High-Brightness Microfocus Sources for Chemical Crystallography

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Since its introduction in 2006, the Incoatec Microfocus Source IµS has become the gold standard for home-lab X-ray sources. The IµS combines a low power microfocus X-ray sealed tube with dedicated multilayer mirrors and delivers intensities beyond those of traditional rotating anode sources. With more than 600 sources sold world-wide, the IµS is the market-leading microfocus source for X-ray diffraction applications, such as single crystal diffraction on small molecule and protein crystals as well as small angle scattering. The latest generation of the IµS, the IµS 3.0, is the first microfocus X-ray source that is designed for X-ray diffraction resulting in a gain in intensity of about 30%. Here, we present selected examples for applications of the IµS in single crystal diffraction.

**IµS for Cu-K Radiation**

Due to the strong interaction of the Cu radiation with soft matter samples, the IµS for Cu radiation is the ideal home-lab source for most challenging and poorly diffracting organic samples and macromolecular crystallography delivering more than 2 x 10^9 ph/s/mm². It also provides a sufficiently large anomalous signal for both absolute structure determination from chiral organic samples and SAD phasing from proteins. The figure below shows an example of a tiny MOF crystal. MOF’s are known to crystallize as small and would likely have required synchrotron intensity. The example below shows results from data collection on a Mo-IµS and a Cu-IµS. Very weak diffraction was observed even on a Mo-IµS. A mouse click later, however, good quality data could be collected by switching to the Cu-IµS. The softer radiation in combination with long exposure times provided the key to solve the structure of this tiny MOF crystal, which otherwise would likely have required synchrotron intensity. The example below shows results from data collection on a tiny MOF crystal.

**IµS for Mo-K Radiation**

Data collections to a resolution beyond 0.8 Å, which is the typical resolution limit of Cu sources, require the use of sources with a shorter wavelength. The Mo-IµS delivers more than 2 x 10^9 ph/s/mm² and enables the collection of high quality data beyond 0.4 Å within a reasonable amount of time. This allows not only a more accurate modelling of the electron density by using spherical scattering factors, but also enables a reliable determination of the absolute structure, despite the significantly lower anomalous signal obtained with Mo radiation. The figure below shows the electron density distribution and the data statistics after a multipolar refinement of a sucrose crystal.

**IµS for Ag-K Radiation**

Ag-K radiation is the optimum X-ray wavelength for studying absorbing materials and for high pressure experiments in the home lab. The reduced absorption and extinction minimizes the bias of the structure model by systematic errors. High-pressure X-ray diffraction experiments using a diamond anvil cell (DAC) benefit from the compression of the q-space.

As the area of reciprocal space accessible during data collection is primarily restricted by the geometry of the DAC, a larger portion of the reciprocal space is accessible when Ag radiation is used instead of Mo radiation. Thus, using a Ag-IµS for high-pressure experiments increases the resolution and the number of observations as well as the completeness of the data which facilitates the structure solution and refinement. Further, scattering from the gasket is reduced due to the small beam diameter and the harder radiation. This reduces the background and improves the signal-to-noise ratio.

**IµS 3.0 - The new Microfocus X-ray Tube with IXT**

The latest generation of the IµS, the air-cooled IµS 3.0 source, contains the new Incoatec X-ray Tube IXT and is the first microfocus X-ray source that is designed for X-ray diffraction. Numerous small improvements make the IµS 3.0 the most user-friendly, yet most powerful microfocus X-ray source ever.

**Upgrading Existing Diffractometers with the Microfocus Source IµS**

You have a Bruker APEX, Marresearch, Nonius, Rigaku, Huber or some other system? Incoatec supports a full integration of the IµS into all common commercial diffractometers as well as into customized set-ups. Over the last years, we have upgraded more than 60 diffractometers world-wide. An international team of engineers, physicists and chemists with a broad scientific background will find the optimal solution also for your specific application. Contact us and challenge us.

**Conclusion**

The Incoatec Microfocus Source IµS has all the advantages of a sealed tube system and a flux density exceeding that of traditional rotating anode X-ray sources. It is therefore a cost effective and user-friendly X-ray source for diffraction applications in the home lab, bridging the gap between conventional sealed tube sources and high performance microfocus X-ray sources, such as microfocus rotating anodes and liquid metal jet sources.

The new IµS 3.0 is the first microfocus X-ray source that is designed for X-ray diffraction and delivers 30% more intensity than the second generation IµS. This makes the IµS 3.0 the most user-friendly, yet most powerful microfocus X-ray source ever.