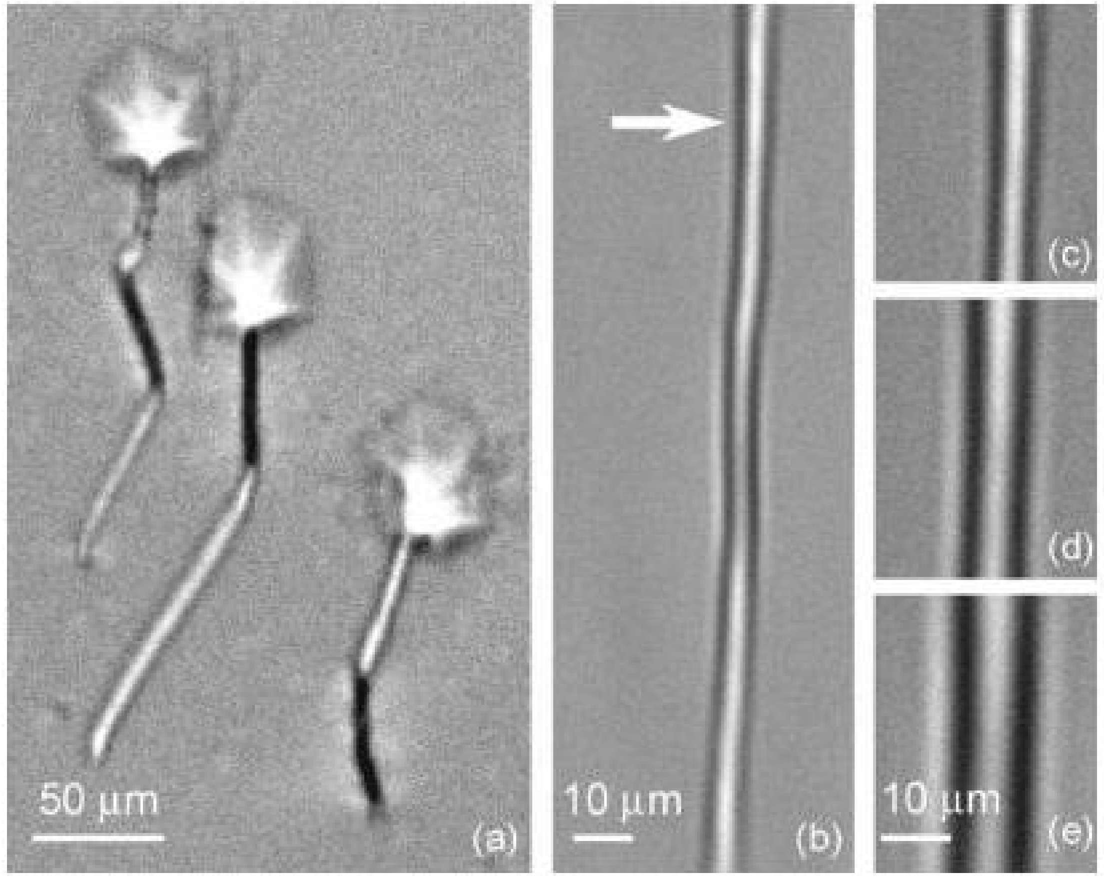



FIG. 1. Typical images of micropipes in SiC wafers cut perpendicular to the [0001] growth direction (a) and along the growth direction (b). The arrow in (b) indicates the fragment shown in (c)–(e) at various sample-to-detector distances: 10, 30, and 50 cm, respectively. Halos in (a) correspond to etch pits on the wafer surface.

# Direct Measurement of Transverse Coherence Length of Hard X Rays from Interference Fringes

V. Kohn,[1] I. Snigireva,[2] and A. Snigirev[2,*]

[1]*Russian Research Centre "Kurchatov Institute," 123182 Moscow, Russia*

[2]*European Synchrotron Radiation Facility, B.P. 220, F-38043, Grenoble Cedex, France*

(Received 17 November 1999)

We propose a simple interferometric technique for hard x-ray spatial coherence characterization, recording a Fresnel interference pattern produced by a round fiber or a slit. We have derived analytical formulas that give a direct relation between a visibility of interference fringes and either the source size or the transverse coherence length. The technique is well suited to third-generation synchrotron radiation sources and was experimentally applied to determine the spatial coherence length and the source size at the European Synchrotron Radiation Facility.

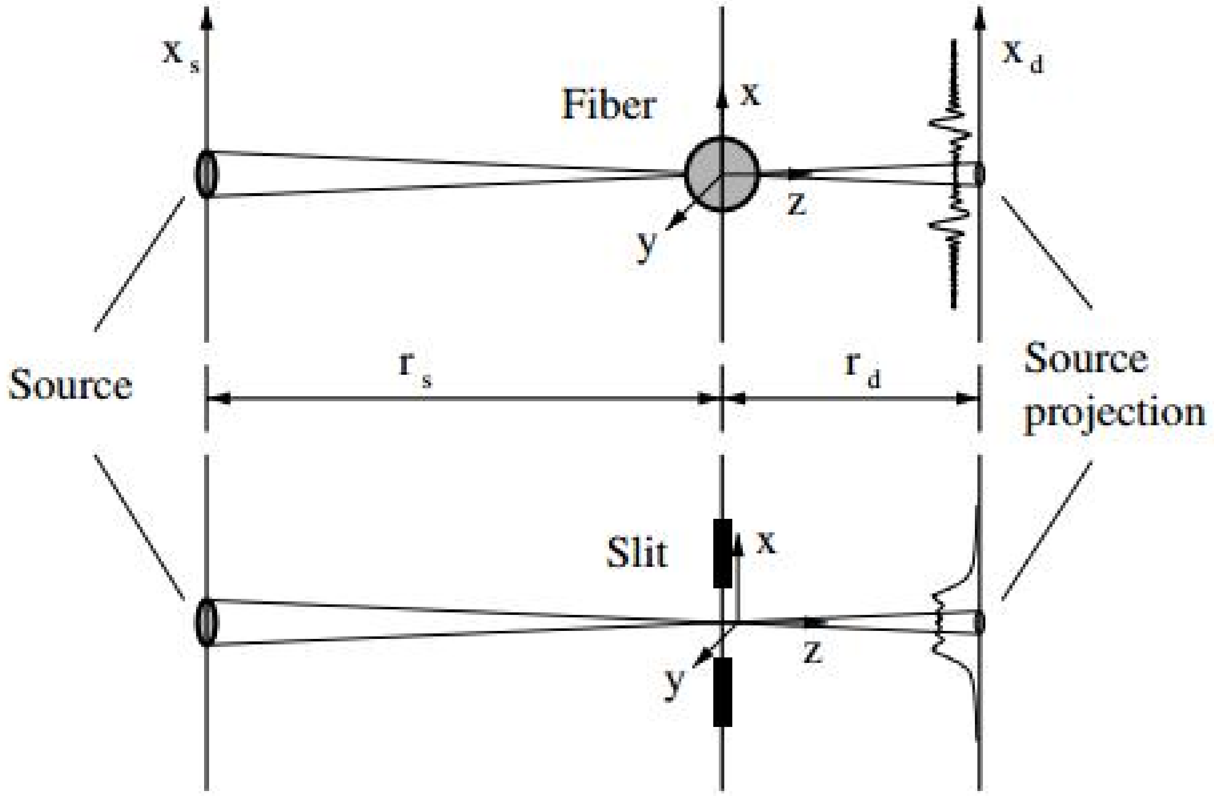



FIG. 1. Schematic drawing of the experimental setup, where $r_s$ is the distance from the source to fiber or slit and $r_d$ is the distance from the fiber or slit to the high resolution detector.

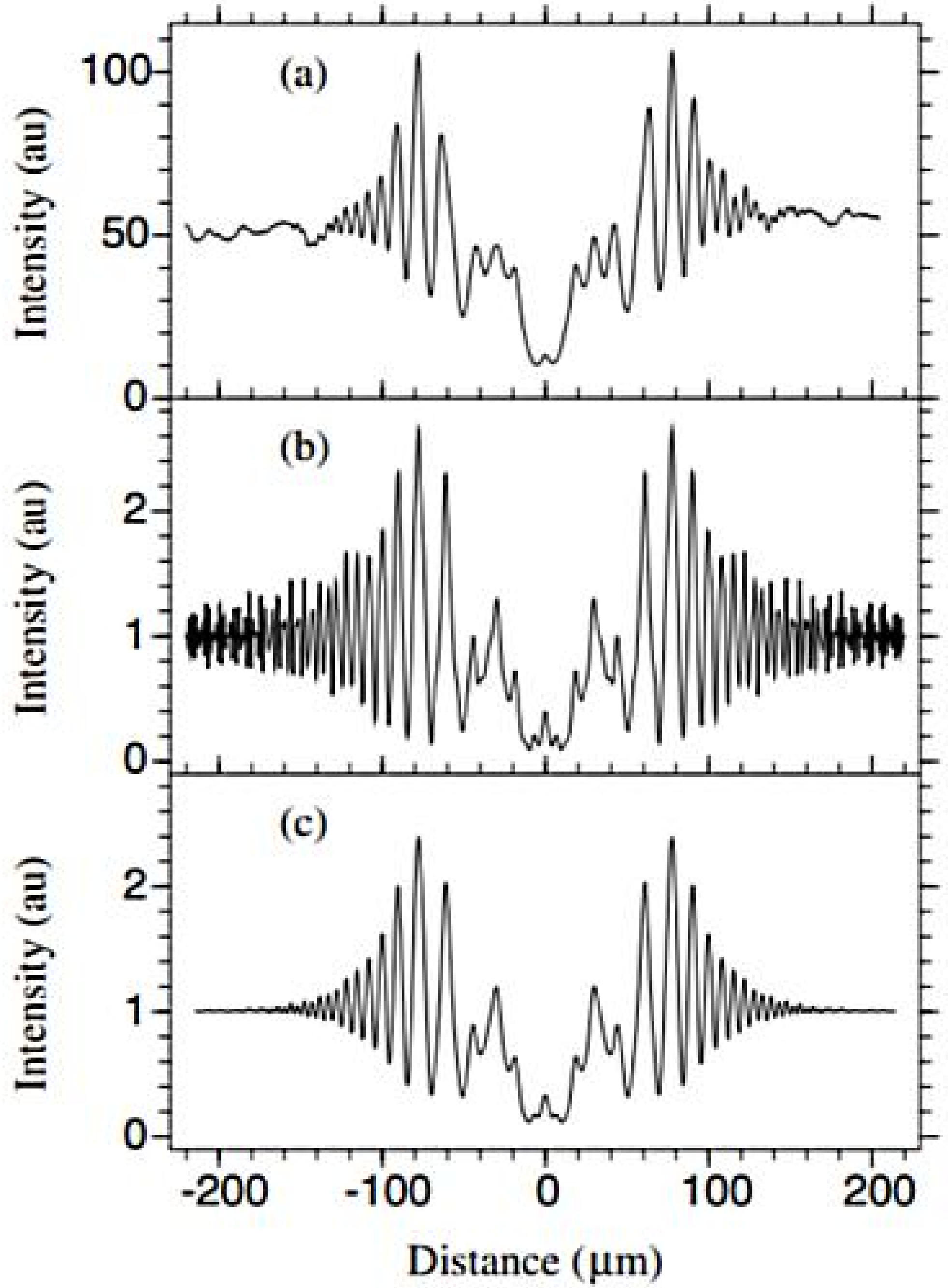
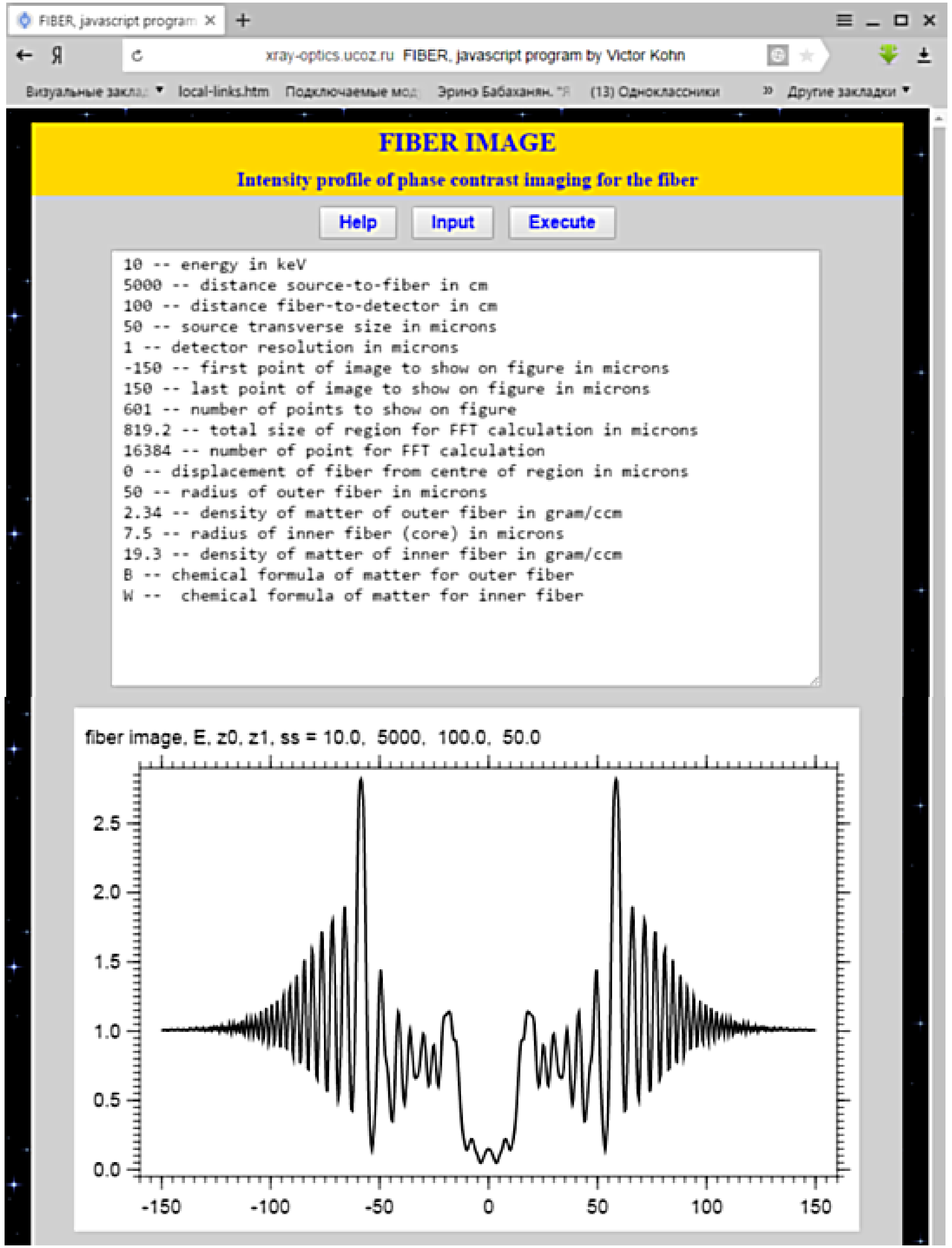
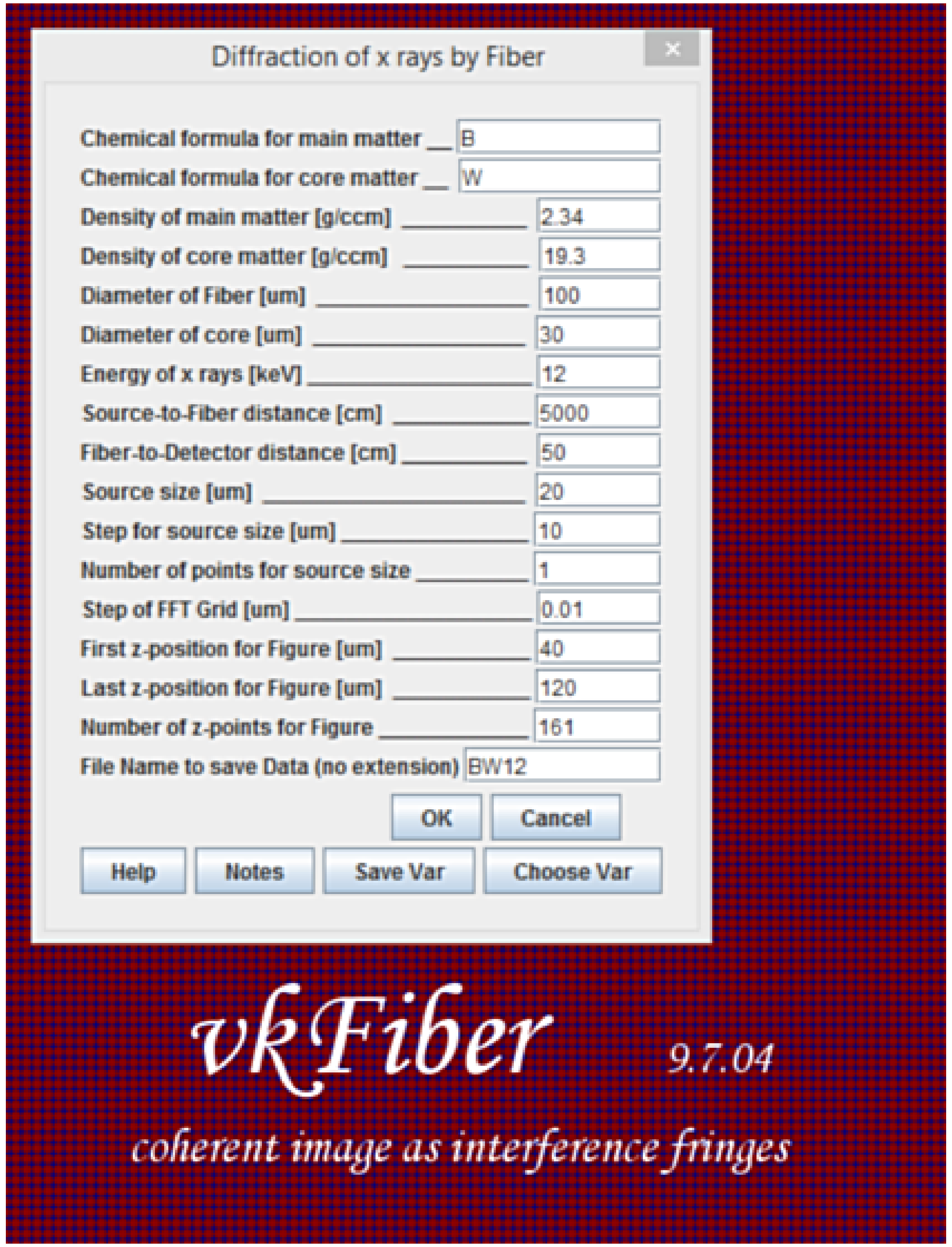


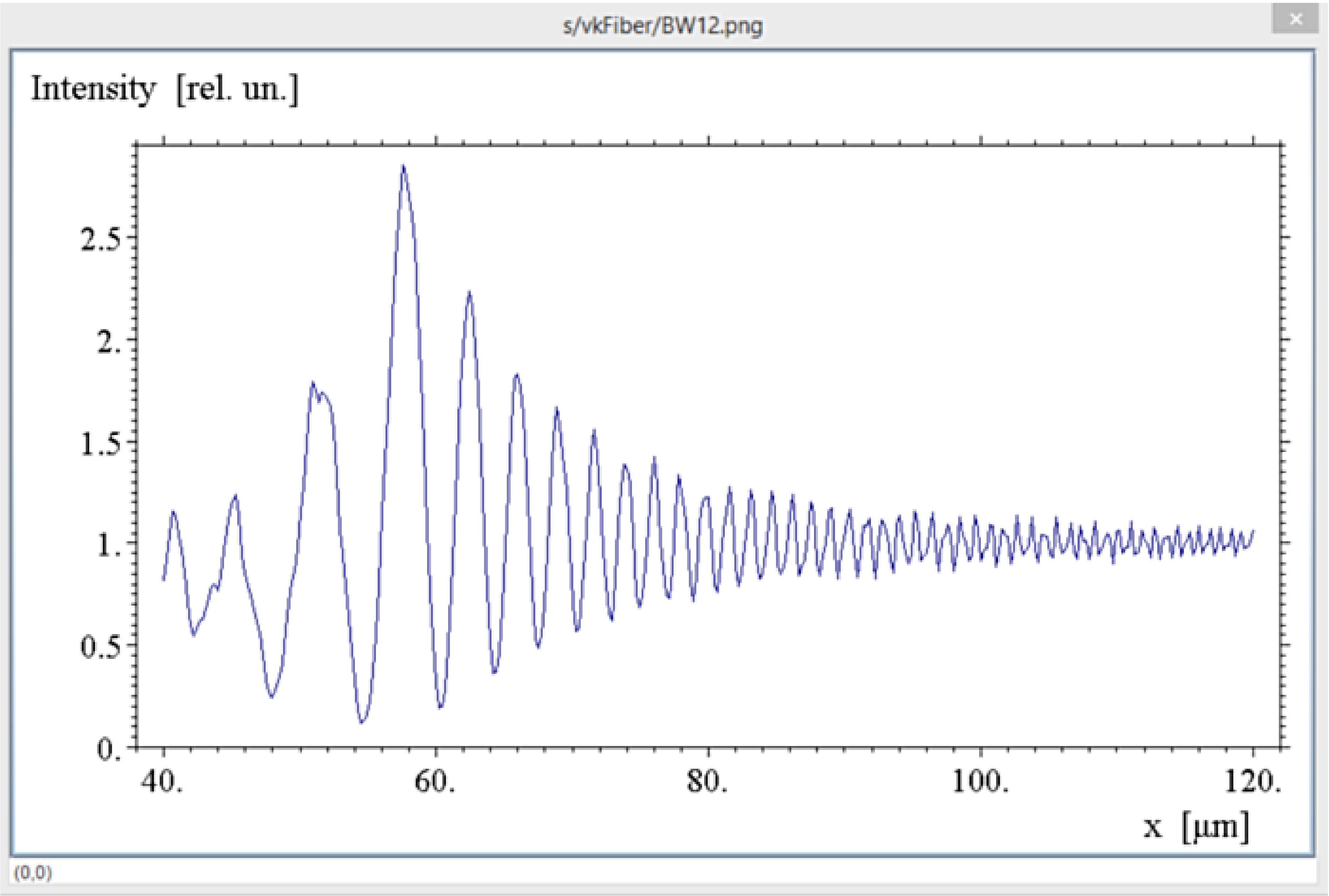

FIG. 2. Diffraction fringes produced by the boron fiber of 100 $\mu$m diameter with a 15 $\mu$m tungsten core. Fiber is placed at 41 m from the source; the distance fiber-to-detector is 5 m; the x-ray energy is 17 keV. (a) The experimental data, (b) theoretical calculation for a point source, and (c) theoretical calculation for a 33 $\mu$m source size.




The method of measuring the effective source size by means of boron fiber with a tungsten core is very useful in many SR facilities. Today I have elaborated several computer programs for simulating the phase contrast of such objects. One of them is working online on my site of internet. At the left part of slide the site is shown.
http://xray-optics.ucoz.ru/js-pro
/fiber-pro.htm




The offline program is written in Java. It can work in any operating system. It has more options and it is more convenient. It can be downloaded from my site as a part of the program vkUtility.

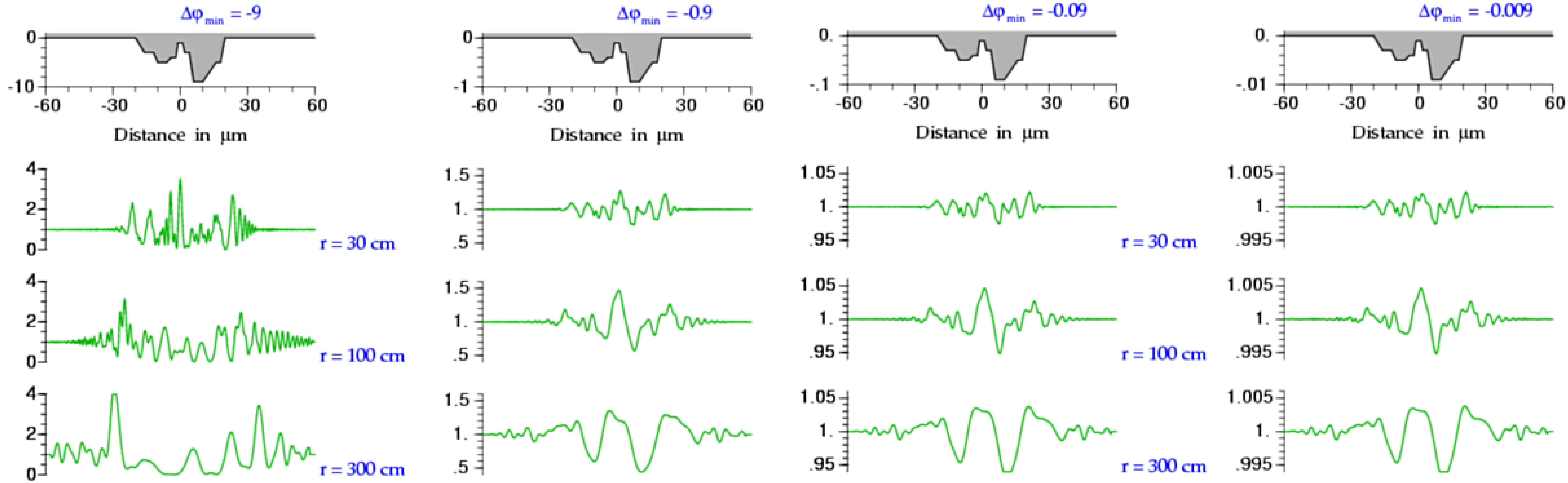


We see that the phase shift profile $\Delta\varphi(x)$ creates the intensity profile $\Delta I(x)$ In general it is necessary to solve the inverse problem, i.e. to obtain $\Delta\varphi(x)$ from $\Delta I(x)$. There are some approaches to this task. If $|\Delta\varphi(x)|_{\max} \ll 1$ then the problem is more easy because a dependence is linear and the inverse problem can be solved by one step.

## Image of complex transparent object

X-ray energy 20 keV, source distance 50 m, source size 30 μm.

Intensity depends on object thickness Δφ and detector distance r



Nuclear Instruments and Methods in Physics Research A 543 (2005) 306–311

# The live lattices become visible in coherent synchrotron X-rays

V. Kohn[a], C. Rau[b], P.M. Sergienko[c,*], I. Snigireva[b], A. Snigirev[b], A. Vazina[c]

[a]*Russian Research Centre "Kurchatov Institute", 123182, Moscow, Russian Federation*
[b]*European Synchrotron Radiation Facility, BP-220, F-38043, Grenoble, France*
[c]*Institute of Theoretical and Experimental Biophysics, RAS, 142290 Pushchino, Russian Federation*

We demonstrate a great potential of the method of phase contrast imaging for a study of muscles and animal organism in normal and pathological states. The method is applied to image biological tissues that have the unique feature of structure–translation symmetry of 0.1–10 μm periodicity. The cross-striated muscle is the most interesting example of such objects. The experiment was done using high-brilliant coherent X-rays, delivered by synchrotron radiation source of third generation (ESRF, Grenoble), and high-resolution 2D-detector.

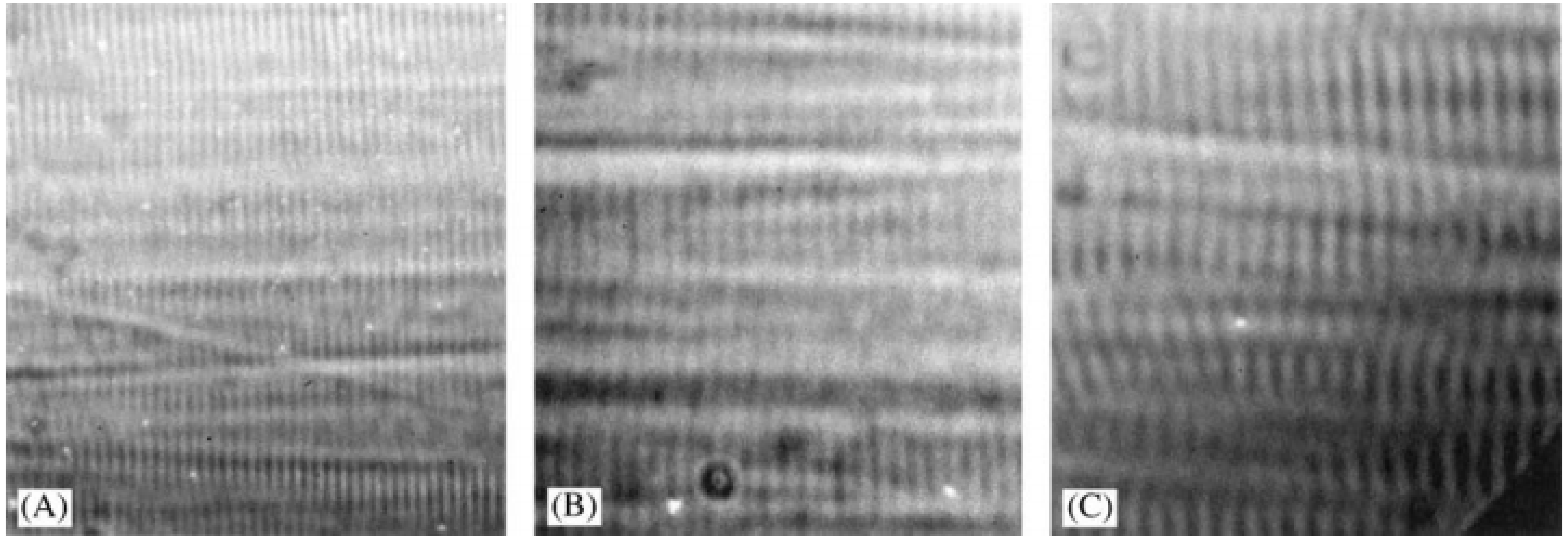



Fig. 3. The X-ray phase contrast imaging of living cross-striated skeletal *Sartorius* muscle of frog *Rana ridibunda*: (A) in rest, sarcomere length 2.2 μm; (B) after stretching to the sarcomere length 3 μm; (C) stretched to no overlap, sarcomere length 4 μm.

# The theory of weak phase contrast imaging

In the case when the object produces a weak phase modulation of the wave field and the transmission amplitude has the form

$$T(x) = I_0^{1/2} \exp(i\varphi_0 + i\Delta\varphi(x)), \quad |\Delta\varphi| << 1 \qquad (1)$$

we obtain the formula for the intensity distribution $I_h(x')$ on the hologram (the phase contrast image). Let the normalized intensity be

$$r(x_0) = ( I_h(x') - I_0 )/I_0 \qquad (2)$$

where $x_0 = x'z_0/z_t$, $z_t = z_0 + z$, $z_0$ is a distance from a point source to the object, $z$ is a distance from the object to a detector. Then we have

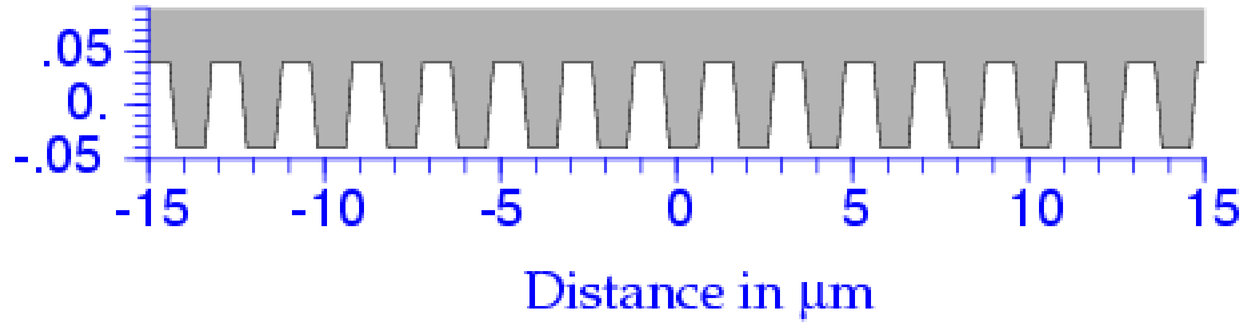
$$r(x_0) = \int dx\, Q(x_0 - x, z_r)\, \Delta\varphi(x) \qquad (3)$$

where $z_r = z_0\, z/z_t$ and

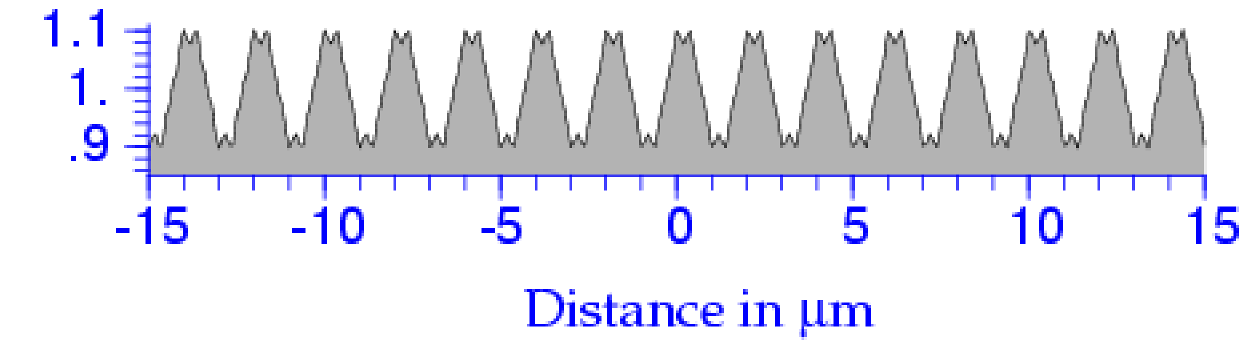
$$Q(x,z) = 2 \sin( \pi[x^2/\lambda z + 3/4] )/(\lambda z)^{1/2} \qquad (4)$$

Hence we have linear connection between the relative phase profile and the relative intensity distribution (contrast).

Obviously, in the case of periodical phase modulation one has to obtain a periodical phase contrast image. As an example we consider the next model phase profile




The result of calculating the phase contrast image for the parameters: $z_0$ = 62 m, $z$ = 10 cm, transverse size of source 40 µm, x-ray energy 20 keV is shown below



# The theory of weak phase profile reconstruction

The more important problem is to reconstruct the phase profile from the experimental intensity profile. In the case of near field condition this problem is not simple because the twin image and the intermodulation term cannot be neglected. For a weak contrast we have the linear relation (3) where the intermodulation term is neglected. However, the twin image is not small and only the computer reconstruction based on the Fourier transformation is possible. We find that eq. (3) is a convolution of two functions. Therefore we have a simple product for the Fourier images

$$r(q) = Q(q,z_r)\,\Delta\varphi(q) \qquad (5)$$

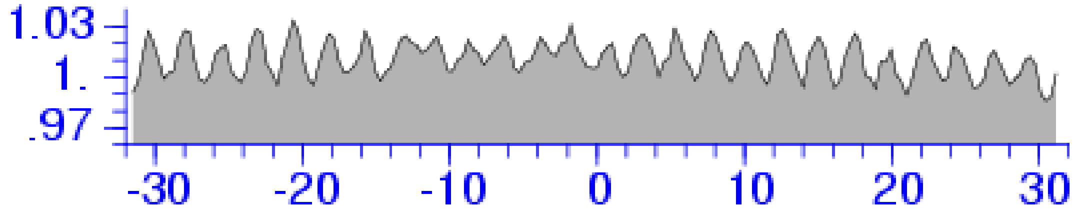
The Fourier image of the propagator is known analytically

$$Q(q,z) = 2\sin(\,[\lambda z/4\pi]\,q^2\,) \qquad (6)$$

This function has zero values and therefore some regularization procedure is necessary. It was verified that the next formula works well

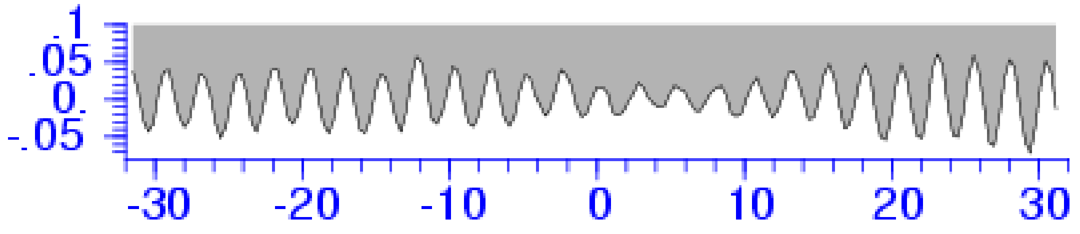
$$\Delta\varphi(q) = \frac{r(q)\,Q(q,z_r)}{Q^2(q,z_r) + \varepsilon} \qquad (7)$$

where ε is the small reqularization parameter.




Distance in µm

We apply the method on the random fragment of the muscle image shown above. The parameters are the same as in the model calculation. The reconstructed phase profile is shown below. One may see the period of oscillation is approximately the same whereas the peculiarities of the profile are different.



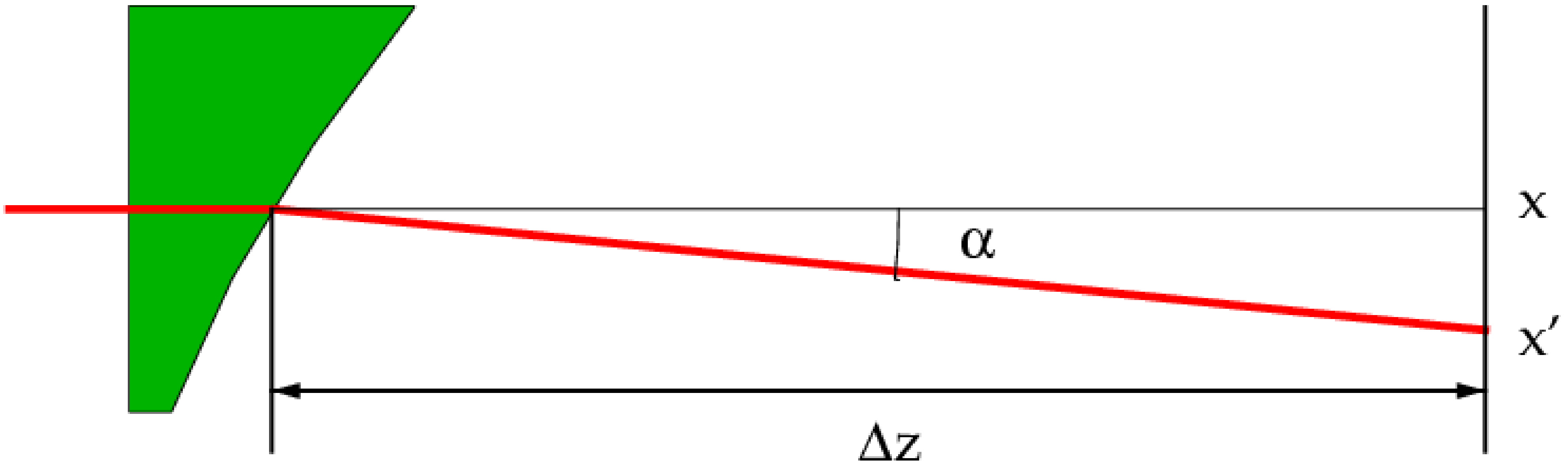

Distance in µm

# Transport of Intensity Equation (TIE)

## for the phase φ(x,y) from the intensity difference ΔI(x,y)

$$-\frac{1}{\lambda I}\frac{\Delta I}{\Delta z} = \frac{1}{2\pi}\left(\frac{d^2\varphi}{dx^2} + \frac{d^2\varphi}{dy^2}\right)$$

is derived from incoherent geometrical optics — ray count




Angle of ray inclination $\alpha = \frac{\lambda}{2\pi}\frac{d\varphi}{dx}$, ray position $x' = x + \alpha\,\Delta z$

Relative ray density $\frac{dx'}{dx} = \frac{I(0)}{I(\Delta z)} = 1 + \frac{\lambda}{2\pi}\frac{d^2\varphi}{dx^2}\Delta z$

# Gerchberg - Saxton Algorithm (GSA)

for the phase $\varphi_F(x,y)$ from two intensities:

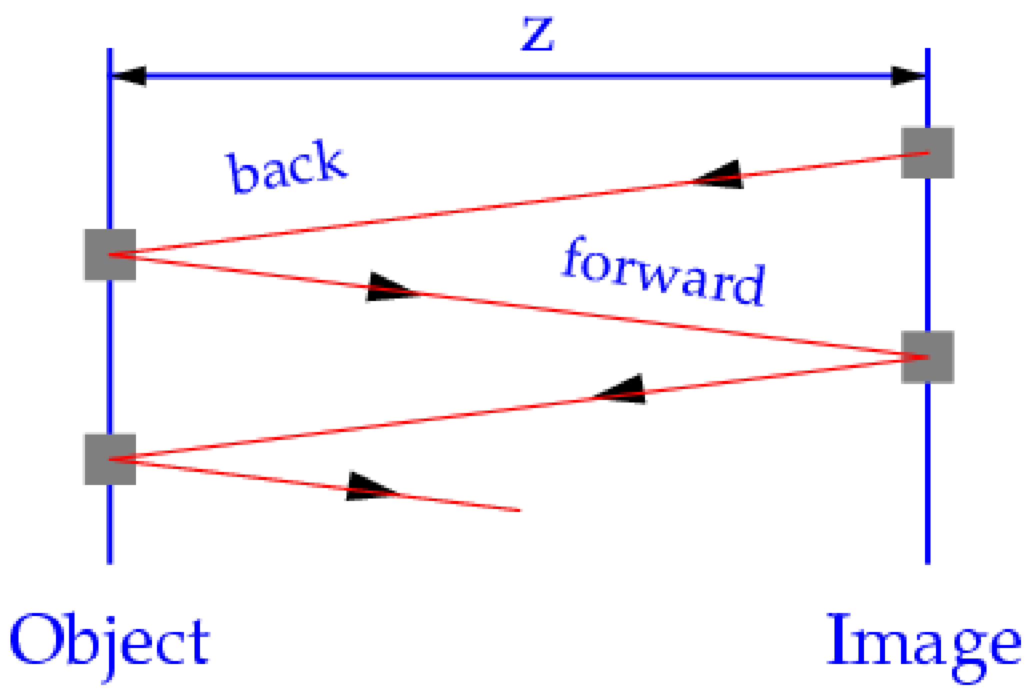
at object $I_O(x,y)$ and at image (hologram) $I_H(x,y)$

Back propagation: $R(x') = I_H^{1/2}\, e^{i\varphi_R}$; $F'(x) = |F|\, e^{i\varphi_F} = P_z^*(x-x') * R(x')$

Forward propagation: $F(x) = I_O^{1/2}\, e^{i\varphi_F}$ $R'(x') = |R|\, e^{i\varphi_R} = P_z(x'-x) * F(x)$

$A(x'-x) * B(x)$ means a convolution $\int dx\, A(x'-x)B(x)$

1D Propagator: $P_z(x) = \dfrac{1}{(i\lambda z)^{1/2}} \exp\left( i\pi \dfrac{x^2}{\lambda z} \right)$




Start with any $\varphi_R$, for example $\varphi_R = 0$,
then back and forward propagations
are repeated iteratively

Physica Scripta. Vol. 56, 14–19, 1997

# The Method of Phase Retrieval of Complex Wavefield from Two Intensity Measurements Applicable to Hard X-rays

Victor G. Kohn

A novel algorithm for a reconstruction of the phase shift profile produced by a transparent object in a coherent wave, from a set of two recorded intensity distributions is presented. Contrary to well known algorithms of in-line holography, the method works under the near-field condition where the size of the first Fresnel zone is much less than the characteristic size of the object's details. Such a condition is typical for an in-line holography experimental setup with the use of coherent high energy X-rays ($E > 20$ keV) produced by synchrotron radiation sources of the third generation like ESRF. The novel algorithm is fast and insensitive to a partial loss of coherence or weak detector resolution. The method can be applied to X-ray refraction tomography.

The method is close to TIE method, but is derived from calculation of Kirchhoff integral by the Stationary Phase Method. It can be used for partiallly coherent beams.

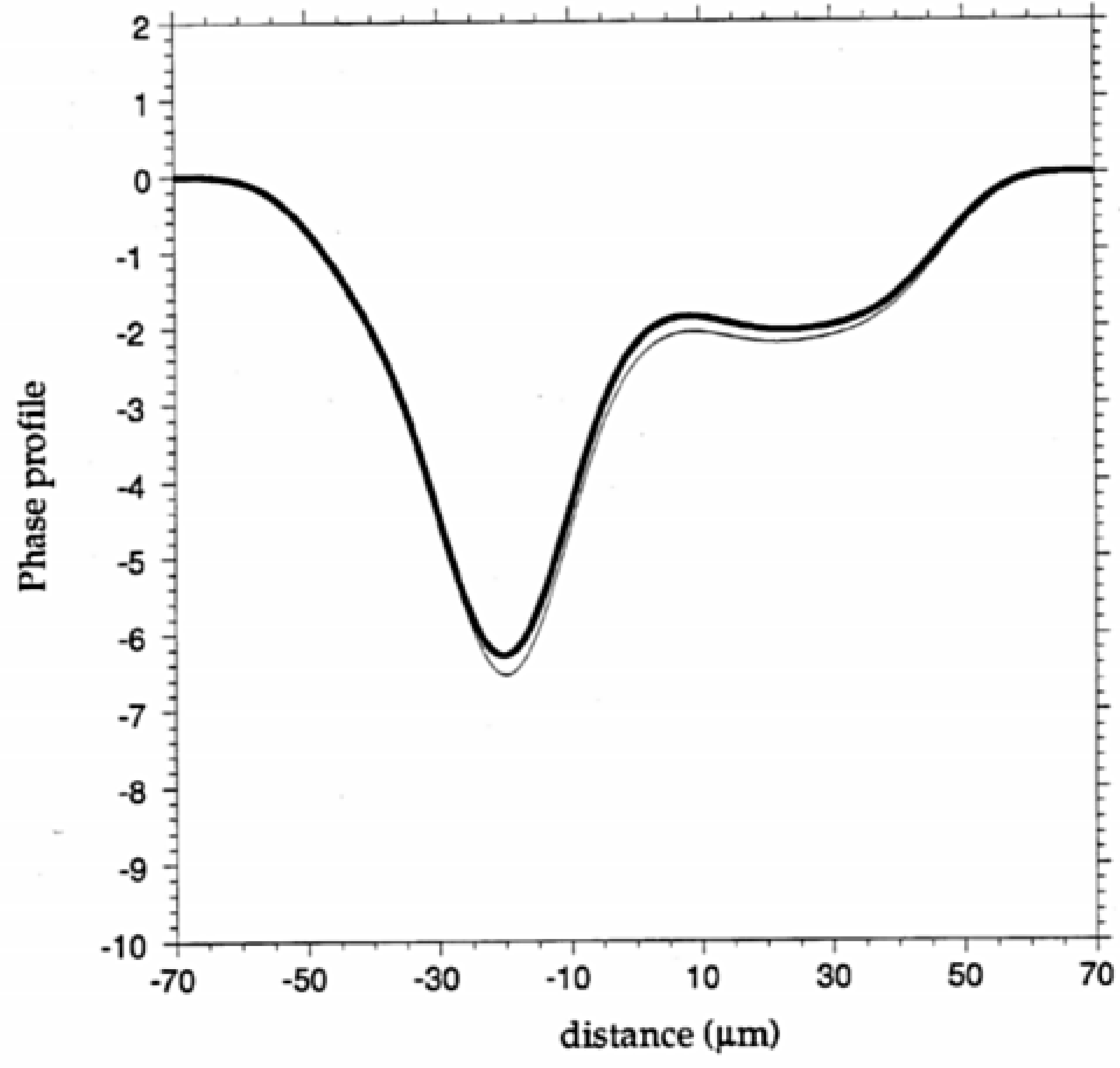
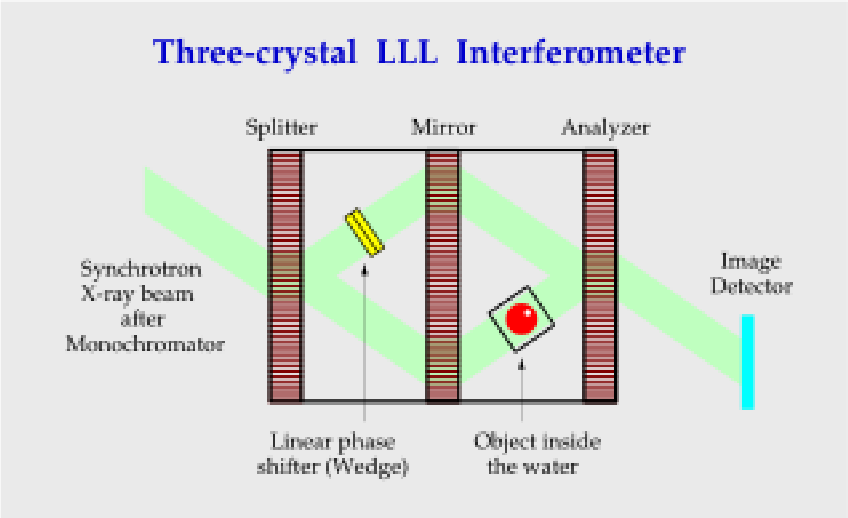



*Fig. 3.* Original (thin curve) and reconstructed (thick curve) phase shift profiles for a smoothed object.

# Methods of Phase Sensitive Imaging

## Interferometry




Proposed by:

**Momose et al., Japan**

Advantage:

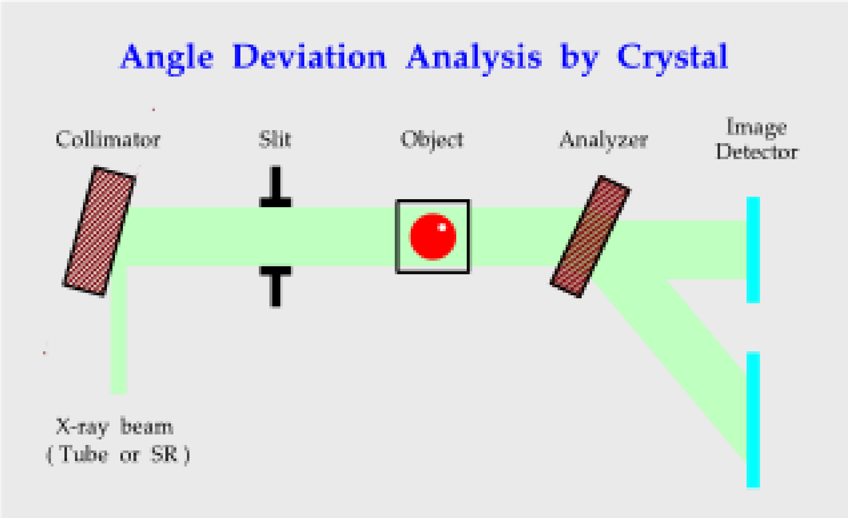
φ from Experiment, CT

Conditions:

Small dφ/dx,

Small object size

## Diffraction




Proposed by:

**Ingal et al., Russia**

Advantage:

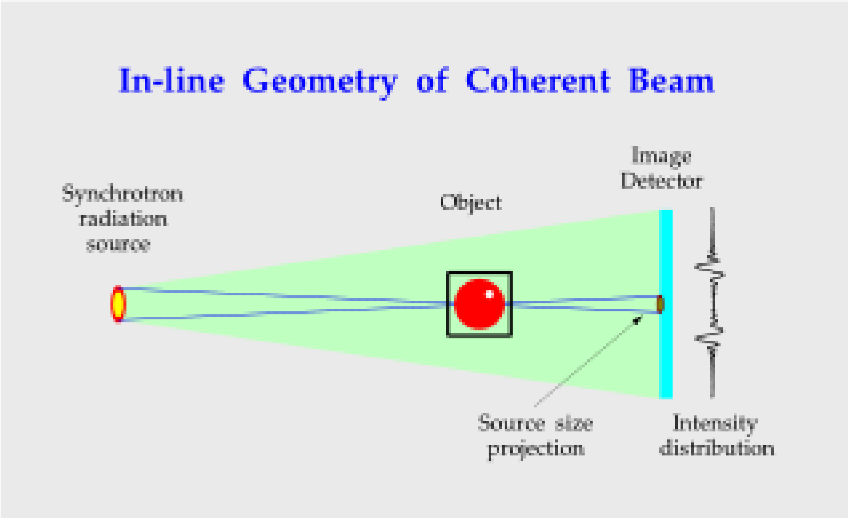
Any X-ray source

Conditions:

Limited dφ/dx,

Simple image treatment

## Holography




Proposed by:

**Snigirev et al., France**

Advantage:

Objects of any kind and size

Boundary image and CT

φ retrieval is possible

Any coherent X-ray source

MANY THANKS

FOR

ATTENTION