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A numerical method for indexing uniaxial powder patterns. By I. R. TANNENBAUM*, B. J. LEMKE, and D. KRAMER, *Atomics International, A Division of North American Aviation, Inc., Canoga Park, California, U.S.A.*

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The numerical method of Hesse (1948) for the indexing of powder patterns of hexagonal and tetragonal materials has been modified to permit computation on digital computers.

In broad outline the test utilized by this method for tetragonality and for hexagonality rests upon the fact that both of these crystal systems give reflections such that

$$\sin^2 \theta = AM + Cl^2, \quad (1)$$

where $M = h^2 + k^2$, $A = \lambda^2/4a^2$ for the tetragonal case and $M = h^2 + k^2 + hk$, $A = \lambda^2/3a^2$ for the hexagonal case. $C = \lambda^2/4c^2$ in either case. The other symbols have their usual crystallographic meaning.

To solve a pattern the program computes from the observed diffraction angles, θ_i , the values for $\sin^2 \theta_i$ and tabulates these values, the values of $2 \sin^2 \theta_i$, and all cross sums of the types $2 \sin^2 \theta_i$, $\sin^2 \theta_i + \sin^2 \theta_k$, $3 \sin^2 \theta_i$, and $2 \sin^2 \theta_i + \sin^2 \theta_k$ (where the i and k range from one up to the total number of lines).

Each entry in this table of sums is compared with all other entries to find all equations of the type

$$\sum g_j \sin^2 \theta_j = 0 \pm \epsilon. \quad (2)$$

In equation (2) the summation is taken over four terms, the g_j have the possible values 0, ± 1 , ± 2 , ± 3 , and ϵ is the previously assigned limit of error.

Since M , l , A , and C are all positive, equation (2) implies that the sum of the products of the g_j by the M_j must equal zero and that the sum of the products of the g_j by the l_j^2 must equal zero. These are the working equations.

The trial and error solution to these equations is obtained by utilizing a starting combination of permissible M or l numbers in the equation containing the smallest number of variables. The numbers obtained from this starting combination are then substituted into the remaining equations in order of increasing numbers of unknowns. Each value obtained is checked against the

list of permitted values for the crystal system under consideration. When a set of numbers is obtained which is internally consistent, the pattern is considered solved.

If a solution is obtained the highest values of θ for which M_i and l_i were obtained are substituted in equation (1) and A and C are obtained by simultaneous solution.

The values of M and l are obtained for the θ_i 's which did not appear in the working equations by means of the newly determined, approximate, values for A and C and equation (3).

$$\sin^2 \theta_i = AM_i + Cl_i^2 \pm \epsilon. \quad (3)$$

The lattice parameters are then computed from the three most reliable high angle lines by the method of Cohen (1935, 1936).

Hesse's method does not apply to cubic crystals so that the tests for tetragonality and hexagonality are preceded by a test to determine if the sample is cubic. Cubic samples are, therefore, excluded from further computation.

This program was checked using data from the American Society for Testing Materials Diffraction Data Cards for indium, zirconium, and nickel. The angles were reported in degrees, using five significant figures although the machine used, IBM-709, automatically carries eight. Running time for the cubic sample tested (8 lines) was 30 seconds; for the tetragonal sample (19 lines), 75 seconds; for the hexagonal sample (25 lines), 2 minutes. If no solution is found, running time is less than three minutes. Running time is almost independent of number of lines. As it now is programmed, the code requires 10,200 locations and, hence, will run on any sixteen thousand word computer. On a sixteen thousand word computer, there is space for 40 angles, of which 15 are utilized to obtain up to 100 working equations. Reduction of the dimensions to 25 angles and 50 equations should permit the use of eight thousand word machines.

References

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Lattice-parameter changes in the pseudo-binary system of titanium and zirconium dihydrides. By A. D. MCQUILLAN and N. PESSALL, *Department of Physical Metallurgy, University of Birmingham, England*

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When titanium and zirconium are saturated with hydrogen they form dihydrides in which the metal atoms are arranged, at room temperature, in a face-centred cubic and face-centred tetragonal structure respectively, and the hydrogen atoms lie in the tetrahedral interstices. Sidhu *et al.* (1956) found, however, that below about 30 °C. the structure of titanium dihydride becomes face-centred tetragonal, and Yakel (1958) later showed that

the extent of tetragonality increased progressively with decreasing temperature. He also observed that the tetragonality of zirconium dihydrides decreased with increasing temperature but still remained tetragonal at 500 °C. The form of his parameter-temperature curves for zirconium dihydride at 500 °C. suggest that the structure may very probably become face-centred cubic in the temperature range 550–600 °C., and the behaviour