MS45 Measuring data quality

Chairs: Phil Evans, Alexandre Urzhumtsev

MS45-P1 Current Status of Microfocus X-ray Sources for Chemical and Biological Crystallography

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Modern microfocus X-ray sources define the state-of-the-art for most applications in X-ray diffraction. These sources are usually combined with multilayer X-ray mirrors which are excellent X-ray optical devices for beam shaping and preserving the brightness of the source.

Microfocus rotating anode generators and liquid metal jet systems deliver flux densities in the range of 10^{11} photons/s/mm^2. However, these sources are expensive and need regular and sometimes time-consuming maintenance. Low power microfocus sealed tube sources, such as the Incoatec Microfocus source IμS, represent an interesting low-maintenance alternative to rotating anode generators. Power loads of several kW/mm^2 in anode spot sizes of < 50 µm deliver a small and bright beam. Flux densities of up to 10^{10} photons/s/mm^2 can be achieved in a focused beam suitable for most protein crystals and poorly diffracting small molecule samples. The latest generation of the IμS, the IμS 3.0, is the first microfocus X-ray source that is optimized for X-ray diffraction resulting in a gain in intensity of about 30% compared to its predecessor.

In this presentation, we will be reviewing the current performance levels of different microfocus X-ray sources. Further, we will be discussing the main features of the newest generation of the IμS. We will be presenting selected results to demonstrate the impact of these modern microfocus X-ray sources on the data quality for applications in chemical and biological crystallography.

Keywords: X-ray optics, microfocus X-ray source, new XRD technology, multilayer thin films

MS45-P2 2D spherical-polar visualization of data completeness using equal-volume units of reciprocal space

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In Macromolecular Crystallography (MX) completeness plays an important role in the assessment of data quality. Lack of completeness often results in the distortion of the related electron density map, with the ensuing difficulty in the building of a macromolecular model. Data completeness is typically quantified as percentage in spherical resolution shells; the specific region of the reciprocal space covered by the data is not normally reported in plots. This poses little or no problem when dealing with data from a single crystal, but becomes a complication when multiple crystals are involved. In the BLEND software [1] for the management of multiple crystals, for instance, the specific selection of groups of crystals is mainly guided by the criterion of isomorphism, while data completeness, especially related to reciprocal space coverage, is only dealt with after many trial-and-error combinations. One of the reasons why completeness is calculated only as a function of resolution is that the number of reflections in the case of MX is very high, thus requiring CPU or GPU intensive tools for their visualization. Even when computing resources make this feasible, three-dimensionality does not immediately render data completeness as an overall function of reciprocal space, because multiple rotations are needed to highlight regions poor in reflections. Here we introduce a new type of completeness diagram made out of two 2D plots, a resolution-dependent (radial) and an angular-dependent one. An example of the two plots is shown in Figure 1. This diagram gives an instantaneous and immediately intuitive picture of data completeness in terms of specific coverage of reciprocal space. Two or more diagrams related to individual crystals can be added without loss of information as data multiplicity is displayed by gradient or hue colouring. The main algorithmical innovation behind the creation of these diagrams is the one used already in the field of robotics, more specifically in the rotational movement of robotic parts. One of the problems addressed and solved in that field is the partition of a spherical region of space in regions of equal volumes [2]. The same type of partition, this time applied to the crystallographic reciprocal space, has been used for the completeness diagrams presented in this work.

[1] J. Foadi et al. (2013) - Acta Cryst D [2] G. Yang & I-M Chen (2006) - IEEE Trans on Robotics