POWDER PATTERN INDEXING

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The indexing of a powder diffraction pattern is an essential requirement in *ab initio* structure determination from powder data. The objective of indexing is to restitute the 3-dimensional reciprocal lattice points from the length of diffraction vectors measured from 1-dimensional diffraction data. This reconstruction is not only a crystallographic and algebraic problem, but also depends on the accuracy of the data. The most popular automatic procedures for indexing, regardless of symmetry, are the zone-indexing method based on the principles derived by Runge, Ito and de Wolff (ITO, Visser, *J. Appl. Cryst*. 2, 89, 1969), the index permutation method based on a permutation of Miller indices for selected base lines (TREOR, Werner *et al*., *J. Appl. Cryst*. 18, 367, 1985) and the exhaustive direct-space method based on a dichotomy algorithm (DICVOL, Boultif and Louër, *J. Appl. Cryst*. 24, 987, 1991). Reviews on methods and practical aspects have been reported (Louër, NIST, Spec. Publ. 846, 92, 1992; Werner, 'Structure Determination from powder diffraction data', IUCr/OUP, 118, 2002).

Long ago de Wolff claimed that the indexing problem 'would be quite an easy puzzle if errors of measurement did not exist' (*Acta Cryst*. 10, 590, 1957). Accurate data is then requisite for successful indexing and the success rate of computer-based indexing programs is high ($|\Delta(2\theta)| < 0.03$ °2θ). The respective merits of modern instruments, operating with conventional X-ray sources and synchrotron radiation, are discussed. The choice of the optics (reflection, transmission, capillary) must be decided according to the X-ray absorption of the material. There is no absolute criteria to judge the correctness of a solution. Nevertheless, several conditions must be fulfilled, such as high figures of merit. The crystal symmetry can be studied from absent reflections, using the peak positions (e.g. NBS*AIDS83) or the full trace of the pattern combined with a primitive cell, by means of a pattern matching procedure available in most popular Rietveld programs. The incorporation of indexing programs in software like WinPLOTR (http://www-llb.cea.fr/fullweb/powder.htm) makes convenient such analysis.

Difficulties in pattern indexing can be due to geometrical ambiguities, e.g. with hexagonal cells, or to particular cases, e.g. cells having a short axis as frequently found with pharmaceutical materials. Examples of pattern indexing will be discussed, including the polymorphs of piracetam, a drug with potential applications in therapeutic areas.