MS13-2-4 High-brightness MetalJet X-ray source for MOFs/COFs structure determinations
#MS13-2-4

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Abstract
Organic Frameworks is the 3D porous materials that have been rapidly developed since 21st century, among which metal organic frameworks (MOFs) is so far the most well-known category in the family of organic frameworks. In recent decades, covalent organic frameworks (COFs) have also shown the great potential in the applications of gas absorption, chemical separation, catalysis, and energy storage and conversion, etc. Such applications are closely related to the physical and chemical properties of MOFs and COFs, which are determined by their crystal structures. Therefore, understanding the structure-property relationships from the level of atomic arrangement becomes crucial for a desired application. However, due to the interplay of nucleation and crystal growth processes, numerous cases have shown that it is often not easy to obtain large enough and well-ordered MOFs/COFs crystals for conventional in-house single crystal X-ray diffraction (SC-XRD) experiment. On the other hand, many MOFs/COFs crystals are relatively instable which undergo quick structure transitions during the SC-XRD data collections.

Therefore, high-end SC-XRD techniques for small size crystals such as MOFs/COFs are in high demand to overcome the above-mentioned challenges, which rely heavily on the X-ray source brightness for high-resolution data and short data collection time. Traditional solid or rotating anode X-ray tubes are typically limited in brightness by when the e-beam power density melts the anode. This limit is overcome by the liquid-metal-jet anode technology that has demonstrated brightness in the range of one order of magnitude above current state-of-the art solid anode sources. This is possible due to the regenerative nature of this anode and the fact that the anode is already molten, which allows for significantly higher e-beam power density compared to conventional solid anodes.

Over the last years, the liquid-metal-jet technology has developed from prototypes into fully operational and stable X-ray tubes running in more than 100 labs over the world, among which many researchers are focusing on the structure determinations of MOFs/COFs using SC-XRD since this application benefits greatly from small spot-sizes, high-brightness in combination with a need for stable output. To achieve a single-crystal-diffraction platform addressing the needs of the most demanding crystallographers, multiple users and system manufacturers has since installed the MetalJet X-ray source into their SCD set-ups with successful results.

This contribution reviews the evolvement of the MetalJet technology specifically in terms of flux and brightness and its applicability for pushing boundaries of what is possible in the home lab. Recent user examples will illustrate how the MetalJet has enabled faster turnaround time of research and also enabled easy and convenient 24/7 access to the highest quality of crystallography data.