MS24-2-2 Implementation of a Dose-Symmetric Tomography Scheme in 3D Electron Diffraction #MS24-2-2

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Abstract
3D electron diffraction (3DED) has established itself as a powerful technique to elucidate atomic structures of nano-sized crystals[1]. One of the most commonly encountered issues in the 3DED field is beam damage to crystals under electron exposure, which causes diffraction intensity loss and a decay in data resolution from sensitive crystals[2]. Here we implement the technique of dose-symmetric tomography (DST)[3] employed in the field of cryo-electron tomography (cryoET) into low-dose electron diffraction tomography (LD-EDT)[4] to further improve the signal-to-noise ratio in 3DED.
Starting the acquisition in the low-tilt region, which often provides high-resolution data due to lower apparent thickness, assures that these data are recorded while the crystal is not beam yet damaged (**Figure 1**). The high-tilt frames of the damaged crystal are used for unit cell determination only. Damage-free low-tilt data from multiple particles is then merged for structure determination (**Figure 2**).
We present results obtained on two test samples $Sr_5CuGe_9O_{24}$ and Mn-formiate. Results on $Sr_5CuGe_9O_{24}$, containing 9 independent cation and 13 independent oxygen positions, show that it is possible to get an accurate structure by solely using frames in the +/-10° range from 3 particles. Model accuracy often improves with data completeness by merging more particles, but this is not always the case. Particles that yield only very weak diffraction intensities generate difficulties in the rescaling process and tend to worsen the data quality. The same is true for thick crystals subjected to higher dynamical scattering effects. For Mn-formiate the high tilt diffraction frames clearly showed beam damage effects and it was possible to reduce the range to +/- 8° for the structure solution in SIR2014. All non-hydrogen atom positions were directly obtained with a high accuracy (average distance to the DRX refined positions of 0.1 Å). Dynamical refinement is possible on dose symmetric electron diffraction tomography (DS-EDT) data but requires a certain amount of data completeness.Instead of a tilt range of around 100° in standard 3D ED, DS-EDT only needs a tilt range of 20° or less on an individual crystal to obtain exploitable data. At the same signal-to-noise ratio, the necessary dose can therefore be reduced by an order of magnitude.

References
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Figure 1: Representation of dose-symmetric tomogram

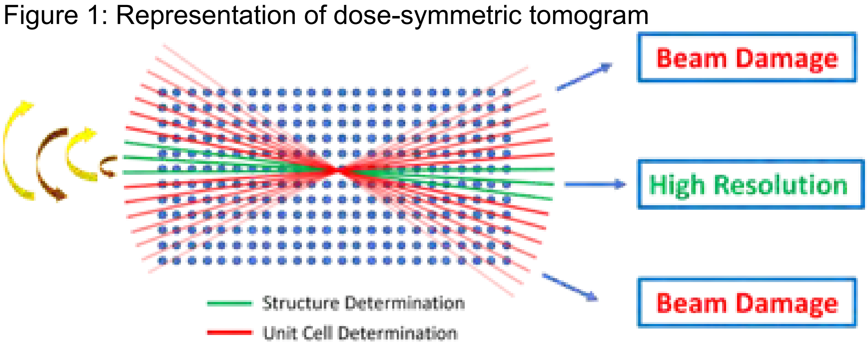

Figure 2: Representation of sub-tomogram averaging