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Electron Diffraction vs aperiodic crystal: from indexation to structure solution

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Can we solve aperiodic structures using intensities from electron diffraction? Yes! How? No mystery about it: the data analysis and the tools used for structure solution are essentially the same as the ones used in X-ray crystallography. The trick actually lies in new approaches used in electron crystallography.

In analogy to X-ray diffraction, the so-called Electron Diffraction Tomography (EDT) [1] corresponds to a phi-scan data collection on a single crystal. There lies one major advantage of this technique: a powder sample is easily converted to infinitely large number of single crystals for electron diffraction. In case of aperiodic crystals this makes the difference over X-ray or neutron powder diffraction where, often, the lack of peaks clearly assignable to satellite reflections prevents any indexation and further analysis of the structure [2]. EDT allows for an accurate estimation of the modulation vector and a good guess of the super space group. These informations can be advantageously used as an input for X-ray or neutron powder diffraction. Not limited to indexation, EDT combined with Precession Electron Diffraction (PED) [3], offers a unique tool for solving modulated structures when crystals suitable for X-ray diffraction are missing. By limiting the paths for multiple scattering, PED makes the diffracted intensities closer to kinematical approximation so that they can be used efficiently for structure solution. Regarding aperiodic crystals, the superspace electron density map, generated as an output of the charge flipping algorithm used in Superflip, can be interpreted to obtain a structural model. This will be illustrated on a series of layered materials closely related to the Aurivillius phases belonging to the pseudo-binary Bi5Nb3O15-ABi2Nb2O9 (A=Pb, Sr, Ca, Ba). Limitations and possible combination with powder diffraction patterns will be discussed.

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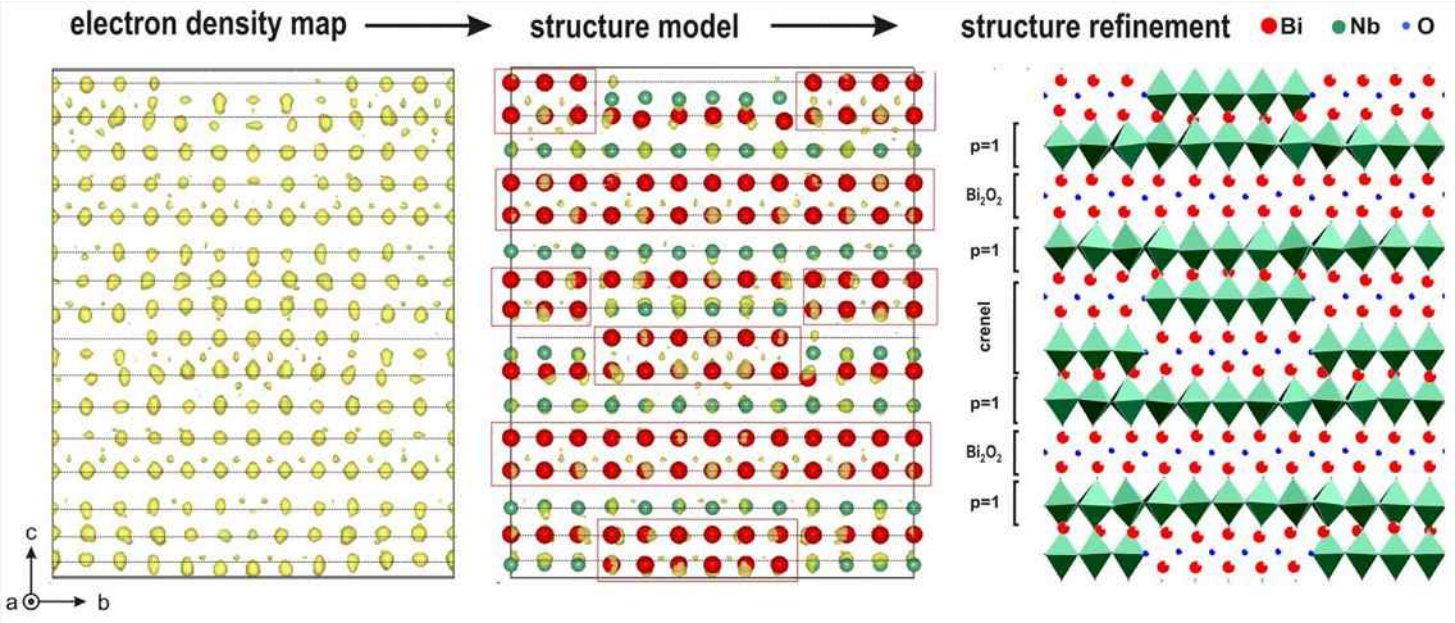

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