18.1–4 ANALYSIS OF INTERATOMIC VECTOR-SETS BY THE S-FILTRATION METHOD. By T.I.Malinowski, Inst. of Applied Physics Ac.of Sc.MSSR,Kishinev;B.M.Schedrin,N.M.Andrushevsky,Moscow State University, Moscow, USSR

While determining the crystal structure by Patterson function analysis, the information about the space symmetry G(T,S) with the translation group $T(\underline{t}_1,\underline{t}_2,\underline{t}_3)$ and the group $S=\{A_k|A_k=(N_k|\nu_k)$, $k=\overline{1,p}\}$ is very important. For representation of the three-dimensional Patterson function - the vector set of interatomic distances the problem is to determine the point structure $Q(X,S)=\{S_k(\underline{x}_i)$, $i=\overline{1,n}; k=1,p\}$ from a vector set $V(X,S)=\{A_k\underline{x}_i - A_q\underline{x}_j\}$. Since $V(X,S)=\{Im\ (Q,A_q\underline{x}_j)$, $q=\overline{1,p}$; $j=\overline{1,n}\}$ where $Im(Q,A_q\underline{x}_j)=\{S_k(\underline{x}_i) - A_q\underline{x}_j$, $i=\overline{1,n}$; $k=\overline{1,p}\}$ is the image of the structure shifted by the vector $-A_q\underline{x}_i$, then $Q(X,S)\subset[V(X,S)\oplus\underline{x}_0]$, $x_0\in X$ - is one of the basic vectors of the structure. Hence, the filtration algorithm from $[V(X,S)\oplus x_0]$ of the symmetric-equivalent vectors of the group S, deduces the image of the structure Q(X,S) relative to the fixed coordinate base $(\underline{t}_1,\underline{t}_2,\underline{t}_3)$. The isolation of additional copies $Q(\underline{\omega}\pm X,S)$ is possible, if for some $A_k\in S$ and $\overline{x}_j\in X$ the condition $\underline{x}_0 \mp A_k\underline{x}_j = \underline{\omega}^*$ is fulfilled, where $\underline{\omega}^*\in\Omega(G)$ is the set of the shift vectors in the equivalent origins and is determined by the solution of the equation set $(N_k - E)\underline{\omega} = \underline{n}$, $k=\overline{1,p}$; $\underline{n}=(n_1,n_2,n_3)$, $n_i\in Z$. It may be noted, that in all the polar groups such a transformation A^* and $\underline{\omega}\in\Omega(G)$, can be found, so that the condition $\underline{x}-A^*\underline{x} = \underline{\omega}^*$ is fulfilled for any $\underline{x}$, i.e. the vector sets of the structures with the appointed symmetry are solved unsynonymously. The mentioned conditions of synonymity of the solution supplement the earlier known ones (Cochran W. 1958 Acta Cryst. v.11). The S-filtration method is especially effective for structures with heavy atoms, when $V_0(X,S)$ is perhaps not a full set, but contains a full (or nearly full) image of the structure reflected in the heavy atom. The use of information about the transformation of group G(T,S) permits to determine from $V_0(X,S)$ one or several basic shift vectors with the help of the procedure "prediction - correction".

Symbol interpretation: | such that; C contained in; ∈ element of; ⊕ direct sum.

18.1–5 ON THE SINGULAR EXPANSION METHOD APPLIED TO THE ANALYSIS OF A DIFFRACTION LINE SHAPE. By N.V.Shokhirev,Inst.of Chem.Kinetics Sib.Branch of Academy of Sciences, 630090 Novosibirsk and Yu.A.Rosenberg, I.L.Lunev, L.G. Andrievskaya, L.I.Kleshchinsky, V.S.Korkushko, Inst.of Transp.Engineers,664074 Irkutsk, USSR.

The observed X-ray diffraction profile is connected with the physical profile of a crystal through the Fredholm integral equation of the first kind with an instrumental function as the kernel. The kernel form determines unambiguously the singular values and two conjugate sets of singular functions (for a symmetric operator these are eigenvalues and eigenfunctions). The experimental profile is expanded in functions of one of the sets, the physical profile is expanded in those of conjugate set. The expansion coefficients of the physical profile are determined by the corresponding expansion coefficients of the experimental profile and by singular values. In contrast to the standard Fourier deconvolution procedure the present method does not assume a difference kernel and does not impose strict limitations on the range of measurements which makes it possible to work with weakly resolved lines. Moreover, the method proposed allows to reliably control the accuracy of the physical profile reconstruction determined by experimental errors and the range of measurements. The present method has been applied to the analysis of lattice imperfection parameters for polycrystals of synthetic diamond, tin dioxide and aluminium. The data are discussed.

18.2–1 SLANT, CONTUR, AND PLOT: COLOUR GRAPHICS PROGRAMS FOR THE XTAL SYSTEM By N. Spadaccini, M.A. Spackman and A. Imerito, Crystallography Centre, University of Western Australia, Nedlands 6009, Australia.

Recent additions to the XTAL Program System (Hall et al., Acta Cryst. (1980) A36, 979) display atomic information as contours or ellipsoids. Modifications of existing XTAL routines ORTEP and PLOT enable thermal ellipsoids to be displayed in a variety of modes and output devices. CONTUR contours a density map for either the programs FOURR or SLANT. Both ORTEP and CONTUR generate plot commands that are translated by PLOT into specific code for a range of output devices. All routines are written in portable RATMAC code. Special features of SLANT, CONTUR and PLOT will be described, along with some recent applications.

CONTUR is a general contouring program for producing low-resolution maps (e.g. an E-map) or high resolution maps of accurate difference densities. Single or multiple layers are permitted; linear or cubic interpolation and several types of contour level input may be specified. Curves with arbitrary dash and gap sequences are allowed.

SLANT calculates densities in any general plane by interpolation from a map of the asymmetric unit. A plane is defined by 3 points and linear (8 points) or cubic interpolation (64 points) is used to calculate each point in the plane.

PLOT converts plot commands from ORTEP or CONTUR into code suitable for a selected output device. Current versions of PLOT support matrix and character printers; pen plotters and graphics terminals. Adaption to the local plotting environment is achieved via the redefinition of a small number of macro commands, and the possible addition of local subroutines.