Poster

Automated MicroED as a powerful powder diffraction tool for complex samples

J. Unge¹, J. Lin¹, S. J. Weaver¹, A. Sae Her¹, T. Gonen^{1,2,3}

¹Department of Biological Chemistry, University of California, Los Angeles, 615 Charles E. Young Drive South, Los Angeles, California 90095, United States, ² Department of Physiology, University of California, Los Angeles, 615 Charles E. Young Drive South, Los Angeles, California 90095, United States, ³ Howard Hughes Medical Institute, University of California, Los Angeles, Los Angeles, California 90095, United States

Johan.Unge@umu.se

MicroED enables structures from sub-micro-meter sized crystals and forms a niche complementary to X-ray Crystallography, NMR as well as to CryoEM. By combining MicroED and automation, which enables data collection of thousands of crystals, more of the intrinsically difficult samples can be analyzed. From the selection of thousands of data sets, a few coherent data sets can be found and the structure solved. For complex powder mixtures, the content of the samples can be estimated and the constituents identified. Identification can be done from crystal properties only. As the sample is analyzed grain by grain, peak overlap in complex mixtures that tend to make powder diffraction difficult can be avoided.

Diffraction from nano-sized crystals offers opportunities and challenges. Application of MicroED currently tend to be in projects with non-ideal crystals displaying limited diffraction, powder with limited number of crystalline grains and crystals that can not grow large enough for X-ray based methods. These have often be approached using single crystals synchrotron radiation or powder diffraction techniques. Automation in MicroED effeciently enhance analysis of complex samples.

An automated approach to MicroED is presented using the commonly used SerialEM software. This allows unattended data collection after initial setup of typically 1000 data sets per day, where typically 20-30 data sets would be collected manually. The protocols and pipelines together with examples and applications of using an automated approach to MicroED is presented.



Figure 1. Workflow for automated MicroED for powder analysis.