18. COMPUTING

18.1-1 MODELS FOR EVALUATION OF THE CRYSTALLIZATION PROCESSES. By Evgeny, 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:  
\[ \Delta = \text{opt} \left\{ \delta \right\}, \quad \delta \in \left\{ \text{Integers} \right\} \]

Another model needed for calculation of the objective values, such as  
\[ \sigma(g) = \text{opt} \left\{ f(g, \delta) \right\}, \quad f \in \left\{ \text{Integers} \right\} \]

These conclusions have been checked by comparison with the measured ones to satisfy the symmetry operations from a space-group symbol and the evaluation of subgroups. The evaluation of the symmetry operations from a space-group symbol and the evaluation of subgroups. The evaluation of the symmetry operations from a space-group symbol and the evaluation of subgroups. The evaluation of the symmetry operations from a space-group symbol and the evaluation of subgroups. The evaluation of the symmetry operations from a space-group symbol and the evaluation of subgroups.

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. The program for this part is in preparation. The program for this part is in preparation.

To solve the problem of indexing we used the trial-and-error method. Different known algorithms of the method have been analysed with relation to the computing time minimization. A new and more effectve algorithm with dynamical choice of indexing schemes has been proposed. At \( I_{\text{min}} = 5 \), \( N = 9 \), the indexing of Laue patterns of a cubic crystal by this algorithm requires no more than 0.01 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 (2) the computing time is less than 1 min even at \( I_{\text{min}} = 10 \). 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 (3xN x 3) 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 F-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 and the E-program 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 2. Krist.) for the derivation of symmetry operations from a space-group symbol and EPSO (Zimmermann, to be published in 2. 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.