extinction (T.M. Sabine, *Aust J Phys*, 1985,38,507), thermal diffuse scattering, transparency, structural defects (*eg* A.J.C. Wilson, *Mathematical Theory of X-ray Powder Diffractometry*, 1963, Eindhoven: Centrex), partial crystallinity, such as can occur in polymers and glassy materials (J.N. Hay *et al*, *Polymer Commun*, 1984,25,175), and contamination of the diffraction pattern by impurities (P.J. Bendall *et al*, *J Appl Cryst*, 1983,16, 164).

Limitations on an analysis of the data can be imposed by the nature of the diffraction pattern; background determination and the separation of peaks with severe overlap in complex patterns (J.I. Langford *et al*, *Powder Diff*, 1986,1,211) and a paucity of lines all affect the results of profile refinement. Inadequacy of the function used to model peak shapes is often a source of systematic error (R.A. Young & D.B. Wiles, *J Appl Cryst*, 1982,15,430), as is the model used in any size-strain analysis.

The significance of these factors depends on what information is to be extracted from pattern fitting. In general, requirements of the Rietveld method are less stringent than for size-strain analysis, for example, and for *ab initio* indexing of powder data precise peak positions are more important than other profile parameters. Some problems in profile analysis can be avoided, or at least minimised, by a suitable design of the experiment and by systematic sample preparation (G. Will *et al*, *J Appl Cryst*, 1983,16,611). Others can be treated analytically, but there can also be residual problems, often originating in the sample, for which there is no remedy; these must be taken into account when presenting the results of profile refinement.

12.X-6 NEW TECHNOLOGIES IN SEARCH-MATCH PROCEDURES. By R. Jenkins, International Centre for Diffraction data, U.S.A.

First systematic attempts to identify mixtures of polycrystalline phases by unscrambling their composite x-ray powder patterns dates back to the mid-1930's, and the original idea of searching small subsets of the d/I lists (the search), and then comparing potential candidates with the full pattern (the match), is still used today. In the mid-1960's, the first attempts to automate the search-match process were made using large, main-frame computers. More recently, the advent of fully automated powder diffractometers and the increasing use of personal computers have led to widespread interest in computer search-matching.

Earlier search algorithms required some judgment on the part of the operator in the estimation of data quality, and problems arose due to uncertain quality of "d" spacings, and/or to the effects of solid solution. More recently, this situation has improved due to a better knowledge of the accuracy of measured and standard "d" values, combined with matching techniques based on statistical probabilities. A second problem is that of unreliable intensities due mainly to preferred orientation of the specimen. Where subtractive techniques are used to remove an "identified phase" from the composite pattern, too much or too little intensity may be removed. A recently employed alternative is the use of an additive method, in which a comparison is made with a composite pattern comprising each identified phase.

Other problem areas include the method of handling the polychromaticity of the source, use of elemental data before or after the d-spacing search, and the allocation of "figures of merit" for "hits" based on a given search strategy. This paper reviews, with practical examples, recent advancement in the treatment of these problems.

12.X-7 USE OF THE RIETVELD METHOD FOR DETERMINING COMPONENT PHASE ABUNDANCE AND PARTICLE SIZE/STRAIN CHARACTERISTICS: APPLICATIONS TO CERAMICS AND BATTERIES. By R.J. Hill, CSIRO Mineral Chemistry, PO Box 124, Port Melbourne, Vic 3207 Australia, and C.J. Howard, AAEC Applied Physics, Lucas Heights Res Labs, Locked Bag No. 1, Menai, NSW 2234 Australia.

The Rietveld method was developed to refine crystal structures from neutron and X-ray powder diffraction patterns and has been extensively used for this purpose (Hewat, Chemica Scripta, 26A, 119, 1986). While most applications continue to be in structure refinement, it is now recognized that the method can also be used to obtain information on phase abundance in mixtures and on particle size, shape and strain.

Codes for multiphase Rietveld analysis were first developed to deal with impurity phases in otherwise standard crystal-structure refinement studies. However, the scale factors obtained in a multiphase analysis are directly related to the masses of the crystalline phases in the mixture. This relationship is the basis of a method for obtaining an accurate phase analysis without the need for standards or laborious experimental calibration; it is particularly powerful in the case of neutron diffraction.

Improvements in the description of peak shapes have been devised to provide better fits to the recorded diffraction patterns and thereby increase confidence in the derived crystal-structure parameters. In so doing, the analysis provides information on crystallite size and strain, which can also be of considerable interest.

In this presentation, we outline how the nonstructural parameters derived as a byproduct of Rietveld analysis are related to the physical state of the material. We also outline some current and potential applications, with particular emphasis on ceramics and batteries.

12.X-8 THE APPLICATION OF NEUTRON DIFFRACTION TECHNIQUES TO INDUSTRY. B.M. Powell, Chalk River Nuclear Laboratories, Chalk River, Ontario, K0J 1J0, Canada.

Neutron diffraction is utilized increasingly as a commercial examination technique. Its advantage lies in the great penetration depth of neutrons in materials of common industrial use. Consequently, neutron diffraction can probe the interior of large industrial components or can investigate the bulk properties of a complete component. An application of fundamental industrial importance is the ability to measure the residual strain in the interior of a structural component. By masking the neutron beams appropriately, the spatial distribution of strain within a specified region or the average strain within the region can be measured. Welds, rolled joints, bent tubes and components as large as pipelines have been examined. Components produced in industrial processes often show pronounced texture, which can have a drastic effect on performance. Neutron diffraction can measure texture in large samples, thus minimizing inaccuracies due to grain size. The complete texture can be specified by construction of the orientation distribution function from measured pole figures. For industrial materials which contain secondary phases or develop them in use, neutron diffraction can investigate the volume fractions of these minority phases. High resolution neutron diffraction measurements analyzed with multicomponent refinement methods are more sensitive to the presence of such phases than most other detection methods. Certain industrial applications require large single crystal components e.g. semiconductor wafers, turbine blades. The quality of these crystals can be examined by neutron Bragg reflection. Various neutron techniques and their utilization will be discussed.