18.1–1 MODELS FOR EVALUATION OF THE CRYSTALLIZATION PROCESSES. By Zeng Hong, 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:

$$G^*=\mathrm{Opt}\{G^\eta \mid G^\eta \in \{G^1, G^2, \ldots, G^k\},\ 0<k<\infty,$$
$$k \in \{\text{Integers}\}\}.$$

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

$$\sigma^*(G)=\mathrm{Opt}\{\sigma^\eta(G^\eta) \mid \sigma^\eta(G^\eta) \in \{\sigma^1(G^1), \sigma^2(G^2), \ldots, \sigma^k(G^k)\}$$
$$,\ \eta \in \{1,2,\ldots,k\},\quad 0<k<\infty,$$
$$k \in \{\text{Integers}\}\},$$

have also been obtained by us.

Where,

G^* = the optimal system of crystallization processes;

η = 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 (Ploc, J.Appl.Cryst.(1978) 11, 713; Hart and Rietman, Acta Cryst. (1981) Sup. A37, 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 $-(333) \leq (hkl) \leq (333)$ 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 ($-I_{max} \leq h,k,l \leq I_{max}$) of an array of N lattice vectors the angles between which coincide with the measured ones to within $\pm\ \delta$. This problem has been analyzed using the set theory. The expectation of the number of indexing schemes W has been calculated as a function of I_{max}, N and δ. It is shown that $W \leq 1$, when $N \geq \ln(K_s P_0^3)/\ln(n_v P_0^2)$, where n_v is the number of lattice points in the investigated volume; $K_s = n_v/n_{vs}$ (n_{vs} is the number of lattice points having no equivalent with respect to the symmetry operation), $P_0 = 2\delta/\pi$ and $P_0 = 3\delta/2\pi$ for forward and back Laue patterns, respectively. These conclusions have been checked by computer experiment and agree with the results by Ploc (1978).

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 $I_{max}=5$, $N=9$, $\delta=0.018$ rad 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 (<2) the computing time is less than 1 min even at $I_{max} \sim 10$.

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 ($3 \leq N \leq 9$) 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.

S-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 200000 words of core memory, is written in "Fortran-77" as a dialogue. The algorithm design and the program preparation have required about 4000 hs.

18.1–3 SPASY - A COMPUTER PROGRAM FOR THE EVALUATION OF SPACE GROUP PROPERTIES By H. Burzlaff and H. Zimmermann, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Loewenichstr. 22, Universität Erlangen-Nürnberg, FRG.

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 isotranslational 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.