

diameter (2048<sup>2</sup> pixels in 2x2 binning) has been installed in February 2005 to replace an older CCD-system which was in operation since 1996. To increase the quantum efficiency for energies between 20 and 30 keV the detectors are fitted with 100  $\mu\text{m}$  Gd<sub>2</sub>O<sub>2</sub>S<sub>2</sub>:Tb phosphor instead of a standard 40  $\mu\text{m}$  phosphor.

A previously developed software suite [1] for the reconstruction of diffuse scattering from CCD raw data has been adopted to the new data format and successfully applied in a composition- and temperature-dependent study of precursor-induced diffuse scattering in V-diluted lead-phosphates. Compared to pure lead-orthophosphate, the system Pb<sub>3</sub>(P<sub>x</sub>V<sub>1-x</sub>O<sub>4</sub>)<sub>2</sub> displays a complex sequence of phase transitions. The CCD-data show an overall rhombohedral symmetry (R-3m) of the paraelastic high-temperature phase, but broad diffuse intensities are clearly visible even 40 K above T<sub>c</sub>. These maxima are centered around symmetry-allowed Bragg-reflections of the paraelastic HT-phase and must be indexed by half integers. The diffuse scattering shows a slight anisotropic spatial distribution in reciprocal space with an elongation along a\*, indicating a higher degree of disorder along [111]<sub>h</sub>. This effect results from small (ca. 50 Å), dynamic precursor-clusters of the monoclinic ferroelastic LT-phase in an overall paraelastic matrix.

[1] Paulmann C., et al., *Nucl. Instr. Phys. Res. A*, 2001, **467**, 1293.

**Keywords:** CCD detectors, synchrotron X-rays, diffuse scattering

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#### Efficiency of Light Atoms on the Low Energy SAD Phasing

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Recent advancements in the X-ray data-acquisition techniques and phasing algorithms have enabled structure determination using weak anomalous signals from light elements such as sulfur that are naturally present in most proteins. This is rapidly becoming a useful technique for high-throughput protein crystallography because it does not require preparation of heavy atom derivatives. Photon Factory is building a new insertion device beamline BL-17 with emphasis on diffraction experiments with microcrystals and low X-ray energy phasing (around 6 keV) [1]. To establish a standard experimental protocol of the low energy SAD, we carried out diffraction experiments on two lectins [2] and a small GTPase with low energy X-ray beams. In the case of the lectins, it was found that the number of potassium ions in the crystal is critical for the phasing. The crystal structure containing two potassium ions were solved successfully, but crystals with only one potassium ion were not. In the case of the small GTPase, phasing was successful despite the fact that it contains fewer sulfur atoms than the proteins whose structures have been solved by the low energy SAD so far. This is because the phosphates of GDP and the calcium ion bound to the GDP contributed significantly to the anomalous signal. This suggests that the low energy SAD is a successful method especially for nucleotide binding proteins.

[1] Igarashi N., et al., *IUCr2005*, Florence. [2] Satoh T., et al., *IUCr2005*, Florence.

**Keywords:** synchrotron radiation crystallography, low energy SAD phasing, macromolecular crystallography

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#### Testing the Compact Light Source: A Miniature Synchrotron for the Home Lab

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During the past 30 years, synchrotron light sources have become the x-ray probe of choice for physicists, chemists, biologists and research physicians. With their high-quality, intense x-ray beams, these national research facilities have spawned a large number of new

techniques and technologies spanning a broad array of applications. Perhaps the most dramatic examples of this impact come from the detailed 3-dimensional studies of protein structure using powerful crystallographic techniques such as multiple-wavelength anomalous dispersion (MAD). Recent research at Stanford University and Lyncean Technologies, Inc. has led to a new x-ray source, the Compact Light Source (CLS), which will significantly broaden this impact. The CLS is a tunable, homelab x-ray source with up to three beamlines that can be used like the x-ray beamlines at the synchrotrons--but it is about 200 times smaller than a synchrotron light source. The compact size is achieved by using a laser undulator and a miniature storage ring. The photon flux on a sample will be comparable to the flux of highly productive synchrotron beamlines. In this presentation I will introduce the Compact Light Source and show how it will bring the quality, tunability and flux of a synchrotron beam line into an x-ray scientist's local laboratory. At Lyncean Technologies, Inc. we are constructing a prototype of this source with SBIR funding from the NIGMS Protein Structure Initiative. I will report on our recent experiments and long-term outlook for the CLS.

**Keywords:** synchrotron, X-ray source, protein structure

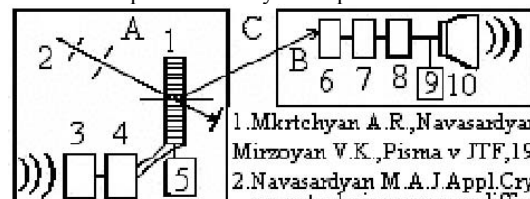
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#### On Forced Reflection and Transmission of Speech, Using X-rays

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Under external influences (temperature gradient, US oscillations and so on) the intensity of the diffracted x-ray beams can be greatly increased (up to ten times or more) and at the same time the transmitted beam can be entirely reflected in the direction of diffraction (in the Laue case). This phenomenon was named by the authors of co called "controllable complete reflection" or "forced reflection" [1,2]. Three settings of the double-crystal spectrometer will be presented for this case. In the case of controllable variation of diffracted x-ray beams, it can be obtained quick increase of the intensity of diffracted x-ray beam using modulated US oscillations. This way it becomes possible to transmit and receive audio information in particular speech by means of an x-ray beam. A scheme for a practical device for transmission and reception of audio information by x-ray beams is presented in Fig. The device operates in the following manner. Single crystal modulator 1 using x-ray beam 2 and goniometer 5 is setup in the Bragg condition for one of reflecting atomic planes of sample. Modulated electromagnetic oscillations from generators 3 and 4 are sent to the crystal modulator on which modulated x-ray beams "C" is excited. We can obtain a beam with changeable counting rate of electrical impulses in detector 6, which becomes electric vibrations (speech) after passing through integrating circuit 7 and amplifier 8. This oscillations can be seen on the screen of oscilloscope 9 or hear by loud speaker 10.



1. Mkrtchyan A.R., Navasardyan M.A.

Mirzoyan V.K., Pisma v JTF, 1982, 8.477

2. Navasardyan M.A. *J Appl. Cryst.* 2001, 34, 763

x-ray techniques, x-ray diffraction

**Keywords:** X-ray techniques, X-ray diffraction, charge densities

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#### High Brilliance X-ray Laboratory System for Microdiffraction Studies

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An X-ray laboratory system is described optimized for diffraction studies of protein crystals and crystals under high pressure. The system is also suitable for phase contrast analysis, small-angle scattering and other investigations.

The system is based on a micro-focus X-ray source of 50W