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Application of a pnCCD in protein crystallography

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The fast and precise determination of crystal structures using the Laue diffraction method requires a simultaneously position- and energy-resolved detection of photons. By means of a back side illuminated pnCCD with frame-store operation [1] the spatial distribution of Laue spots as well as their energies can be measured at the same time. The sensitive volume consists of a fully sideward depleted n-Si layer of 450µm thickness subdivided into 256x256 pixels of 75µmx75µm size with a typical readout frequency of about 120Hz. The system has found applications for soft and hard X-rays [2,3].
Using white synchrotron radiation the pnCCD delivers a three-dimensional intensity distribution spanned by two pixel directions and an energy direction covering a 3D data volume in reciprocal space which is expanded to 4D in case of dynamic measurements. In this sense the system provides a good possibility to investigate unknown crystal structures in arbitrary orientations in space as well as structural phase transitions at fixed scattering geometry. Previously it was shown that the crystallographic unit cell of a tetragonal LiAlO2 crystal can be determined from the three-dimensional pnCCD data sets without any a priori information about the sample [4]. Consequently the energy-dispersive Laue diffraction is a powerful technique for single shot structure analyses in protein crystallography. In the subsequent application the potential of the pnCCD is exploited to investigate small organic crystals exhibiting complex structures and weak scattering signals. As a test example the energy-resolved Laue pattern of a hen egg white lysozyme single crystal is considered in transmission geometry and used for structure determination. In such kind of experiments the detector system is operated in a combined energy-dispersive single photon counting and integration mode.
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