Poster Presentation

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Ultra-high resolution charge density studies in the home lab

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Data acquisition for the analysis of the core-electron density distribution of light element containing crystals as well as highly absorbing crystals containing very heavy elements have been almost exclusively carried out at synchrotron facilities in the past. Hybrid Photon Counting (HPC) detectors have the potential to move such data acquisition from the synchrotron to the home lab thanks to various advantages over other currently available X-ray detector technologies. The absence of readout noise and detector dark signal ensure high data quality irrespective of exposure time or number of acquired frames. Direct detection of hard X-rays in CdTe-sensors provides high quantum efficiency and a small, sharp point-spread function. This renders the typically required oblique angle correction obsolete. The high dynamic range of a digital counter allows the collection of low- and high-resolution data simultaneously, reducing potential errors introduced in scaling procedures.

We will present results acquired using a PILATUS3 R CdTe 300K detector and an Ag-microfocus source with α-boron and CeB6 reference crystals. Both crystals yielded datasets of ultra-high quality up to resolutions of 0.3 Å with excellent statistics and quality indicators such as Rint, Rsigma, and Rmerge as well as crystallographic R-values and residual electron densities. These outstanding datasets have the potential to allow the analysis of the core electron density distribution of light element crystals as well as the charge density refinement of very heavy element crystals in the home lab.
Keywords: core-electron density distribution, charge density refinement, X-ray detectors