

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

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

"LSI" (Least Squares Indexing) operates on d-values extracted from reasonable quality powder data. Critical to its success is the use of least squares in an iterative manner for solving 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.