Experimental implementation of X-ray powder diffraction by polychromatic synchrotron radiation in the range of 20-30 keV

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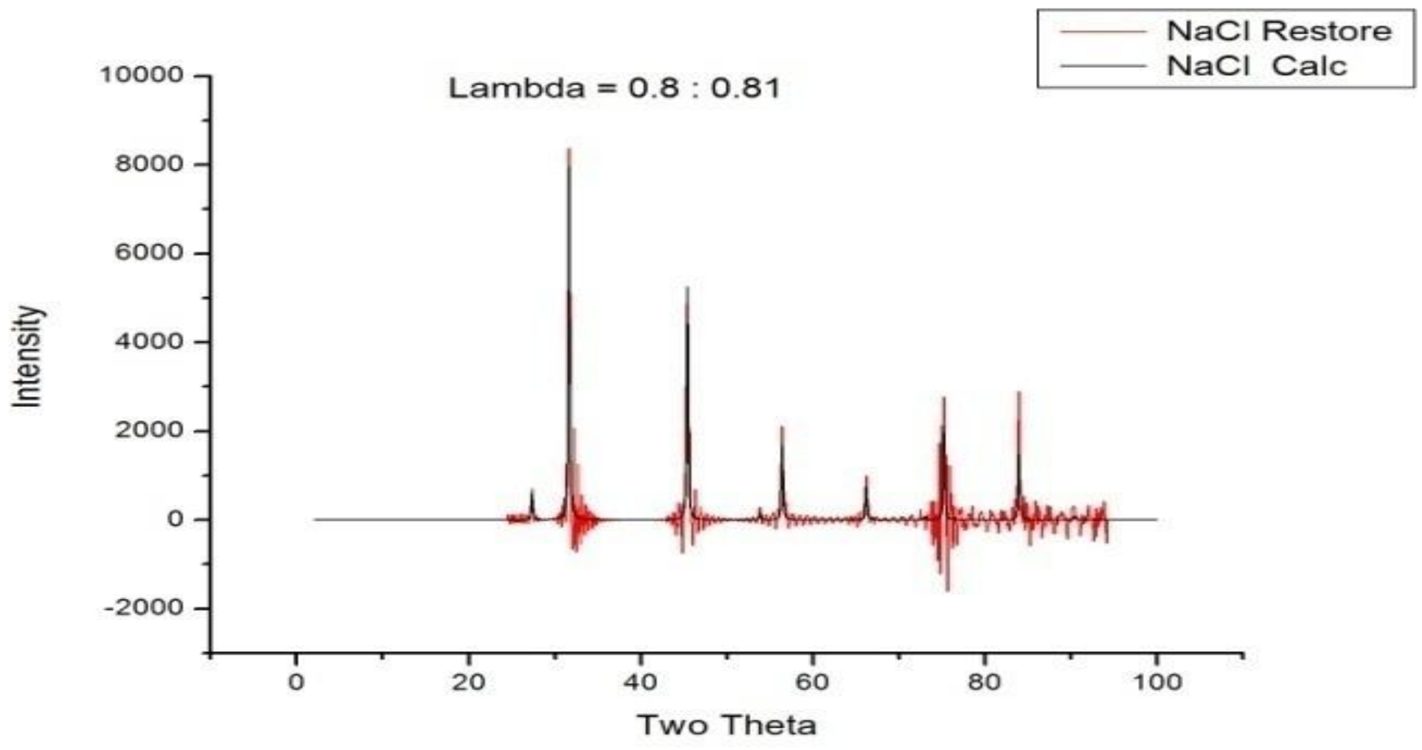
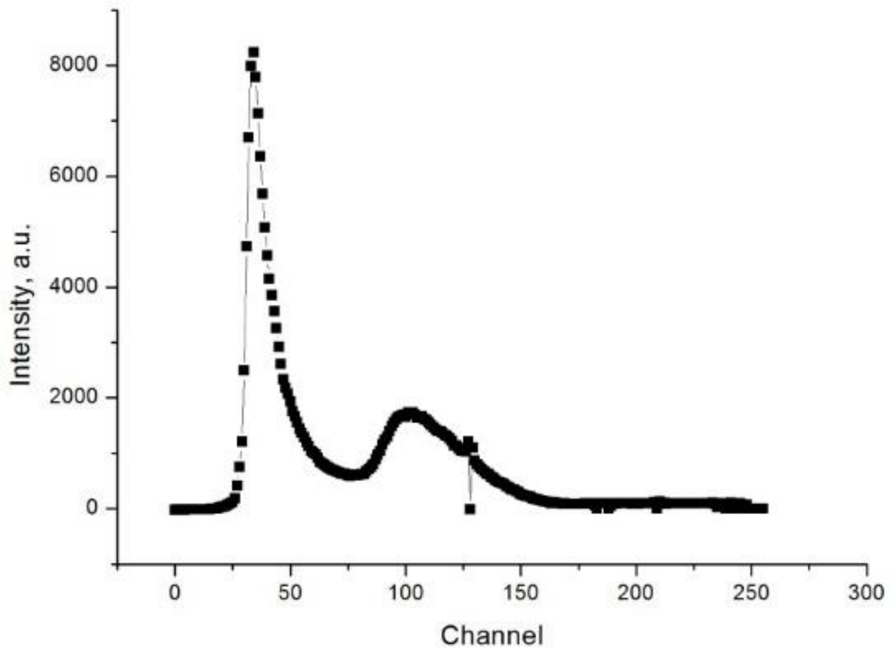


Рисунок -1. Компьютерное моделирование восстановления рентгенограммы NaCl. Из расчетной дифрактограммы, полученной с использованием полихроматического спектра была восстановлена дифрактограмма, получаемая при использования узкой спектральной полосы 0.8-0.81 А.

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.



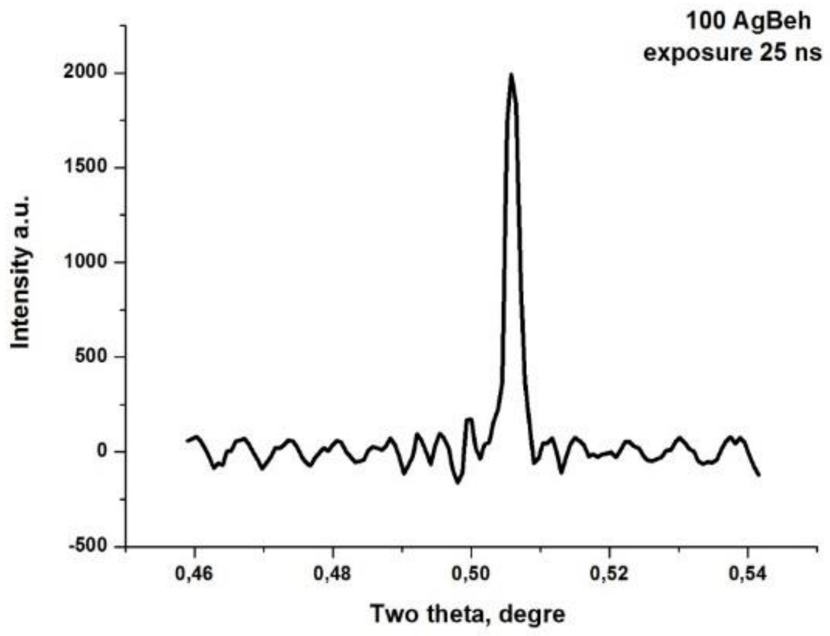


Рисунок -2. Экспериментальная кривая дифракции от бегената серебра, полученная при экспозиции 25 нс

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.

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.
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