Poster Presentation

Why go to synchrotrons? charge-density experiments at home!

Tobias Stuerzer¹, Holger Ott¹, Jens Lübben², Birger Dittrich² ¹Bruker AXS GmbH, Karlsruhe, Germany, ²Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany E-mail: tobias.stuerzer@bruker.com

Modern laboratory instruments with high performance X-ray sources and sensitive detectors facilitate in-house charge density experiments, making synchrotron trips unnecessary in many cases.

The improvements in microfocus sealed tube technology significantly increase primary beam intensities, boosting diffraction from charge density samples at high resolution, while maintaining outstanding tube lifetimes (I μ S), minimizing the cost of ownership. The higher energy X-rays of the Ag source improve the reachable resolution of the experiment and strongly reduce absorption, extinction, and scattered X-ray background. With the In source (METALJET), these benefits can be enhanced even further.

On the detector side, the latest generation of CPADs (charge-integrating pixel array detector) have proven to outperform classical CCDs and image plates both in background noise and read-out times. Their thin and extremely efficient high Z-element scintillators, overcome shortcoming of Si-sensor based HPADs (hybrid pixel array detectors). The non-linearity at high count rates, charge sharing noise, read-out deadtime, and parallax effects of thick sensors hamper charge-density data quality.

At synchrotrons, there are additional considerations, such as beam instability, variable experimental setups that have not been optimized for this special application (alignment, available degrees of freedom), and above all a work environment that is unfamiliar, even for a regular synchrotron user (control and data processing software, detectors, goniometer, sample mounting, etc.). Furthermore, the available flux often reduces the experiment times to a critical minimum, for which data quality is sacrificed.

Even with modern home laboratory sources, a charge density data collection will still take several hours to a couple of days. However, this time investment pays off in terms of data quality, especially when you can work in your own lab under optimized conditions without additional time/success pressure, and with no wait for access.

This presentation will highlight charge density results from modern home lab systems and compares them to state-of-theart synchrotrons.



Keywords: Charge density, CAPD, In-house instruments