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powder pattern and comparison with a "pure" powder pattern calculated from structural models offers several advantages:
1)It requires no standards or calibration procedures and can be performed with both X-ray and neutron powder diffraction.
2)Analysis can be extended to more complex powder patterns. As the extractable information does not increase linearly with the addition of more and more phases due to line overlap, the limit of multiphase analysis depends on the overall density of the Bragg reflections in the pattern, i.e. on cell dimension and crystal symmetry of the phases, on the purity and wavelength(s) of the radiation and on the resolution of the diffractometer.
3)Systematic errors such as preferred orientation, extinction, line broadening or surface roughness may be detected more easily. Recent progress in modelling these phenomena e.g. use of symmetrized harmonics to describe preferred orientation or of anisotropic line broadening to model crystal imperfections have aided with numerical corrections.
4)Unidentified phases may better be detected through careful refinement and analysis of the difference between the sum of all calculated phases and the observed intensity.
5)Better analytical or graphical modelling of the background considerably enhances the precision of the method. Addition of an amorphous reference material or analytical modelling of an amorphous component permits it's quanitative determination.
6)More precise assessment of the quality of the analysis can be achieved by use of phase specific reliability factors (Rw-Bragg and GOF-Bragg) in addition to the conventional overall profile reliability factors Rwp and GOFwp.
7) The accuracy of the method can more easily be assessed by internal or external consistency checks: a)Extinction or surface roughness may be detected by a comparison of high and low angle data. b)Preferred orientation can be varied by use of different sample geometries, i.e. reflection, transmission or capillary. c)Extinction or micro-absorbtion may be varied through choice of different wavelengths (Cu, Mo..). d)neutron data are barely affected by preferred orientation, extinction or micro-absorption.
Ease of use of the method has been greatly enhanced by set up of dedicated compilations of structure data and by interfacing to large crystal structure data banks. The method will become even more popular through increasing ease of software handling such as multiphase Rietveld programs on PC's, automatic parameter turn on sequencing and automatic multisample refinements.
More complex X-ray powder patterns may be analysed in the future by use of strictly monochromatic radiation, more flexible profile functions and increased instrument resolution offered by Guinier or Synchrotron diffractometers.
Technical applications such as the determination of mineral contents in rock specimens and analysis of clay minerals in ceramics will be discussed.

DS-20.02.05 QUANTITATIVE ANALYSIS OF MULTIPHASE MATERIALS USING THE TWO STAGE METHOD. By G. Will, Mineralogical Institute, University Bonn, Poppelsdorfer Schloß, 5300 Bonn 1, Germany.

Besides the conventional methods of phase analysis of multiphase materials using search match methods and the standard procedures for qualitative analysis, like the standard-less method by Zevin, a novel approach is being developed in the last years based on the procedures used in crystal structure refinements. Considerable progress has been made in recent years. In general two different methods are being tested and used today: the Rietveld method or Total Pattern Refinement, and the Two-Stage Method.

The Two-Stage Method is a very promising strategy especially in cases were preferred orientation may cause difficulties and may lead to wrong results. In the two-stage method, the diffraction diagram is decomposed into its individual peaks and thus its contribution to the different phases. The intensity data are normally used for crystal structure refinement, for example by the program POWLS. This procedure of refinement by POWLS also calculates a scale factor K besides positional and other structural relevant parameters. In case of several phases present each structure refined by itself thus yields its own several scale factors K_i. The scale factors K_i are directly related to the amount of material in the sample. By refining two or more crystal structures in the multiphase sample a quantitative analysis can be performed.

Since the whole diffraction pattern enters the analysis and since the crystal structures of the individual components are known, preferred orientation problems are easily recognized and can be taken into account. The biggest advantage of this method is found therefore in samples with considerable preferred orientation, like materials with calcite- or calcite-related-structures or clay and mica minerals.

Besides our own developments efforts and progress has been made in several laboratories, for example by Karimat and co-workers on kaolin samples. A review of recent developments will be presented.

