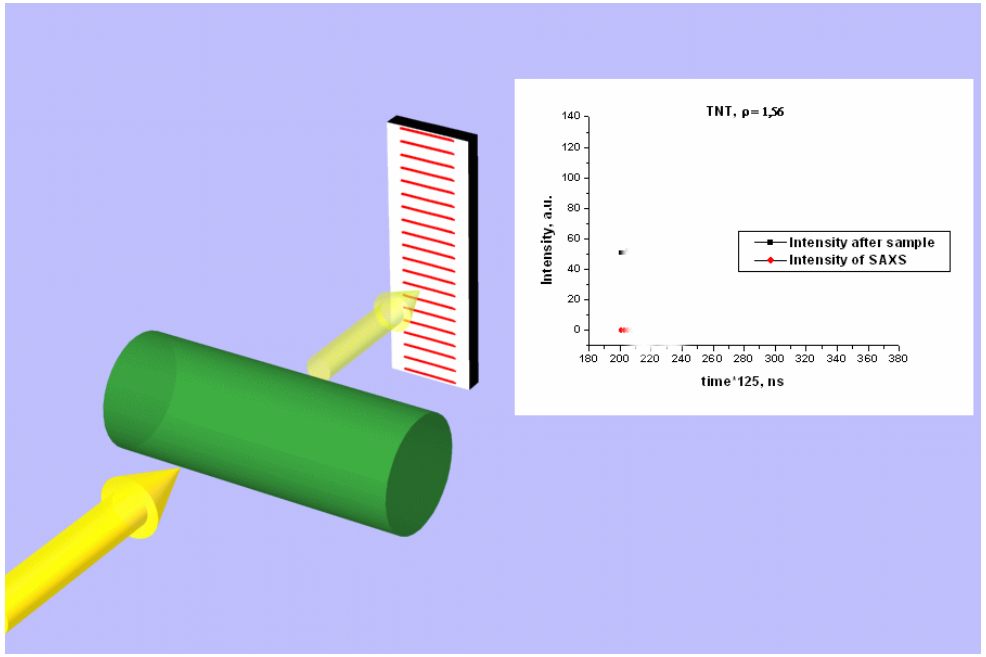
The use of polychromatic synchrotron radiation to study fast processes in solids. Advantages and challenges.

Prof. TOLOCHKO, Boris (Institute of solid state chemistry and mechanochemistry)
Dr. ARAKCHEEV, Aleksey (Budker INP); Mr. AULCHENKO, Vladimir (BINP); Dr. SHEKHTMAN, Lev (Budker Institute of Nuclear Physics); TEN, Konstantin (LIH SB RAS); Dr. ZHULANOV, Vladimir (Budker INP), Vinokurov N.A. (Budker Institute of Nuclear Physics)

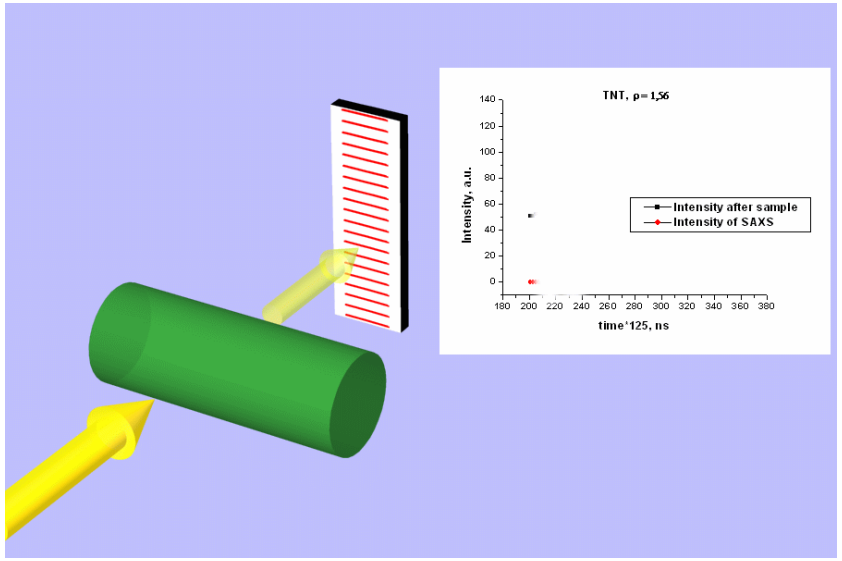
Introduction



The aim of the work is to develop a method that allows X-ray analysis using a synchrotron radiation wide spectral band (polychromatic radiation) by EXAFS, PXD, SAXS, tomography.
This will make it possible to increase the number of photons in the primary beam by 2-3 orders of magnitude and, accordingly, reduce the time for determining the composition of the sample to nanoseconds.
PXD, SAXS, tomography SAXS is currently experimentally implemented at VEPP-3 / VEPP-4.
In this work, we propose optimizing the undulator parameters for the implementation of the EXAFS and XANES method.

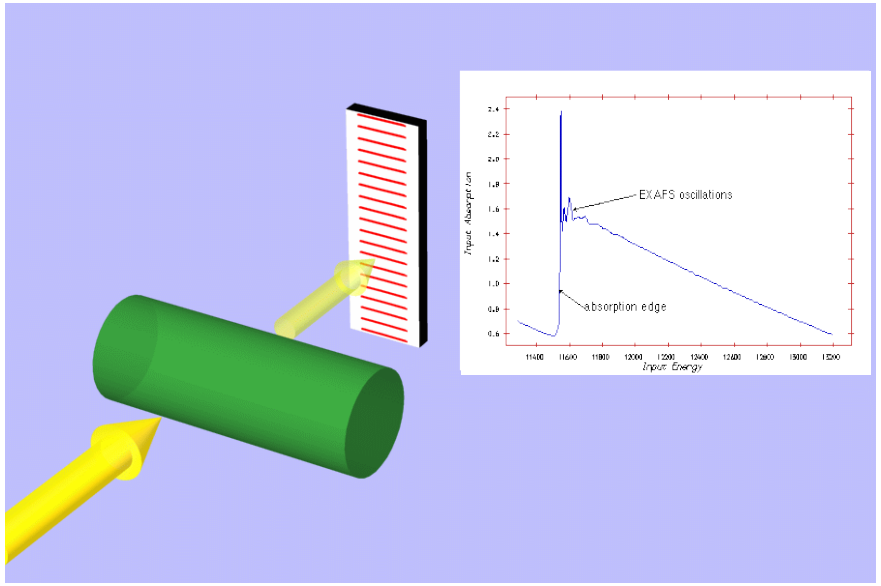
The scheme of SAXS experiment during detonation of explosive trotyl with using a polychromatic synchrotron radiation .

Introduction

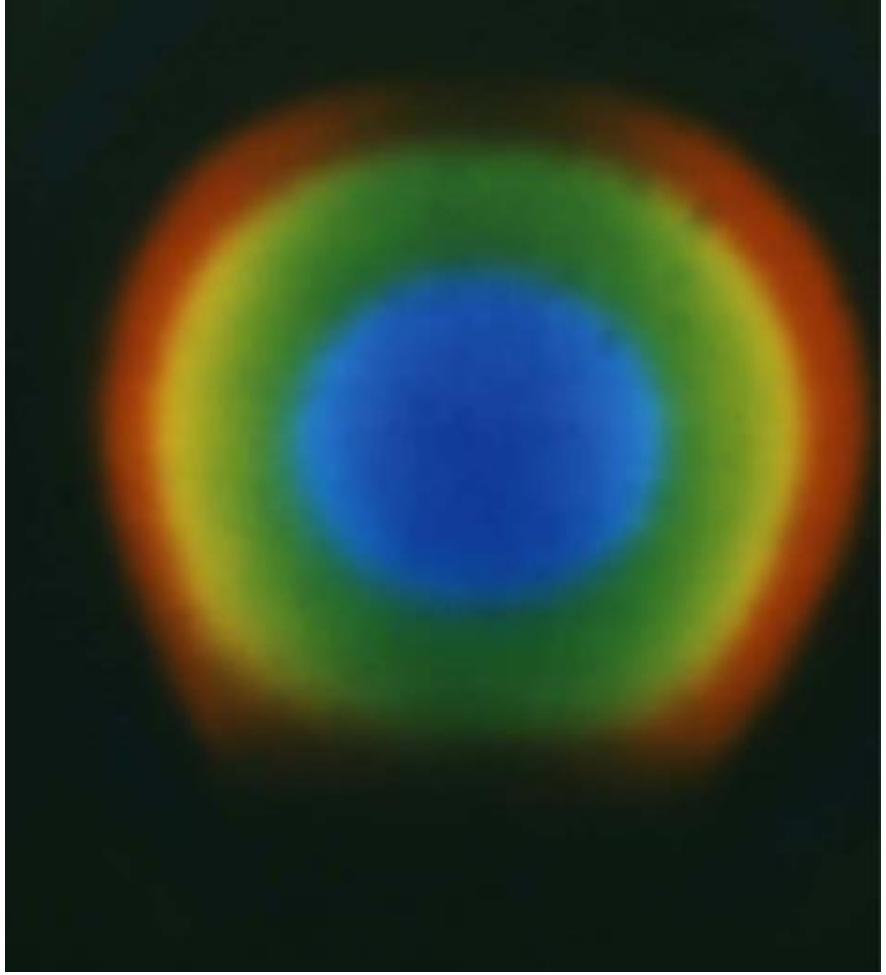


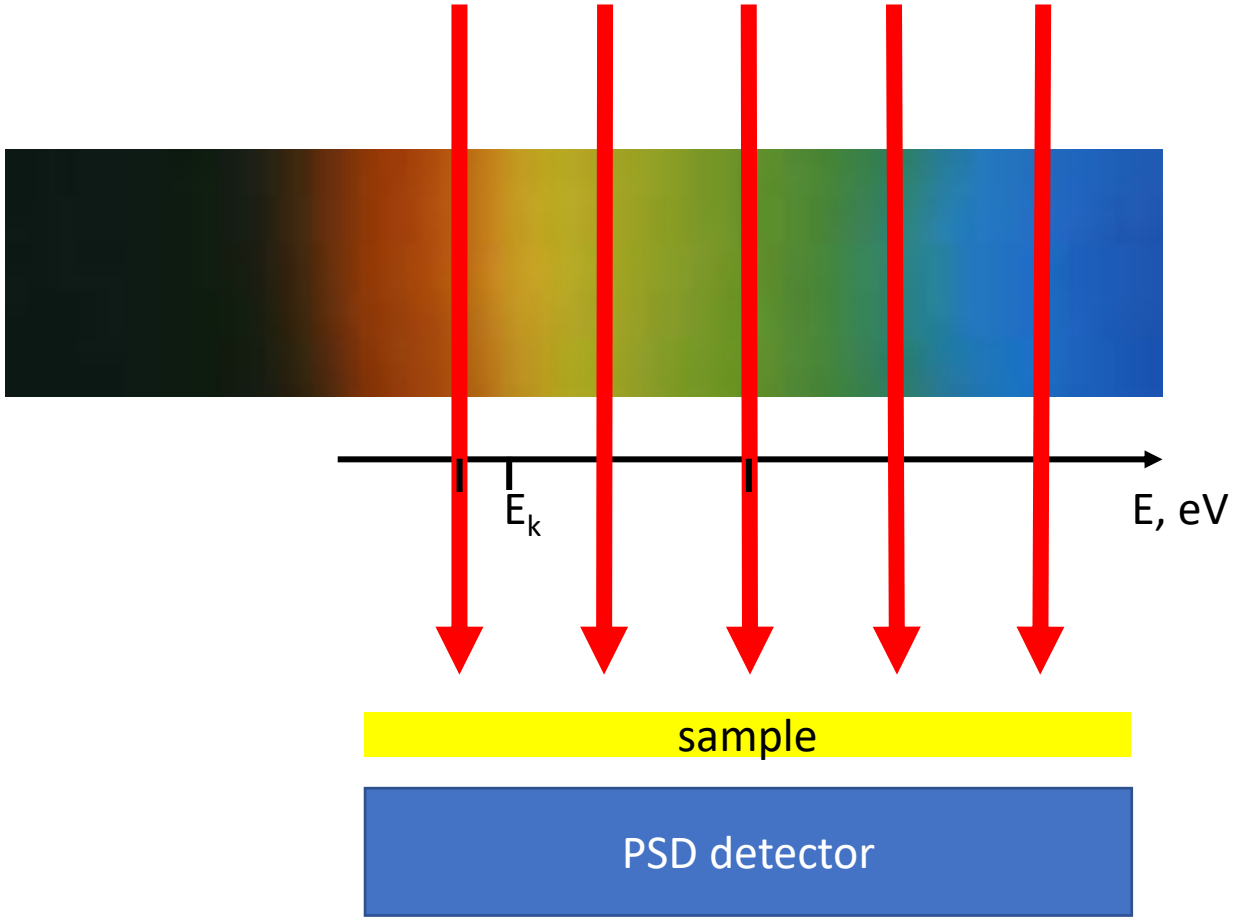
The aim of the work is to develop a method that allows X-ray analysis using a synchrotron radiation wide spectral band (polychromatic radiation) by EXAFS, PXD, SAXS, tomography.
This will make it possible to increase the number of photons in the primary beam by 2-3 orders of magnitude and, accordingly, reduce the time for determining the composition of the sample to nanoseconds.
PXD, SAXS, tomography SAXS is currently experimentally implemented at VEPP-3 / VEPP-4.
In this work, we propose optimizing the undulator parameters for the implementation of the EXAFS and XANES method.

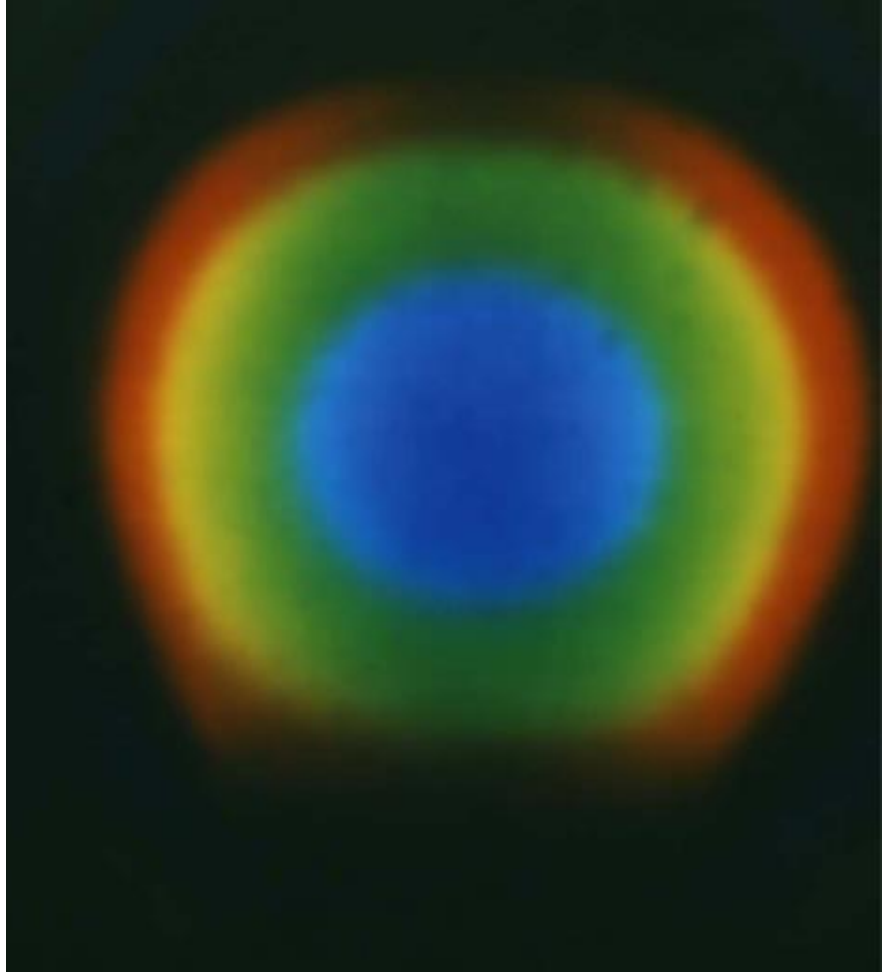
The scheme of SAXS experiment during detonation of explosive trotyl with using a polychromatic synchrotron radiation .

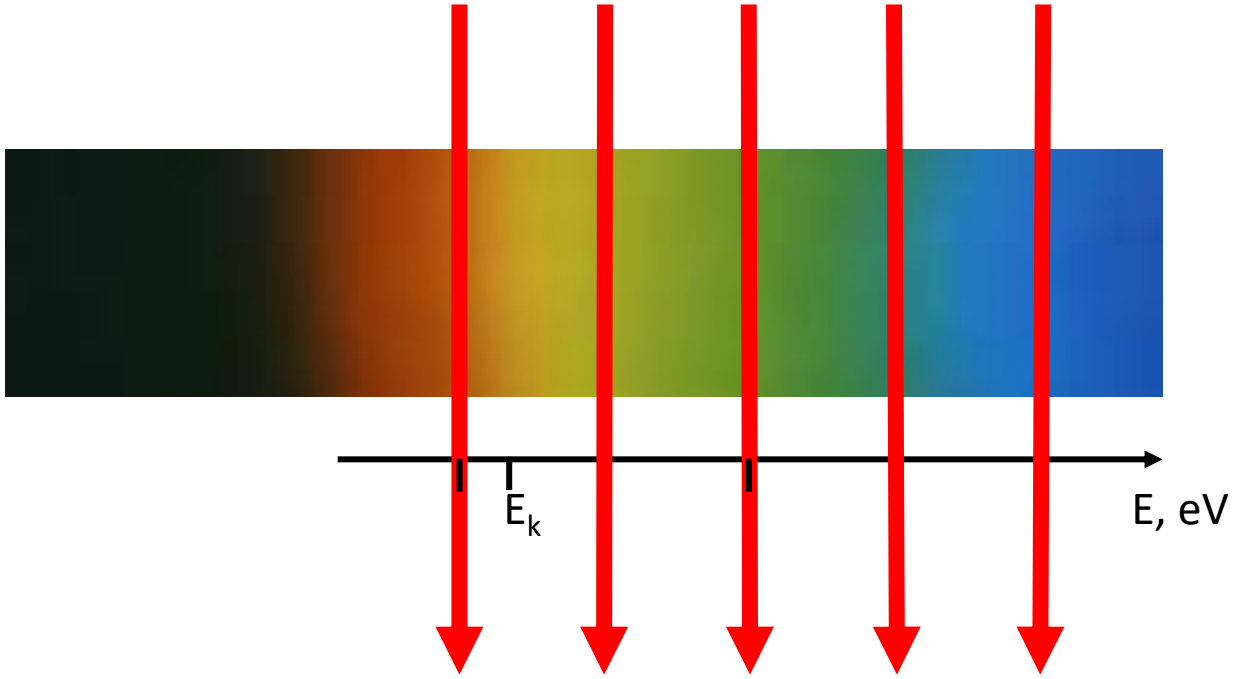


Flash EXAFS



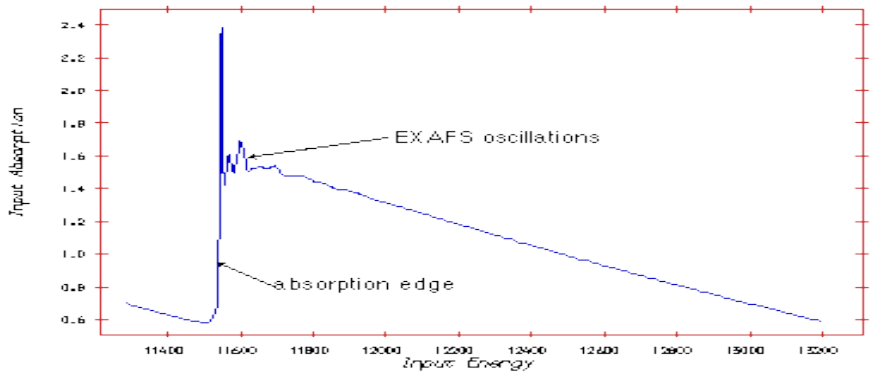

E$_k$
E, eV
sample
PSD detector

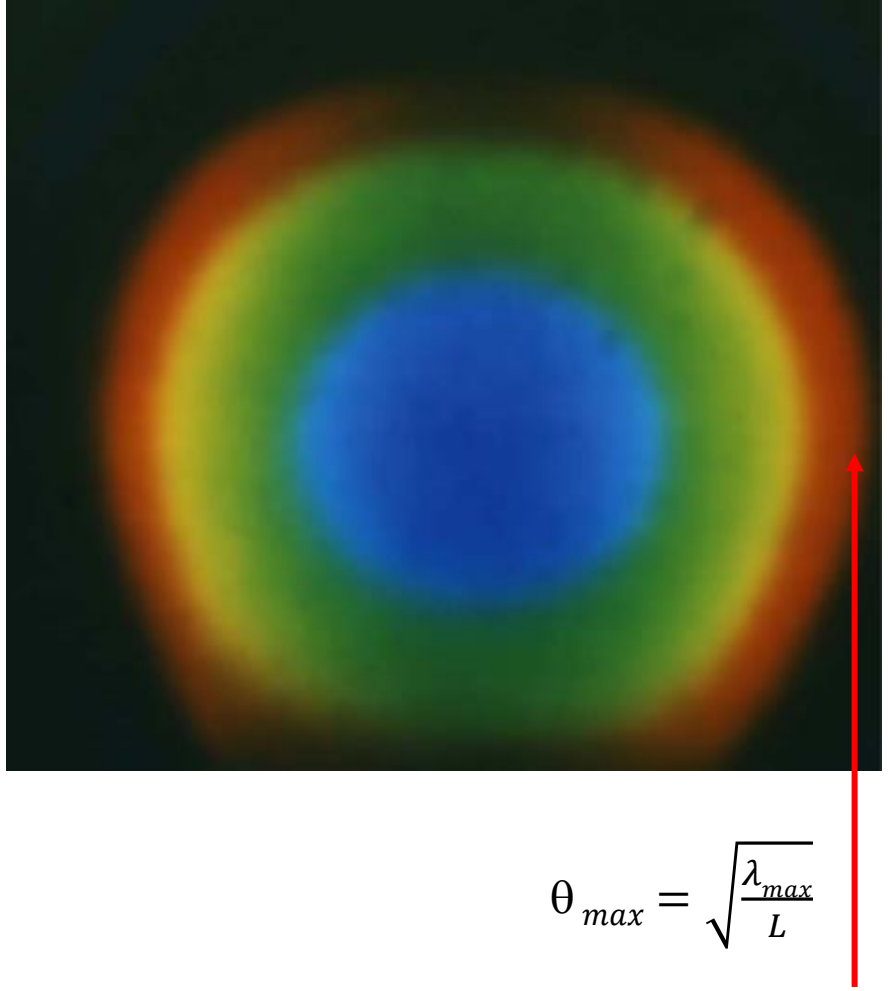




sample

PSD detector

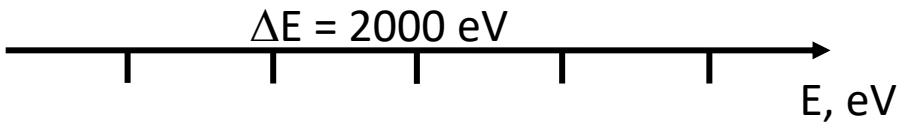




$$\theta_{max} = \sqrt{\frac{\lambda_{max}}{L}}$$

L - undulator length

$$\lambda = \frac{\lambda_u}{n}\left(\frac{1+\frac{K^2}{2}}{2\gamma^2} + \frac{\theta^2}{2}\right),$$



Requirements for spectrum:

$\Delta E = 2000$ eV $\qquad \frac{\Delta E}{E} = 0.001$

Requirements for detector:

2000 detector strips

$\Delta l = 100$ mm (50 mkm strip)

Requirements for undulator:

L - ? λ_u - ? K - ? H - ?

Undulator optimization

Длина волны λ излучения на гармонике с номером *n* ондулятора с периодом λ_u при энергии электронов $\mathrm{E} = \gamma mc^2$ равна

$$\lambda = \frac{\lambda_u}{n}\left(\frac{1+\frac{K^2}{2}}{2\gamma^2} + \frac{\theta^2}{2}\right), \qquad (1)$$

где *K* – параметр ондуляторности, пропорциональный амплитуде поля ондулятора.

The wavelength λ of the radiation at the harmonic with the number n of the undulator with the period λ_u at the electron energy E = γmc^2 is equal to

$$\lambda = \frac{\lambda_u}{n}\left(\frac{1+\frac{K^2}{2}}{2\gamma^2} + \frac{\theta^2}{2}\right),$$

where K is the undulator parameter proportional to the amplitude of the undulator field.

Ширина линии излучения ондулятора длиной $L = N\lambda_u$ равна $\frac{\Delta\omega}{\omega} = \frac{1}{nN} = \frac{\lambda_u}{nL}$. При этом относительный сдвиг частот соседних гармоник равен $\frac{1}{n} = N\frac{\Delta\omega}{\omega}$, т. е. в N раз больше ширины спектра одной гармоники. Находим отсюда нужный номер гармоники $\frac{\lambda_u}{n} = L\frac{\Delta\omega}{\omega}$. Тогда из (1) при $\theta = 0$ следует

$$K = \sqrt{\frac{4\gamma^2\lambda}{L\frac{\Delta\omega}{\omega}} - 2}. \qquad (2)$$

The width of the radiation line of an undulator of length $L = N\lambda_u$ is $\frac{\Delta\omega}{\omega} = \frac{1}{nN} = \frac{\lambda_u}{nL}$.

In this case, the relative frequency shift of neighboring harmonics is $\frac{1}{n} = N\frac{\Delta\omega}{\omega}$, i.e., N times higher than the spectral width of one harmonic (!). From here we find the desired harmonic number $\frac{\lambda_u}{n} = L\frac{\Delta\omega}{\omega}$. Then from (1) for $\theta = 0$ it follows

$$K = \sqrt{\frac{4\gamma^2\lambda}{L\frac{\Delta\omega}{\omega}} - 2}.$$

Минимальная необходимая амплитуда поля ондулятора определяется из условия превышения длиной волны половины критической длины волны синхротронного излучения

$$B > \frac{2\pi mc^2}{3\gamma^2 e\lambda} = \frac{10{,}7\text{кГс}\cdot\text{см}}{3\gamma^2\lambda} = \frac{0{,}0107\text{Тл}\cdot\text{м}}{3\gamma^2\lambda}. \quad (3)$$

Пример

$$\frac{\Delta\omega}{\omega} = 0{,}002, \quad \lambda = 0{,}2\text{нм}, \quad L = 2\text{м}, \quad \gamma = 6000$$

Меньшая ширина спектра невозможна, т. к. энергетический разброс электронов 0,001.

$$B > \frac{0{,}0107\text{Т}\cdot\text{м}}{3\gamma^2\lambda} \approx 0{,}5\text{Т}. \quad (4)$$

$$K \approx 2{,}3. \quad (5)$$

Example:

$$\frac{\Delta\omega}{\omega} = 0{,}002, \quad \lambda = 0{,}2\text{нм}, \quad L = 2\text{м}, \quad \gamma = 6000$$

A smaller spectrum width is impossible, because the energy spread of electrons is 0.001.

$$B > \frac{0{,}0107\text{Т}\cdot\text{м}}{3\gamma^2\lambda} \approx 0{,}5\text{Т}. \qquad (4)$$

$$K \approx 2{,}3. \qquad (5)$$

The undulator must satisfy conditions (4) and (5).

From (4) and (5) it follows:

$$\lambda_u = \frac{K\ 2\pi\ mc^2}{eB} = \frac{K\ 0{,}0107\ \text{Т}\cdot m}{B} < 0{,}05\text{м}. \qquad (6)$$

Choosing $\lambda_u = 0.04$ m we get

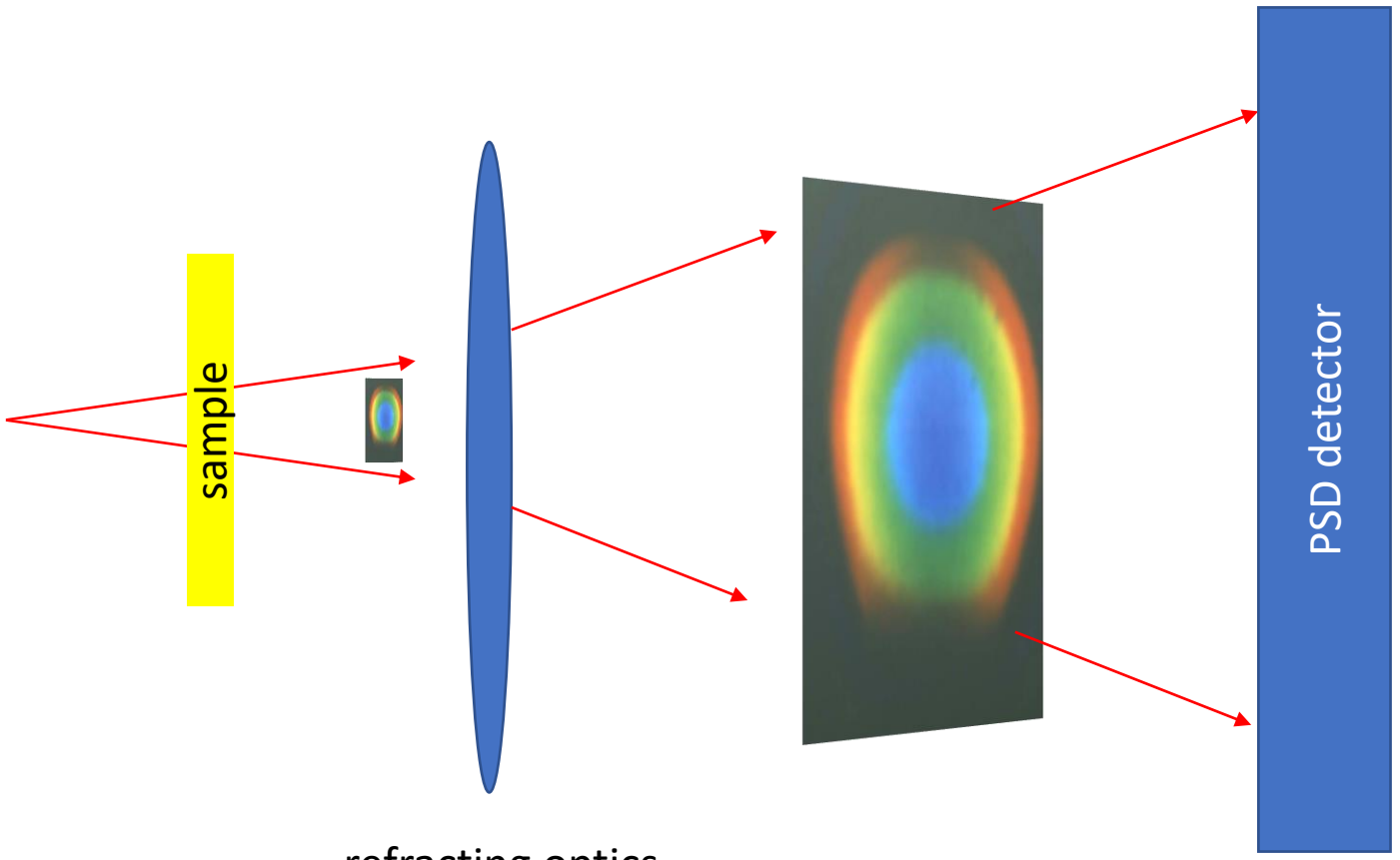
N = 50

$$B = \frac{K2\pi mc^2}{e\lambda_u} = \frac{K0{,}0107\text{Т}\cdot m}{\lambda_u} \approx 0{,}6\text{Т}.$$

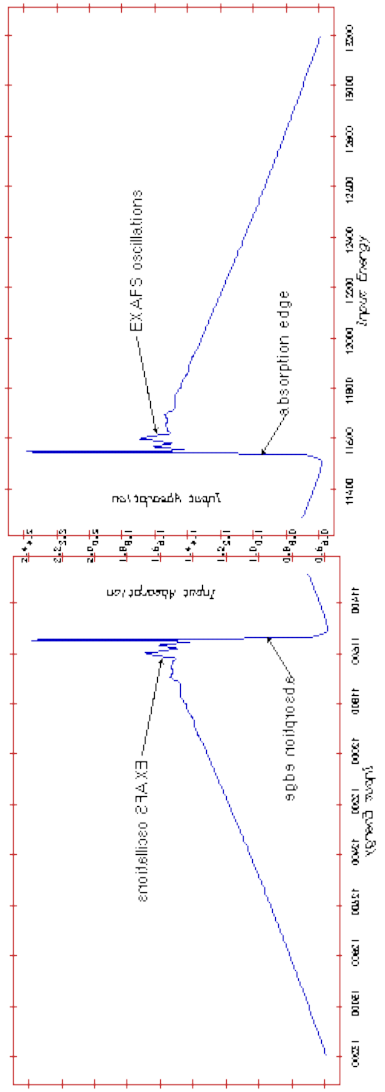
This is a very simple undulator, for example, with permanent magnets.

PSD detector optimization

The refracting optics using for spectrum adaptation for space resolution of PSD detector



refracting optics



Flash powder X-ray diffraction

The aim of the work is to develop a method that allows X-ray phase analysis using a wide synchrotron radiation (SR) spectral band (polychromatic radiation). This will make it possible to increase the number of photons in the primary beam by 2-3 orders of magnitude and, accordingly, reduce the time for determining the composition of the sample to nanoseconds.
The relationship between the angular dependence of the scattering intensity of polychromatic radiation and the angular dependence of the scattering intensity of monochromatic radiation by an object is described by the Fredholm equation of the first kind and is an incorrect task. The solution of this equation in the case of significant experimental errors (which is inevitable in experiments with extremely high time resolution) is quite problematic.
The idea of the method is to form a sharp short-wavelength boundary in the SR spectrum and approximate the X-ray diffraction pattern from the polycrystalline sample by the sum of Gaussian peaks, which allows one to determine the intensities and interplanar distances from polychromatic X-ray diffraction patterns using the procedure of minimization by peak parameters. Computer model experiments showed that in this case, the initial values of the peak parameters to minimize are determined with sufficient accuracy for a successful procedure, and the errors in determining the interplanar distances and their corresponding intensities are equal in order of magnitude to the errors associated with traditional experiments.
The purpose of this work is the experimental implementation of the proposed method, debugging it on test samples and using fast processes to study.
The work is aimed at methodological support of the fundamental task - obtaining previously inaccessible information about the atomic structure of matter during fast processes (explosion, solid-phase reactions). The results obtained will allow us to determine such process parameters as pressure, temperature, density and phase composition in the local region (several microns), as well as the dynamics of their changes in real objects.
To date, obtaining direct structural information about the state of a substance during fast-moving processes and the dynamics of its change has been impossible. This hindered the development of the theory of fast-flowing chemical reactions and processes occurring in matter during the passage of the front of shock and detonation waves. The use of polychromatic synchrotron radiation (SR) opens up new possibilities and will allow to obtain previously inaccessible information on the kinetics of phase formation in explosion products after passing through a detonation wave.
Synchrotron radiation, as a source of x-ray radiation, has a number of unique properties, the main of which are a large flux intensity, which allows the use of a very short exposure time (<1 ns), high periodicity in time (5-250 ns) and a small angular divergence. This compares favorably with SR from ordinary x-rays and allows one to obtain a multi-frame picture of the density distribution in shock waves and in a detonating explosive with good resolution when registering radiation passing through a substance. In addition, the registration of SR rays deflected by a small angle makes it possible to extract information on density fluctuations in the measurement zone, which in carbon-containing explosives can be associated with the synthesis of condensed carbon phases - ultrafine diamonds or low-density graphite-like substances.
This work was supported by RFBR grants # 19-29-12045, # 16-29-01050, # 14-03-00770 and Ministry of Science and Education of Russia grant # AAAA-A17-117030310280-6.

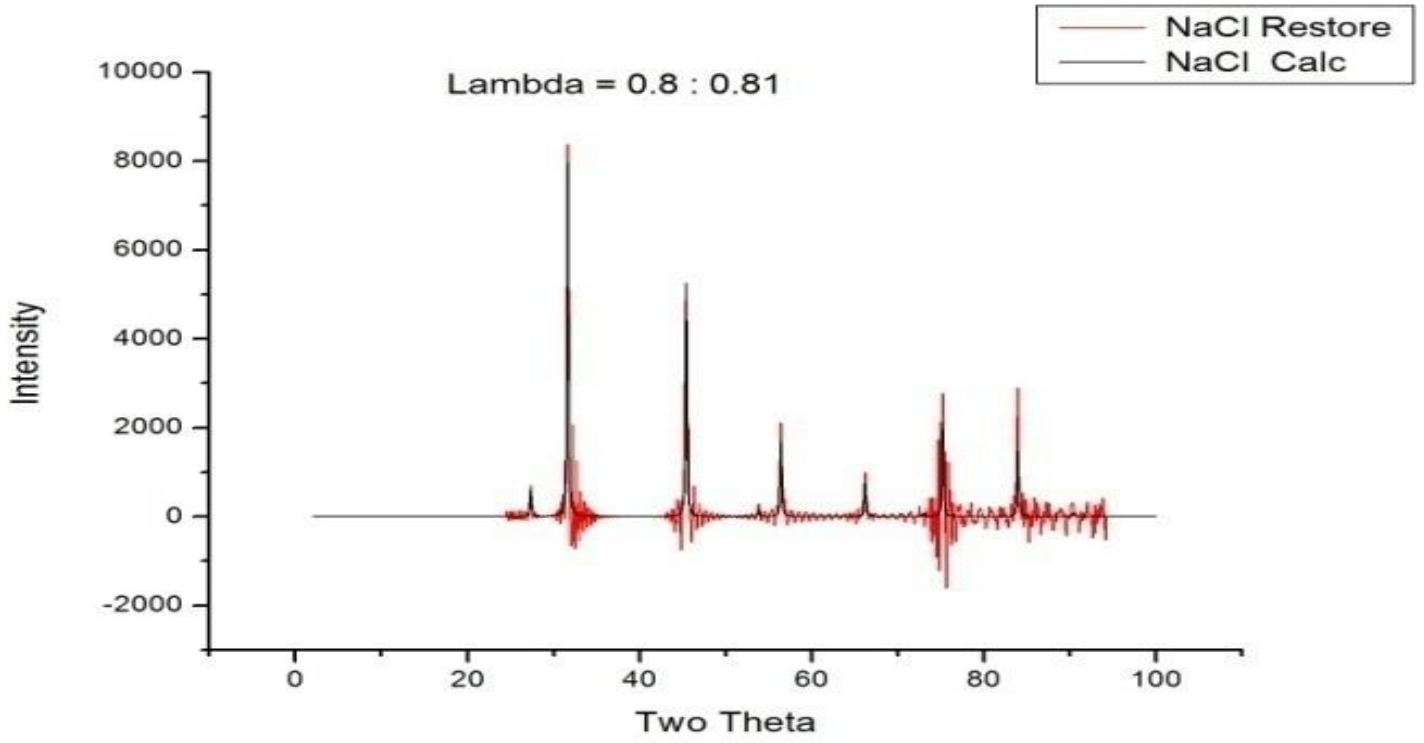
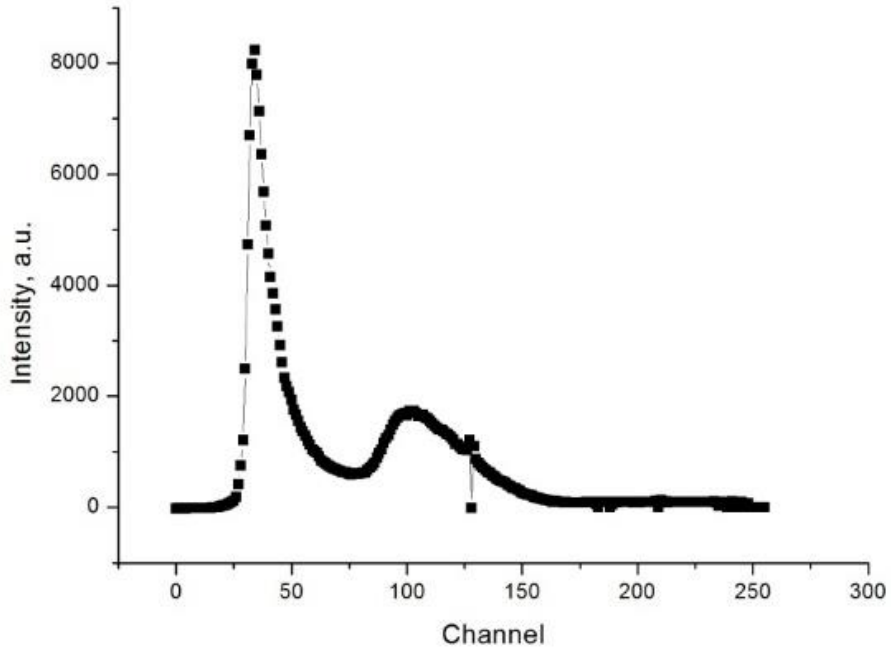


Рисунок -1. Компьютерное моделирование восстановления рентгенограммы NaCl. Из расчетной дифрактограммы, полученной с использованием полихроматического спектра была восстановлена дифрактограмма, получаемая при использования узкой спектральной полосы 0.8-0.81 А.

Picture 1. Computer simulation of the restoration of the x-ray NaCl. From the calculated diffractogram obtained using the polychromatic spectrum, the diffraction pattern obtained using a narrow spectral band of 0.8-0.81 A was reconstructed.



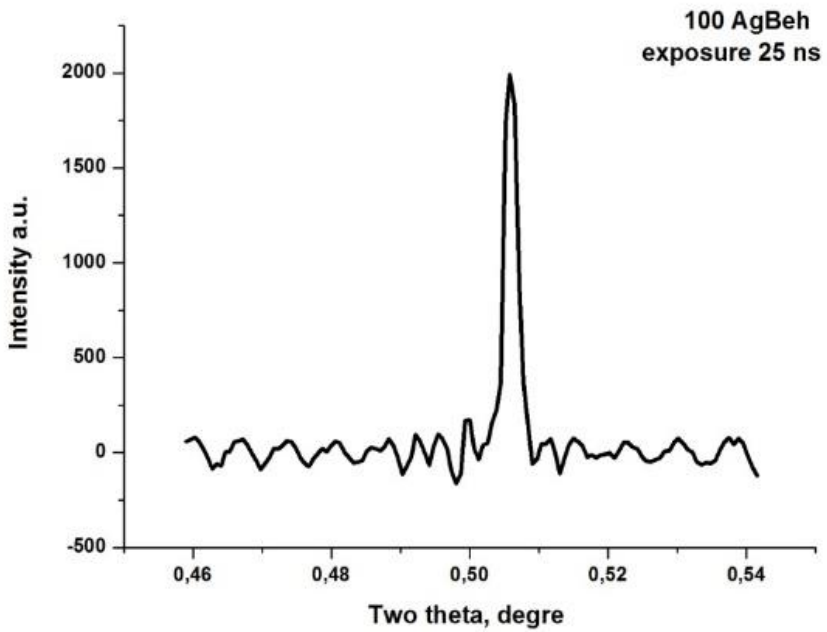


Рисунок -2. Экспериментальная кривая дифракции от бегената серебра, полученная при экспозиции 25 нс

Figure-2. Experimental diffraction curve from silver behenate obtained at an exposure time of 25 ns.

Рисунок -3. Восстановленная кривая дифракции от бегената серебра, полученная при экспозиции 25 нс.

Figure-3. The reconstructed diffraction curve from silver behenate obtained at an exposure of 25 ns.

Thank you