18.1-1 MODELS FOR EVALUATION OF THE CRYSTALLIZATION PROPERTIES. By Ev. K. Zhukov, Department of Chemical Engineering, Chengdu University of Science & Technology, Chengdu, Sichuan, People's Republic of China.

Model for evaluation of the crystallization processes has been derived as follows:

\[ \tau = \text{opt} \{ \dot{\gamma} \} \in \{ \dot{\theta}, \dot{\phi}, \ldots, \dot{\tau} \}, \quad \text{opt} \{ \dot{\gamma} \} \in \{ \text{Integers} \} \]

Another model needed for calculation of the objective values, such as

\[ \sigma = \text{opt} \{ \sigma_{\text{a}}, \sigma_{\text{b}}, \sigma_{\text{c}}, \ldots, \sigma_{\text{k}} \}, \quad \sigma_{\text{i}} \in \{ \text{Integers} \}, \quad \text{opt} \{ \sigma_{\text{i}} \} \in \{ \text{Integers} \}, \]

have also been obtained for us.

Where,

- \( \gamma^* \) = the optimal system of crystallization processes;
- \( \gamma \) = the index of the system considered.

Example has been given.

18.1-2 COMPUTER SOLUTION OF INVERSE DIFFRACTION PROBLEM IN LAUE METHOD. By E.V. Shulakov, Solid State Physics Institute, Chernogolovka, Moscow district, 142432 USSR.

The investigations performed recently have shown that the development in this direction looks promising (Floco, J. Appl. Cryst. (1978) 11, 712). Hart and Rietman, Acta Cryst. (1961) Supp. 337, 337. However, the known computer solutions require preliminary analysis of Laue patterns, i.e., of reflections or zones which have low indices. This procedure is necessary because the processing time and the number of indexing schemes drastically increase as the considered (hkl) range is increased. Typically, the range \((333),(222),(333)\) is used. This limits the application of known programs and necessitates further investigation.

In the present report the problem of Laue pattern indexing reduces to determining in a confined volume of the reciprocal or real space \((1, 3, 4) = (1, 3, 4)\) of an array of N lattice vectors the angles between which coincide with the measured ones to within \(\delta\).

This problem has been analyzed using the set theory. The expectation of the number of indexing schemes \(N\) has been calculated as a function of \(1, 3, 4\) and \(\delta\). It is shown that \(N(1, 3, 4)\) when \(\delta \leq 0.01\), where \(\delta = \max\{\phi, \psi, \gamma\} \in \{\text{Integers}\}\), \(\phi, \psi, \gamma\) are the angles between the measured and the calculated reflection angles.

To solve the problem of indexing we used the trial-and-error method. Different known algorithms of the method have been analyzed with relation to the computing time minimization. A new and more effective algorithm with dynamical choice of indexing schemes has been proposed. At \(1, 3, 4 = 9, 9\), the indexing of Laue patterns of a cubic crystal by this algorithm requires no more than 30 s at the computer speed of the order of \(10^6\) operations/s. In case the first reflection (or the zone axis) has low indices \(\leq 1\) the computing time is less than 1 min even at \(1, 3, 4 = 10^6\).

These ideas were realized in the computer program LAUE which comprises three main blocks. These are:

- F - program which simulates the Laue pattern for the given crystal orientation;
- R - program which indexes the reflections or zone axes \((9, 9, 9)\) by using the trial-and-error method and calculates the crystal orientation with respect to the laboratory coordinate system. The correctness of this procedure is checked by comparing the simulated and the experimental Laue patterns. The probability of ambiguous interpretation is thus excluded. The R-program allows for the redetermination of the crystal orientation by means of optimizing the crystal to film distance.

E-program establishes intercommunication between the F and the R programs and provides service routine for the LAUE program. The F-program can be used independently of the R-program and has wide applications.

The program requires about 20 000 words of core memory, is written in "Fortran-77" as a dialogue. The algorithm design and the program preparation have required about 4000 hs.


The program SPASY is constructed as a tool for the treatment of symmetry in structural relations. The two programs SYMOP (Burzlaff & Zimmermann, accepted for publication in Z. Krist.) for the derivation of symmetry operations from a space-group symbol and EPOS (Zimmermann, to be published in Z. Krist.) for the derivation of equivalent positions in a space group are combined. The resulting program is extended by a special procedure for the evaluation of subgroups. The evaluation of the maximal isoclass and isomorphous subgroups follows the idea used for the derivation of the symmetry operations from the space-group symbol. The handling of isomorphic or equivalent subgroups follows another concept. The procedure for this part is in preparation.