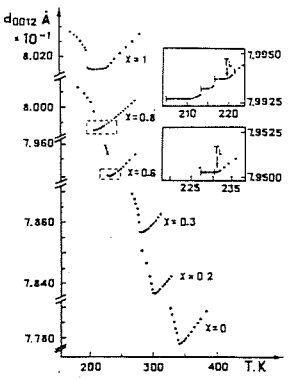
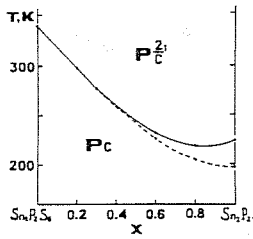
20.4-12 INCOMMENSURATE PHASES AND INVAR EFFECT. V.Sh. Shekhtman, T.K. Barsamian, S.S. Khasanov, Institute of Solid State Physics Academy of Sciences of the USSR, Chernogolovka

As has been found (S.S.Khasanov, V.Sh.Shekhtman Ferroelectrics, 1986, v67, 47-54), three-dimensional modulation is observed in proustite ($Ag_3AsS_3$)(R3c) in the incommensurate phase (IC) range (50-60 K). $Sn_2P_2Se_6$ ($P2_1/c$) displays one-dimensional modulation (T.K.Barsamian, S.S.Khasanov, V.Sh.Shekhtman, Yu.M.Vysochanskii and V.Yu.Slivka, Ferroelectrics 1986, v67, 47-54) in the IC range (197-225K) adjacent to the ferroelectric transition. In the temperature ranges indicated these crystals showed satellite reflections and the temperature dependences of wave vectors were measured by X-ray diffraction methods. However, the characteristic feature of the main reflection in the IC range, that is, the temperature dependence of the interplanar spacing of the basic lattice and the intensity, are most noteworthy. The invar effect, that is, the temperature independence of the lattice parameter, was observed in the IC range on the temperature dependence of the interplanar spacings of the main lattice, $d_{100}$ and $d_{001}$, for proustite and $Sn_2P_2Se_6$, respectively. In this respect it is of interest whether an invar effect exists in the IC range, when the concentration of one of the components of the mixed compound $Sn_2P_2(SeS)_6$ whose phase diagram depicts the Lifshitz point (Fig.2), is varied. The temperature dependence of d(0012) of system $Sn_2P_2(Se_{1-x}S_x)_6$ was measured for X=0; 0.2; 0.6; 0.8 and 1 (Fig.1). An invar effect was found to exist or compositions with X=0.6; 0.8; and 1. Satellite reflections, whose wave vectors varied smoothly with temperature, were observed for the same compositions in the ranges, corresponding to the invar effect. This is an indication that the limits of the invar effect fix unambiguously the IC ones. When the crystal composition concentration is changed, the linear coefficients of thermal expansion vary essentially beyond the IC range, whereas the invar effect remains stable. The temperature range of the invar effect was used for constructing the T-X phase diagram (Fig.2). The triple point on the phase diagram terminated the line separating the para- ferroelectric second order phase transition, then the line diverges into the para- IC second order phase transition line and the IC - ferroelectric first order phase transition line. So, the triple point is by defination the Lifshitz point. The width of the IC temperature range satisfies the relation $T_i-T_c=A(X-X_L)$, where A=53.7 and $X_L=0.28$.




20.4-13 STATIC AND DYNAMIC STRUCTURE OF QUASICYSTALS AND OTHER INCOMMENSURATE CRYSTAL PHASES. By R. Currat and T. Janssen, Institut Laue-Langevin, Grenoble , France and Institute for Theoretical Physics, University of Nijmegen, The Netherlands.

Incommensurate crystal (IC) phases in general and quasicrystals in particular, have symmetry properties that are appropriately described in a space with more than 3 dimensions (de Wolff, Janner and Janssen). This higher-dimensional "superspace" approach may be applied to describe the structure, the diffraction pattern and certain physical properties.

The general expression for the geometric structure factor, fundamental for the structure determination, as given for IC phases by de Wolff (1977) and Yamamoto (1982) may be used ,for example, in the particular cases of modulated structures, discommensuration type structures and quasicrystals. The central idea here is that the structure factor for an IC phase is in one-to-one correspondence with that of a periodic structure in more dimensions.

It has been shown that macroscopic properties as the morphology yield information on the microscopic structure as well (Rasing, Dam and Janner). The higher-dimensional approach to the morphology may also be generalised to the case of quasicrystals.

For the dynamic structure factor a general description may be given in terms of the eigenmodes of the structure. It requires a formulation of the lattice dynamical problem for IC phases, which can also be given in higher-dimensional space. It is specified for the various classes of IC phases.

Using the treatment of lattice vibrations in the superspace approach one may discuss the behaviour of the Debye-Waller factor for the various classes of IC phases: modulated structures, composite crystals and quasicrystals. The most important contributions to this DW factor will be discussed.

20.4-14 DISORDER, AVERAGE STRUCTURE AND SUBGROUPS By O. Jarchow, Mineralog.-Petrogr. Institut der Universität Hamburg, Germany.

In disordered structures besides diffuse maxima frequently occur groups of sharp maxima, which are describable by a pseudoselection rule. This main maxima belong to an average structure with regular space group.
Taking into account also the diffuse maxima, the cell of the average structure must be enlarged in 1, 2 or 3 dimensions. The disordered structure is built up by many ordered domains of different sizes. Each domain has single crystal character, but unlike domains can be structural different. In most of the OD structures this domains are in close t,k-subgroup relationship to the average structure (Hermann, Z.Krist, 1929).
t= transl. equivalent subgroups. Owing to the decrease in point group symmetry, when the translational group is preserved and k= class equivalent subgroup, with the same point group, but different translation lattices.Such subgroup relations are listet up for disordered polytypes, built up by equivalent layers.
The practical use of subgroup tables in structure determination of polytypes may help to understand the principles. 1.step: The diffraction pattern must be in standard orientation, that means $c^*$ is parallel to diffuse streaks The supercell must be multiples of the average cell (mA, nB, pC with m ›n). 2.Step: The possible space group of the average structure is to be determined from sharp maxima only. 3.Step: The enlargement factors of the supercell are to be determined (usual 2,1,1; 2,1,2; 2,2,1; 2,2,2 for subgroups of the tetragonal system) and also the Bravais type of the a,b-net (P or C-net for 2,2,1 or 2,2,2). The information of 1.-3. are sufficient to find the possible symmetry of the t,k-domains. The space group of the average structure gives the entrance of the row and the enlargement factors the column in the determination tables of subgroups.