

chemical and positional disorder, structural solution from low quality data (powder patterns), joint use of several data sets, resonant scattering and fast *in-situ* data collection. The direct space approach is currently the powder diffraction method mostly used in hydride research for its simplicity of use, ability to work with powder patterns of low quality (broad peaks), easy way to treat the occupation disorder on hydrogen sites and active use of simple geometrical constraints. Crystal structures containing as many as 55 independent atoms (including hydrogen) have been fully characterized using powder diffraction. This is of great importance, because rapid collection of powder data thanks to modern synchrotron and neutron time-of-flight sources opens the possibility for fast *in-situ* studies, mapping of phase transitions induced by the temperature, pressure, hydrogen content, and chemical reactions. The crystallography of important materials for hydrogen storage like LiBH_4 [2,3], $\text{Mg}(\text{BH}_4)_2$ [4,5], $\text{Mn}(\text{BH}_4)_2$ [6] and many others will be discussed.

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Solving Complex Structures by Combining Precession Electron Diffraction and X-ray Powder Diffraction Techniques. Dan Xie^a, Christian Baerlocher^a, Lynne B. McCusker^a. ^aLaboratory of Crystallography, ETH Zurich, CH-8093 Zurich.

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X-ray powder diffraction (XPD) and electron microscopy are remarkably complementary techniques for analyzing the structures of polycrystalline materials. Several ways of combining them have been developed recently to address structures that cannot be solved by either technique alone. Here we present two different ways of using precession electron diffraction (PED) data in combination with XPD data for structure solution. In one case, PED data are simply used to identify the weak reflections in a projection, and then these reflections are eliminated from the XPD intensity extraction procedure. Generally the intensity ratios of overlapping reflections are set to one (equipartitioning), so it is quite possible that weak reflections in an overlap group are assigned medium or even large structure-factor amplitudes. By eliminating these weak reflections from consideration, a more correct partitioning of the remaining reflections in the group is obtained. In the second case, phase information is extracted from 2-dimensional PED data using the charge-flipping algorithm [1-2]. The number of correct phases retrieved in this way was found to be

comparable to that that can be derived from an HRTEM image. These phases are then used in combination with the intensities extracted from the XPD data to initiate structure solution using the powder version of the charge-flipping algorithm [3] in the program *Superflip* [4]. The approaches were first developed using data for the moderately complex zeolite ZSM-5, and then tested on TNU-9 [5], one of the two most complex zeolites known. In both cases, including PED data from just a few projections facilitated structure solution significantly. It should be noted that the methods are generally applicable (i.e. not zeolite specific), so it should be possible to apply them to any polycrystalline material. Furthermore, introducing information from PED data to the structure solution procedure is not restricted to charge flipping. It could also be used to advantage in other programs (e.g. in the form of better intensities in a direct-space global optimization program or as starting phases for direct methods trials). Thus, the PED technique offers a relatively simple route to valuable information that can be used to complements that in a XPD pattern.

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MAD Techniques Applied to the Structure Solution from Powder Data: A New Probabilistic Approach.

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Phase determination *via* multiple-wavelength anomalous dispersion (MAD) techniques, owing to the tunability of the wavelength of the synchrotron radiation, is one of the most popular approaches for the solution of the phase problem in protein crystallography. The classical MAD technique is essentially a three-step procedure: a) the estimation of the structure factor moduli of the anomalous scatterer substructure; b) the location of the anomalous scatterers *via* Patterson or Direct Methods; c) the protein phase estimation. MAD techniques were not very beneficial for powder crystallography owing to the unavoidable peak overlapping in powder patterns. Indeed: a) the reflections F^+ and F^- systematically overlap: consequently, anomalous