

**ADVANCES IN INDEXING OF POWDER DIFFRACTION PATTERNS:
ITERATIVE USE OF SINGULAR VALUE DECOMPOSITION AND
MONTE-CARLO BASED WHOLE POWDER PATTERN DECOMPOSITION**

A.A. Coelho & A. Kern

Bruker AXS GmbH, Östliche Rheinbrückenstraße 50, 76187 Karlsruhe, Germany

Two fast and simple methods for indexing powder diffraction patterns have been developed for large and small lattices of all symmetries: "SVD-Index" and "LP-Search".

"SVD-Index" operates on d-values extracted from reasonable quality powder data. Critical to its success is the use of Singular Value Decomposition (SVD) in an iterative manner for solving linear equations relating hkl's to d-spacings. The method is relatively insensitive to missing high d-spacing reflections where on simulated data little effect in terms of successful indexing has been observed when one third of the d-spacings are removed.

LP-Search is independent of d-spacing extraction and it has been developed for indexing of poor quality powder data. It minimizes on a new figure of merit function that gives a measure of correctness for a particular set of lattice parameters. More specifically the figure of merit function assigns parts of the diffraction pattern to peaks and then sums the absolute values of the products of the diffraction intensities multiplied by the distance to the peaks. The method avoids difficulties associated with extracting d-spacings from complex patterns comprising heavily overlapped lines; the primary difficulty being that of ascertaining the number of lines present.

Both methods have been shown to perform well on lattices of up to at least 4000 Å³ and large diffractometer 2θ zero errors up to 0.05° 2θ. In addition SVD-Index is also successful on d-spacing data comprising random errors of up to 0.03° 2θ.

The performance of "SVD-Index" and "LP-Search" as implemented in the program TOPAS [1] will be demonstrated using several selected examples.

Reference:

- [1] Bruker AXS (2000): TOPAS V2.0: General profile and structure analysis software for powder diffraction data. Bruker AXS, Karlsruhe, Germany.