peaks by the recently developed profile-fitting method [Huang and Parrish *Ad v. X-ray Anal.* (1978), 21, 275].

In the intermediate case of partial overlapping (only some of the values of $K_{i\ell} = 0$), the system of equations (1) and (2) could be solved as was suggested by Majumdar et al. [*J. Appl. Crystal* (1972) 5, 343)] for a similar problem. The following conditions should be derived in order to perform the phase analysis: 1) The number of analytical peaks should be extended up to m > n. 2) For each phase at least n-1 peaks ℓ' with $K_{i\ell'} = 0$ should be found. 3) At least one phase of the remaining n-1 should contribute to these ℓ' peaks. Under these conditions the complete number of equations (1) and (2) nm+n is equal to the number of unknowns: n^2 of X_{ji} and $n[m-(n-1)] = nm-n^2+n$ of K_{li}. A least-squares procedure for the refinement of X_{ji} and $K_{\ell i}$ should be performed if the number of samples and analytical peaks exceeded the above-discussed minimal values of n and m, respectively.

12.2-04 CORUNDUM - A REFERENCE FOR PHASE ANALYSIS WITHOUT PROBLEMS? J.Zábráczky and P.Gadó Res.Eng.& Prime Contr.Center of the Hung.Aluminium Corp.,H-1389 Budapest P.O.B.128 Hungary

Corundum (α-Al_2O_3) has been adopted as a standard material for the experimental determination of the I/I_C reference intensity ratio.Realizing the advantages, in diffraction phase analysis, of the availability of this parameter, recently the PDF of the JCPDS included in the set of data published for each material - whenever practicable - the value of I/I_C. The application of this information is straightforward, provided a batch of the same corundum as used for the original determination is possessed. Having tried some commercially offered good quality corundum samples, we found by texture goniometer measurements that this material is rather sensitive to [001] uni-axial preferred orientation. The absolute intensity diffracted depends a great deal upon the way of preparation (oxidation of metal or via sodium aluminate,temperature history,additives and subsequent grinding). Kiss,A.B.& Gadó,P. (M.Kém.Folyóirat 84,289,1978) showed the effect of Na impurities on the IR and X-ray data of corundum. Probably any corundum will yield observations good for analytical estimates. However,if the accuracy stated for some reference intensity ratios (± 2-3 % deviation) should be fully exploited in quantitative determinations, the 5-10 % deviations measured between the reflected intensities of different corundum samples (Linde,Degussa,Norton,Feldmühle,Hungalu) become disturbing. It can be concluded that further international agreements are needed to diminish this component of uncertainty in comparative diffraction phase analysis.

12.3-01 THE REFINEMENT OF UNIT-CELL PARAMETERS FROM POWDER DIFFRACTION DATA USING STRUCTURE FACTORS. A.V.Chichagov, V.V.Surikov, L.N.Ivanova, Institute of Experimental Mineralogy, USSR Ac, Sci., Moscow District, USSR

A Fortran-Algol program for the refinement of unit-cell parameters,using the automatic indexing of experimental reflections from the list of theoretical reflections allowing for their weight,has been written for the BESM-6 computer. Facilities include:
1. Calculation of the θ-ordered list of theoretical reflections with the θ_k^c angle positions, $(hkl)_k$ indices and J_k^c intensities with rejection of the following reflections: a) forbidden by the space group, b) equivalent c) deliberately forbidden, d) with the angle positions outside the given angle range, e) with the normalized intensities below a given threshold value.
2. Preliminary refinement of unit-cell parameters through the minimization of the Δ-function $\sum_i w_i (Sin^2\theta_i^o - Sin^2\theta_{ik}^c)^2$ by the flexible Simplex method. At each refinement step the optimization process allows for the i-th experimental reflection to be matched to the ik-th theoretical reflection $(hkl)_k$ with the maximum weight $Q_{ik} = \sum_j V_{ik} J_k^c$ j is the summation index for the theoretical reflections that have the same angular position but differ in their intensities). The program allows for three types of the weight factor:

$$V_{ik}^1 = 1 - a/\Delta\theta_{ik}/,$$
$$V_{ik}^2 = [1+(\sqrt{2}-1)(\Delta\theta_{ik}/\sigma_i)^2]^{-2},$$
$$V_{ik}^3 = \exp[-\ln 2(\Delta\theta_{ik}/\sigma_i)^2]$$

($\Delta\theta_{ik} = \theta_i^o - \theta_{ik}^c$; a is the preset constant which determines the angular range where the weight factor operates; if $V_{ik}' < 0$, the weight is ignored; $2\sigma_i$ is the half-width of the i-th experimental reflection calculated from: $(2\sigma)^2 = m tg^2\theta + n tg\theta + l$ (m, n, l are given constants)
3. The final refinement of the unit-cell parameters by minimizing the linearized Δ-function for the set reflection indices obtained at the optimization stage as well as the calculation of confidence limits and correlation coefficients of the parameters.
The program needs as input: the list of the $\theta^o(2\theta^o)$, the trial parameter values, the limiting index values, and the information necessary for calculating the list of theoretical reflections.