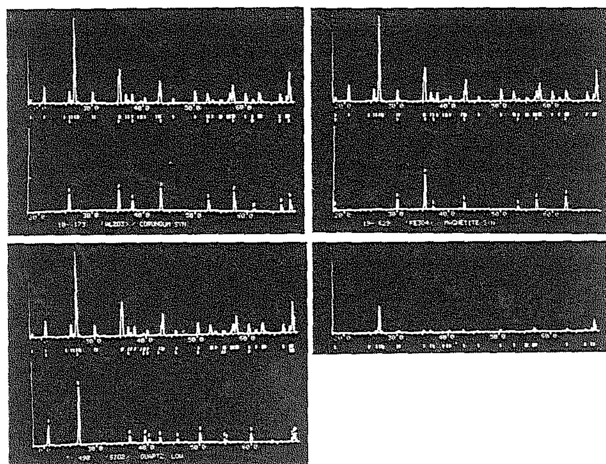
12.2-01 AN ADVANCED SEARCH/MATCH SYSTEM FOR X-RAY POLYCRYSTALLINE IDENTIFICATION. By T. C. Huang, G. L. Ayers and W. Parrish, IBM Research Laboratory, San Jose, California 95193, USA.

A comprehensive computer Search/Match system has been developed for rapid and precise phase identification of polycrystalline materials. It operates on a host computer or a minicomputer using a "question and answer" interactive input. Either full screen menu or line input formats arranged to minimize incorrect entries may be selected.

The data base may be a user created file, or the JCPDS which we have rearranged into four subfiles: inorganics, organics, minerals, and metals and alloys. In each subfile the frequently encountered phases are first, quality data second and the remainder last, which allows stopping at the end of any section when identification has been made. Data may be entered manually or by automatic transfer from Peak Search or Profile Fitting runs or stored data. Systematic errors may be automatically corrected by entering a few correct d's of an internal standard or a known constituent in a mixture. The error limits for matching are selectable and overlapping window limits are used. The program requires the three strongest standard reflections in the experimental range be present in the unknown. However there is an option to remove this requirement if strong preferred orientation is suspected. The chemical information option provides elements present, absent and/or groups of elements absent.

A comprehensive algorithm evaluates each match by computing a figure-of-merit (FOM) based on the matches of the d's, I's and number of reflections. The top FOM standards are listed after each section of the file is completed, and the user may end or continue the search. Interpretation is aided by interactive operations which include graphic terminal displays of the unknown pattern and the standards. The program employs previously determined W*G profile data to generate the standard patterns which appear as if run on the user's diffractometer, and are scaled to correspond to the amount of each phase in the unknown. The identified phases may be subtracted and the remainder plotted to aid in deciding to continue or end the search. This is illustrated below for a 3-mineral mixture; the unknown pattern appears above each standard and the tick marks indicate the peaks. The low right is the residue after subtracting the three standards and results from the differences between the experimental data and the standards. The system has been extensively tested on a wide variety of analyses and round robin data.



12.2-02 PROBABILITY-BASED SCORING METHOD FOR RANKING MATCHES IN X-RAY POWDER DIFFRACTION PHASE IDENTIFICATION. By W. N. Schreiner, Philips Laboratories, Briarcliff Manor, NY, R. Jenkins, Philips Electronic Instruments Inc., Mahwah, NJ.

Computer search/match programs used to identify phases of a polycrystalline material from an x-ray powder diffraction diagram have traditionally found it very difficult to compete with manual searchers, presumably because they lack the intelligence of a human being. While there is no hope of developing intelligent programs in the near future, some "algorithms" that are employed, perhaps unknowingly, by manual makers can be adapted to the computer and improved programs result.

One technique, which we call probability-based scoring, is based on computing event probabilities for a pattern match. The events may be "d-hits", "I-hits", loss in background, line overlap, etc.. An overall pattern match score is obtained by multiplying the event probabilities together in a maximum likelihood fashion. The method has the advantage of eliminating the so-called "windows" traditionally employed by search/match programs. To function optimally, it necessitates the separation of systematic from random errors so that the probability distributions of the events are as narrow as possible.

Probability-based scoring has been implemented in the SANDMAN (Adv. In X-Ray Anal., 24 (1981) in press) search/match/identify system which is part of the APD-3600 Automated Powder Diffractometer. (Norelco Reporter 26, 1 (1979)). It has been found to be extremely effective and has led to the development of additive (as opposed to subtractive) phase isolation. The technique will be described in detail and examples will be shown.

12.2-03 QUANTITATIVE X-RAY PHASE ANALYSIS WITHOUT STANDARDS: GENERAL CASE OF OVERLAPPING PEAKS. By L.S. Zevin, R. Shneck, Research & Development Authority, Ben-Gurion University of the Negev, Beer-Sheva, Israel and I.M. Zevin, Geological Survey of Israel.

The following expression, in matrix notation, is valid for the intensity $I_{j\ell}$ of the ℓ-th diffraction peak ($1 \leq \ell \leq n$) in the j-th sample ($1 \leq j \leq n$). (Assuming that $I_{j\ell}$ is corrected for absorption.)

$$[I_{j\ell}] = [X_{ji}]\,[K_{i\ell}] \qquad (1)$$

where X_{ji} - weight fraction of the phase i ($1 \leq i \leq n$) in the sample j; and $K_{i\ell}$ - coefficient proportional to the intensity of the ℓ-th peak in the i-th phase. If there are no overlapping analytical peaks, the matrix $[K_{i\ell}]$ is a diagonal one; and equation (1) can be solved for all n^2 unknowns X_{ji} and n unknowns $K_{i\ell}$ if the usual condition of complete analysis is added [Zevin, *J Appl. Cryst.* (1977) 10, 147]:

$$\sum_{i=1}^{n} X_{ji} = 1 \qquad (2)$$

In the case of complete overlapping (none of the values of $K_{i\ell} = 0$), the number of unknowns ($2n^2$) exceeds the whole number of equations (1) and (2) (n^2+n). The apparent possibility of increasing the number of significant equations by increasing the number of samples is not viable. The intensity of each diffraction peak 1 in the (n+1)th sample is simply a linear combination of the intensities I_{j1} in the previous n samples [Bezjak, *Anal. Chem.* (1975), 47, 790]. The only viable possibility for the phase analysis is the separation of the