Poster Presentation

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Smart Sensitivity Control with Agilent's New Range of S2 CCD Detectors

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With the recent improvements in the brightness of laboratory X-ray sources, high-quality data can be collected from a wider range of crystal samples on in-house diffractometers. To cope with the resulting increase in workload it is important to be able to collect highest-quality data as quickly and efficiently as possible. Agilent Technologies develop and supply X-ray systems for small-molecule and macromolecular crystallography, which include SuperNova line of diffractometers utilizing the latest generation sealed-tube micro-focus X-ray sources, as well as the new range of Atlas S2, Eos S2 and Titan S2 CCD detectors. Technological improvements allow us to make use of the high brilliance of the sources and the large dynamic range and low signal-to-noise of the new detectors to shift the boundaries of what crystal samples can be successfully measured in the home laboratory. The new S2 detectors incorporate an Intelligent Measurement System, where the exposure time, binning mode, and gain settings are automatically or manually set for each sample. High binning and gain modes are chosen to boost signal detectivity for weakly-diffracting data, whereas low binning and gain modes are selected to increase the dynamic range for well-diffracting samples. This flexibility makes it very easy to collect high-quality datasets for a very large range of samples. In conjunction, our innovative, user-friendly CrysAlisPro software is constantly being updated to make use of all new hardware improvements, as well as making it as easy as possible for the user to effectively screen their samples, gather enough preliminary information quickly, and run the experiments in the most effective way. Key aspects of the detectors, including the notions of absolute detectivity, processing overheads, readout speed, minimizing systematic errors and optimizing data collection protocols will be discussed. To illustrate the benefits of the newly developed technology, a number of protein and small-molecule data collection experiments will be presented and different modes of detector operation compared.

Keywords: Detector technology, In-house data collection, Instrumentation