

temperatures is thought to be from photoelectrons ejected from atoms following the absorption of X-rays. As the photoelectrons traverse the crystal, they lose energy through interactions with atoms in their path resulting in damage. If the X-ray beam is polarized, the photoelectrons are ejected preferentially along the polarization vector. Monte-Carlo simulations [Nave, C., and Hill, M. A. (2005). *J Syn. Rad.* 12, 299-303] suggest that, when the beam size is only a few microns, most photoelectrons escape the illuminated volume. This leads to the peculiar conclusion that the radiation damage due to photoelectrons may be significantly lower within the illuminated volume than in the volume immediately surrounding the irradiated spot. A second prediction of the calculations is that most of the photoelectron's energy is abruptly dissipated within the last few microns of its trajectory. Recently, a long focal length Fresnel zone plate was used to provide a focused beam of ~1-micron cross section at the sample position, and high quality diffraction data was obtained from protein crystals. The 15.1 keV, 1-micron beam was used to probe the geometrical distribution and extent of radiation damage in protein crystals. These data confirm that radiation damage is greater along the polarization vector than in the perpendicular direction, radiation damage is maximal 3-4 microns from the center of the beam, and radiation damage does not extend beyond 6 microns.

Keywords: radiation damage, microcrystals, microcrystallography

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Towards protein structure determination using two-dimensional crystals and powders

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Reliable determination of the structure of integral cell membrane proteins (IMPs) is one of the most important problems in biology today. The structure of the vast majority of IMPs remains unsolved however, mainly due to difficulties associated with conventional crystallisation and the concomitant need for preservation of the active form of the protein as it is taken out of its natural environment within the cell membrane. In order to address these problems, we consider the possibility of using two-dimensional (2D) ordered micro-arrays of proteins, i.e., 2D crystals, in X-ray diffraction (XRD) experiments, instead of conventional three-dimensional crystals. In this work, we discuss the potentials and limitations of using 2D protein crystals for XRD based structure determination. We present a systematic approach to data analysis and fitting based on physical description of X-ray scattering by 2D crystals. Scattering by large assemblies of 2D crystals with random preferential orientations is also considered as a model for XRD with 2D crystal powders. We illustrate how 2D crystal powder diffraction data may be used to reconstruct a 2D projection map of the electron density in the unit cell with reference to preliminary results obtained for 2D crystals of bacteriorhodopsin.

Keywords: membrane proteins, two-dimensional protein crystals, X-ray diffraction

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8C2 high resolution powder diffraction beamline at Pohang Light Source and its recent results

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We introduce 8C2 high resolution powder diffraction (HRPD) beamline at Pohang Light Source. This beamline is designed for a powder crystallography, i.e., very high angular resolution and various sample environments. The technical characteristics of the beamline and some performance indicators are listed, such as the incoming photon flux and the angular/energy resolutions obtainable under typical experimental conditions. We present several recent results using synchrotron x-ray powder diffraction data collected from this beamline, not detected by previous powder diffraction experiments.

Keywords: powder crystallography, powder diffraction, synchrotron X-rays

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Accurate powder diffraction standards: Determination of the lattice parameter of LaB₆ SRM(660)

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We use X-ray powder diffraction and synchrotron radiation to determine the lattice parameter of the NIST standard reference material (SRM 660) LaB₆ to be 4.157580 Å with an accuracy of 12 parts per million (ppm), calibrated relative to the lattice parameter of the Si powder standard ($a_0 = 5.430940(11)$ Å, Si 640b). A discrepancy is observed between the currently accepted lattice spacing of LaB₆ and the measured value, of 0.00048(5) Å, or nine standard deviations from the NIST reference. Twelve different measurements of the lattice parameter are made at beam energies between 10 keV and 20 keV. The observed discrepancy in the lattice parameter is consistent for the different energies used. The absolute values of the mean difference between the measured and calculated 2 theta centroids, are highly consistent, between 0.00020 and 0.00040 for energies from 5 keV to 14 keV, and between 0.00050 and 0.00080 for energies from 15 keV to 20 keV. In order to determine the peak positions with high precision, account must be taken of observed peak asymmetry. Significant asymmetry is due to peak broadening and must be taken into account in order to determine accurate peak locations and lattice spacings. Our approach shows significant advantages over conventional analysis. Our analysis of peak broadening is compared with models used in Rietveld analysis.

Keywords: lattice parameters, powder and single crystal diffraction, synchrotron radiation experimental

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A halogen lamp furnace to synthesize nanoparticles: *In situ* X-ray absorption spectroscopy

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