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Combing electron diffraction techniques for structure solution

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The last few years have seen a revolution in the field of 3D electron diffraction or diffraction tomography. We have moved from only acquiring a few low index zone axis patterns to full tomographic data sets recording all accessible areas of reciprocal space. These new larger data sets have made it easier for structure solution techniques such as direct methods from the x-ray world to be applied to the electron diffraction data for structure solution. While structure solution with tomographic electron diffraction is non trivial when compared to the x-ray case it is significantly easier than it was a few years ago. Mugnaioli et al. We are now in a situation where the most difficult and time consuming step can be the assignment of the space group to a data set. Electron diffraction has many advantages over the x-ray case in terms of the manner in which we can manipulate the electron beam. This allows the collection to convergent beam diffraction (CBD) or large angle convergent beam diffraction (LACBED) patterns, via the recently developed technique by Beanland et al. These techniques can make the assignment of space group significantly easier affair, and the path to structure solution a lot smoother. We will present the combination of data from tomographic, selected area (SA) and nano-beam (NBD) datasets, with diffraction from tomographic LACBED experiments where using the strengths of each technique can be leveraged for a much quicker route to structure solution.

[1] E. Mugnaioli, T. Gorelik, U. Kolb, Ultramicroscopy, 2009, 109, 758-765, [2] R. Beanland, P. Thomas, D. Woodward, et al. Acta Cryst., 2013, A69, 427-434

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