Getting cell parameters from powder diffraction data

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Some keys, hints and tips for the successful indexing of a powder diffraction pattern are given through examples, by using exclusively free access programs for academic research. Summarizing, the sample has to correspond to a single phase; the powder pattern resolution should be maximal, avoiding preferred orientation; the tools used for peak position hunting and indexing should be the best on the market; the figures of merit have to be understood so as to be able to save time by discarding the poor quality suggestions of the indexing programs; further checking by post-indexing visualization is recommended in case of good quality multiple equivalent propositions; finally, whole pattern fitting has to be the ultimate test in order to be convinced enough for attempting the structure solution. Fortunately, indexing powder diffraction data is probably the crystallography topic where the traditional way of sharing openly computer programs remains the more respected (ITO, TREOR, DICVOL, CRYSFIRE, McMaille, etc).

Useful Web address :
CCP14 : http://www.ccp14.ac.uk/
Indexing Benchmarks : http://sdpd.univ-lemans.fr/uppw/benchmarks/
SDPD Internet Course : http://sdpd.univ-lemans.fr/DU-SDPD/

Most recent review papers about indexing :
P.-E. Werner in "Structure Determination from Powder Diffraction Data", Edited by W.I.F David, K. Shankland, L.B. McCusker and Ch. Baerlocher, Oxford Science Publications, Chapter 7 : "Autoindexing", 2002, 118-135.
R. Shirley, "Overview of powder-indexing program algorithms (history and strenghts and weaknesses). IUCr Computing Commission Newsletter 2 (2003) 48-54.
J. Bergmann, A. Le Bail, R. Shirley and V. Zlokazov, "Renewed interest in powder diffraction data indexing", Z. Kristallogr. 219 (2004) 783-790.

Programs for various purposes (indexing, peak position hunting, checking cells):
Chekcell : J. Laugier & B. Bochu, http://www.inpg.fr/LMGP (and CCP14)
CRYSFIRE : R. Shirley, "The Crysfire 2002 system for automatic powder indexing: user's manual. Lattice Press: Guilford, UK (2002).
DICVOL04: A. Boultif & D. Louër, "Powder pattern indexing with the dichotomy method", J. Appl. Crystallogr. 37 (2004) 724-732.
McMaille : A. Le Bail, "Monte Carlo indexing with McMaille", Powder Diffraction 19, 2004, 249-254. http://www.cristal.org/McMaille/
N-TREOR : A. Altomare, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni, R. Rizzi & P.-E. Werner,"New techniques for indexing : N-TREOR in EXPO", J. Appl. Crystallogr. 33 (2000) 1180-1186.
PowderX : C. Dong, "PowderX: Windows-95-based program for powder X-ray diffraction data processing", J. Appl. Crystallogr. 32 (1999) 838.
TREOR: P.-E. Werner, L. Eriksson & M. Westdahl, "TREOR, a semi-exhaustive trial-and-error powder indexing program for all symmetries", J. Appl. Cryst. 18 (1985) 367-370.
WinPLOTR : T. Roisnel & J. Rodriguez-Carvajal,
http://www-llb.cea.fr/fullweb/winplotr/winplotr.htm