MS28-O2 XPAD, an hybrid pixel detector for charge density study on laboratory diffractometers

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The new generation of X-ray detectors, the hybrid pixel area detectors or 'pixel detectors', are based on direct detection and single-photon counting processes. Large linearity range, high dynamic and extremely low noise leading to unprecedented high signal-to-noise ratio, fast readout time (high frame rates) and electronic shutter are among their intrinsic characteristics which render them very attractive. First used on synchrotron beam lines, we will show that these detectors are also promising at laboratory sources, in particular for pump-probe or quasi-static experiments [1] and accurate electron density measurements [2]. An original laboratory diffractometer made from a Nonius Mach3 goniometer equipped with an Incoatec Mo micro source and an XPAD pixel area detector has been developed at the CRM2 laboratory. This diffractometer will be presented in the first part of the talk and the second part will be devoted to the first charge density analysis using an XPAD detector : Mo Ka accurate charge density quality data up to 1.21 $Å^{-1}$ resolution have been collected on a sodium nitroprusside crystal using this prototype diffractometer. The multipolar electron density obtained will be compared to already published data (Pressprich et al., 1994, Nelyubina et al., 2008) In the third part of the talk, we will compare the measurements made with three different diffractometers (XPAD, Agilent Atlas CCD and PHOTON100 CMOS) on the same crystal of a relatively weakly scattering pure organic compound, 4-benzyloxy-3-methoxybenzaldehyde ($C_{15}H_{14}O_3$) to 0.96 $Å^{-1}$ resolution. The three charge density models obtained after multipolar refinements with identical strategies will be compared with unbiased criterions, like residual electron density maps and agreements factors.

[1] Diffraction studies under in-situ electric field using a 2D hybrid pixel XPAD detector : P. Fertey, P. Allé, E. Wenger, B. Dinkespiler, S. Hustache, K. Medjoubi, F. Picca, C. Lecomte and C. Mazzoli, *Journal of Applied Crystallography*, **46**, 1151-1161, 2013.

[2] XPAD X-ray hybrid pixel detector for charge density quality diffracted intensities on a laboratory equipment : E. Wenger, S. Dahaoui, P. Allé, P. Parois, C. Palin, C. Lecomte and D. Schaniel, Acta Crystallographica B, 70, 5, 783-791, 2014.

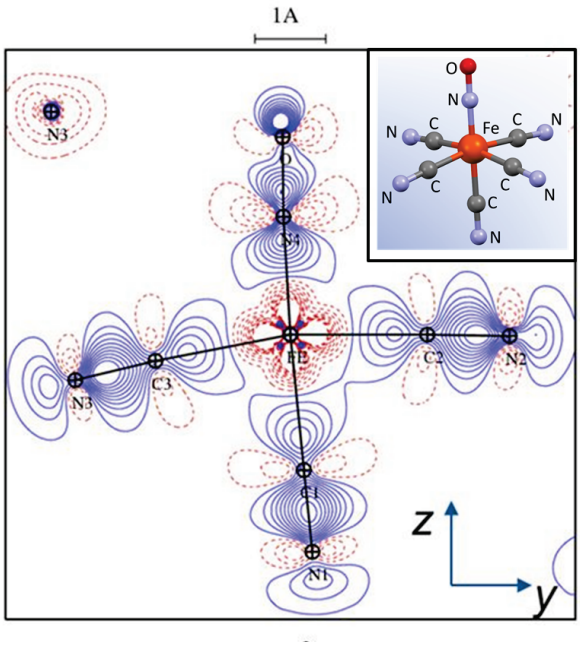

Figure 1. Deformation electron density after spherical atoms refinement in SNP and iron coordination polyhedron.

Keywords: Hybrid pixels detector, CCD X-ray detectors, CMOS X-ray detectors, charge density study, accurate X-ray diffraction data.