MS25-P07 | DYNAMICAL STRUCTURE REFINEMENT FROM DATA OBTAINED WITH A DOSE OF LESS THAN 1 E-/Å²

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Solving the structures of beam sensitive materials is one of the current challenges in crystallography. This challenge is even bigger when it comes to the refinement of their structures. The fact that it is notoriously difficult for many beam sensitive materials to grow large single crystals doesn't make it easier. As a consequence, in certain material classes like metal-organic frameworks (MOF) many compounds have been synthesized but stay in the drawer because they lack a suitable structure investigation method.

Electron diffraction is the most sensible choice in these cases. Not only can we exploit single crystals that are a million times smaller than in X-ray diffraction, but for the same amount of useful signal the dose can also be three to four orders of magnitude lower. On this basis we recently developed the low-dose electron diffraction tomography (LD-EDT) that is optimized for dose by eliminating all periods of irradiation except those actually used for data acquisition.

In this contribution we show that the data quality of LD-EDT is suitable for dynamical refinement of the structures even when the total dose used for data acquisition is less than 1 electron / Å². We present the results of the refinements of complex oxides as well as MOF.