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Electron and X-ray diffraction – two worlds united

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Small crystals structure solution usually done with X-ray powder diffraction (XRPD) provides bulk information and is powerful for in-situ investigations. Peak overlap in the one-dimensional data causes problems e.g. for polyphasic or impure samples and large cell parameters thus peak indexing and intensity extraction are the main issues where x-ray powder data may be supported by extra information. Electrons sample smaller volumes but strong coulombic interaction cause multiple scattering effects changing intensities often so strong that a structure solution is becoming impossible. Nevertheless, oriented electron diffraction patterns may provide sufficient information to support indexing or the assignment of impurity peaks in the case of low quality x-ray powder pattern. Reciprocal space tomography [1] uses a series of non-oriented diffraction patterns for which dynamical effects are significantly reduced and an enhanced amount of independent reflections sampled allows “ab-initio” crystal structure solution using established X-ray structure solution packages. Although structure refinement based on kinematical intensities is stable, achievable R values of 10-30% are high and final refinement may be performed based on X-ray powder data. Scanning transmission electron microscopy (STEM) for crystal tracking and nano electron diffraction (NED) is suitable for beam sensitive material, agglomerated particles, twins or intergrown phases on crystals down to 30nm size [2, 3]. Interesting properties of nanocrystalline materials are driven mainly by twinning, defects, disorder in one or two dimensions down to the amorphous state. Here low data completeness or uncertain intensity determination causes problems in structure solution. Here a mean structure may be determinable serving as a basis for disorder description and being used as a starting model being refined onto X-ray powder data maybe supported by a combination of the diffraction methods or by adding extra information.

[1] *U. Kolb in: Uniting Electron Crystallography and Powder Diffraction, Kolb et al. (eds.), Springer, The Netherlands, Series B: Physics and Biophysics. (2012),* ***[2]*** *E. Mugnaioli, I. Andrusenko, T. Schüler, et al., Angewandte Chem. Int. Ed., 2012, 51(28) 7041-7045,* ***[3]*** *U. Kolb, T. Gorelik, E. Mugnaioli, A. Stewart, Polymer Reviews, 2010, 50, 385-409*

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