High-Throughput Structure Determination Using Serial Electron Diffraction Method

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Abstract

X-ray diffraction crystallography has been used for many years as a standard method for atomic structure determination, and the majority of structures have been obtained using this method. Over the past two decades, transmission electron microscopy (TEM) techniques including cryo-EM and electron diffraction have been used as alternative methods to the x-ray diffraction. Electron diffraction needs much less material compared to x-ray diffraction and it is applicable to nanocrystalline materials. Serial electron diffraction (Serial ED) is a newly developed method that minimizes the radiation damage by sequentially hitting thousands of randomly oriented crystals with electrons, instead of rotating one crystal during the data collection. The focus of my research project is to expand the applications of the Serial ED method, and improve it in terms of data collection/analysis and structure solution protocols. The results of data analysis and structure solution of a metal-organic framework (MOF) are presented. I have also worked on diffraction acquisition of nanocrystals with ultrafast applications, and diffraction of radiation-sensitive crystalline polymers. Finally, scanning-TEM or STEM-based diffraction acquisition using a collimated nanobeam has been used to get diffraction of nanocrystals from a low-magnification image map of the crystals. The future work is to program the microscope to do the serial STEM-based nanobeam diffraction automatically, and to use this method for structure determination of a various range of materials to demonstrate the Serial ED method.

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