

**Figure 1.** Diagrams to represent data completeness in reciprocal space. The plot on the left is a traditional completeness in resolution shells. The plot on the right provides angular (spherica-polar) completeness on the same data

**Keywords:** data completeness, reciprocal space representation, multiple crystals, BLEND

## MS45-P3 Advances in Data Quality in Area Detector Diffraction Experiments.

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Achieving good, reliable data for structure research and subsequent publication is the end goal for most users of single crystal diffraction equipment. It is important that all factors affecting data quality of are taken in to consideration and to understand how best to control them.

The following elements of the diffraction experiment will be discussed:

a) The hardware, which revolves around notions of absolute detectivity, overhead, readout speed, minimizing systematic errors and diffractometer access. Advances in area detector technology and data collection approaches will be presented. Rigaku Oxford Diffraction's new generation of HPC detectors will be described. The CCD camera generation S2 with 'Smart Sensitivity Control' will be put in context of existing CCD detectors.

b) Selecting the sample, method of mounting and protection environment is controlled mainly by the user. This presentation offers suggestions on how to select your sample whilst being conscious of the fixed characteristics of your diffractometer.

c) The experimental procedure comprises the choice of wavelength, the geometric strategy, the mode of scan and detector operation and the decision on absolute detectivity vs. redundancy. Rigaku Oxford Diffraction's CrysAlisPro software implements the fifth generation of strategy software with new features for data quality: The 'Intelligent Measurement System' optimizes experiment conditions for CCD and HPC systems.

d) The data reduction software which should be optimized at extracting consistent area detector data not only under good conditions, but also under real life flaws of the practical experimental procedure e.g. twinned samples. A new data reduction approach for twins, is highlighted, and can significantly improves the data quality of small molecule and protein twins.

**Keywords:** Area detector, data quality, single crystal diffraction