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Keywords: rare earth thioborates; crystal structure analysis; electronic structure calculations

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Powder Diffraction and Pair Distribution Function Analysis by Using Multilayer X-ray Optics and Ag Radiation. R. Dietsch[a], Th. Holz[a], H. Borrmann[b]. [a]*AXO Dresden GmbH, Siegfried-Raedel-Street 31, 01809 Heidenau, Germany.* [b]*Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany.*
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Multilayer X-ray optics are used on diffractometers mostly for Cu, Co or Cr Ka radiation. For these wavelengths the Q-range in reciprocal space is limited to approximately 8Å^{-1} which is not enough for some applications.
This can be overcome by use of harder X-rays like Ag radiation. Advantages of this higher photon energy are the higher penetration depth and the increased number of detectable reflections in the reciprocal space up to 20Å^{-1}. It is also possible to use capillaries with larger inner diameters without having problems with sample absorption.
We will show powder diffraction results measured with parallel beam geometry (TMA – Twin Mirror Arrangement) as well as with focusing geometry.
By using high quality X-ray multilayer mirrors it is possible to resolve even very close reflections within a certain angular range as we will show for a LaB_6 capillary powder sample. The diffraction pattern also shows a vastly increased number of reflections
The large Q-range also allows to determine the pair distribution function even for amorphous and nanocrystalline samples.

Keywords: multilayer(s); X-ray diffraction instrumentation; powder diffraction

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FIDDLE: Powder Pattern Indexing and Structure Solution Hand in Hand. Jan Smits[a], Carmen Guguță[a], René de Gelder[a]. [a]*Solid State Chemistry, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands.*
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The usual scheme for crystal structure determination from powder diffraction data consists of (1) indexing the powder pattern, (2) space group determination, (3) structure solution, and (4) structure refinement. Despite the success of methods for powder pattern indexing there are often cases in which the very first step is non-trivial or simply impossible. This means that the subsequent steps are not accessible and structure determination as a whole fails.
FIDDLE (to be pronounced as 'fit-all') is a direct-space method for the determination of crystal structures from powder diffraction data that uses a different approach for indexing problems. By optimizing *all* model parameters, including the unit cell parameters, the information in peak positions and peak intensities is used simultaneously for finding both the unit cell and the crystal structure. A genetic algorithm, together with a pattern matching technique based on auto- and cross-correlation functions[1], is applied to find the optimal match between observed and calculated diffraction patterns. FIDDLE has the possibility to search through the most common space groups, while varying Z', and does not rely on energy or packing considerations.
Although the method was developed for the complete structure determination process, experience shows that finding the unit cell is very efficient, even when structure solution is not fully complete[2].
Examples of successful applications of the method will be presented.

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Keywords: powder indexing; powder structure determination; optimization algorithms