12.2-4 THE PROBLEM OF COMPUTER IDENTIFICATION OF X-RAY DIFFRACTION POWDER PATTERNS. By E.K.Vasil'ev, Institute Earth's Crust, Sib. Depart. Acad.Sci. USSR, Irkutsk-33, M.S.Nakhmanson, Vses. Nauchno-Issled. Inst. Nauch. Priborostr., Leningrad, USSR.

Theoretical principles of computer identification X-ray diffraction powder and spectral data are described with application of database standards. A generalized structure of identification procedure (Hanawalt's strategy) is considered. The conclusion is made That the majority of computer systems of identification (Johnson-Vand, Frevel, Snyder, Philips, Siemens, IBM and oth.) have been developed on the basis of some empirical assumptions on a series of searching files and criteria of fitting unknown and standard patterns. The theoretical basis of search/match procedures are based on Fiala's vector form of X-ray diffraction powder patterns representation, on statistical distribution of search signs of standards and on study of crystal chemistry features of database. From an analysis of a mineral subfile distributions of peaks in patterns as regarding their locations and intensities and also distributions of standards due to their crystal chemical parameters were obtained. These distributions allow to establish a selection technique of most informative peaks on patterns, to introduce a compressed handling of spectra the form of binary codes, to prepare an expressed way of inwestigation of database structure.

As a measure of closeness between unknown and standard patterns it is advisable to use Euklidian distance between these compared spectra in the sign space. All criteria of closeness, which are used in practice (frequency, Johnson-Vand and oth.) could be obtained and ranged by their exactness if these measures could be simplified and different models of line representation could be used.

An investigation of the structure of mineral subfile has allowed to select series of groups of similar patterns and a group of low informative patterns (6-12 peaks in the pattern) for which the probablity of casual good coincidence with unknown is higher. It is shown, that the autenticity of identification results depends directly on the structure of database. This appears as a result of computer selection of low informative and of similar standards between true phases. It was stated that similar patterns correspond to standards in which linear lattice parameters differ not more, than by 0.1-0.2Å. Patterns are practically indistinguishable by X-ray diffraction method, if the differences of parameters are of the order of 0.02-0.05Å. This circumstance puts a physical limit of possibilities of the method of qualitative X-ray phase analysis.

A formalization of the method is realized in which information on elementary composition of samples is used. It is shown, that in this case most informative elements can be pointed out. Numerical criteria of closeness of samples and standards by their chemical composition can be constructed.

12.3-1 THE FLUX GROWTH AND CRYSTALLOGRAPHIC INVESTIGATION OF A NEW COMPOUND, $Pb_3Bi_{0.1}Nb_2O_{8.15}$, IN THE $PbO-Bi_2O_3-Nb_2O_5$ SYSTEM. By Nie Shuyi, Li Deyu, Pu Zhifen and Xu Yueying, Shanghai Institute of Ceramics, Academia Sinica, China.

According to a method of calculation proposed by Li Deyu et al., the acousto-optical figures of merit of compounds in the $PbO-Bi_2O_3-Nb_2O_5$ system lie in the range 14-19. These values are comparable with that of $PbMoO_4$ crystals, widely used in practice. The studies carried out on this system aim at exploring new acousto-optical materials.

A new compound composed of $3PbO.Nb_2O_5$ and Bi_2O_3 in a molar ratio of 20:1 has been found by using X-ray phase analysis, electron probe and differential thermal analysis. This compound is a congruent one in the $3PbO.Nb_2O_5-Bi_2O_3$ pseudo-binary system.

The transparent dark-orange crystals form hexagonal plates when grown by the flux method. The diffraction symmetry determined from transmission Laue and Weissenberg photographs is D3d - 3m. The unit-cell dimensions determined by means of a CAD-4 diffractometer are a - 7.454, c - 96.277Å. The space-group is P312, P321, P3m1, P31m, P3m1 or P31m. The indices of strong reflections are consistent with the extinction rule for R3m, R3m or R32.

An X-ray powder diffraction pattern was recorded in a Guinier-Hägg focussing camera, diameter 100mm, with highly monochromatic $CuK\alpha_1$ radiation (λ - 1.5405981Å). Finely powdered silicon (a - 5.430880135Å at 25°C) was added as an internal standard. Single-coated Shanghai X-ray Fluorescence Film No. 4 was used. Film measurements were made by means of a computer-controlled LS-18 line-scanner. The unit-cell dimensions after refinement by means of the program PIRUM are a - 7.4600(8), c = 96.356(13)Å.

Comparisons between the unit-cell parameters and space-group of this new crystal and those of compounds in the $PbO-Nb_2O_5$ system lead to the conclusion that the former is a new type of chlorite with a superlattice along the c-axis. The thickness of a sheet in the new type of chlorite structure with superlattice is 3.18Å. The c-axis of the unit-cell of $Pb_3Bi_{0.1}Nb_2O_{8.15}$ consists of 30 sheets.

Homogeneous and perfect single crystals with sizes up to ϕ ~1.5cm and L ≥2cm were grown by the Bridgman method, using the same composition as for the crystals grown by the flux method. An acousto-optical figure of merit M2* ~40 was obtained from the observed values n - 2.589 and v[001] - 3x10⁵ m/s. This showed that the crystal $Pb_3Bi_{0.1}Nb_2O_{8.15}$ is a potential acousto-optical material.