

Table 2. Bond lengths and angles

S - O	O - S - O	O - O
1.578x1	109.58x3	2.543x3
1.534x3	109.36x3	2.504x3

To keep the thermal parameter and the tetrahedron bond lengths to a reasonable value, the following models

(ordered and disordered) are proposed:

Table 3

Atom	Coordinate	Gossner Model	Bellanca Model	Ordered Model (This work)	Disordered Model
M <sub>1</sub>	000	Na	Na	KNa	KNa
M <sub>2</sub>	00½	K	Na	KNa	KNa
M <sub>3</sub>	$\frac{1}{3} \frac{2}{3} z$	K	K	K	KNa

M: Metal atom Na, K or KNa.

Three glaserites  $K_3Na(SO_4)_2$ ;  $K_3Na(CrO_4)_2$  and  $K_3Na(SeO_4)_2 - ((K_3Na(SeO_4)_2)$  have super structures along c-axis, Mehrotra (4)), and are presently under investigation on the basis of ordered and disordered models.

References:

1. Bellanca, A. (1943), Periodicodi mineralogia 14, 69-97.
2. Gossner, B. (1928), Neues Jahrb. Miner. 57A.
3. Mehrotra, B.N.; Eysel, W. & Hahn, Th. (1977) Acta Cryst. B33, 305-306.
4. Mehrotra, B.N. (1977), N. Jh. Miner. Mh., 9, 398-407.

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05.1-62 LOW TEMPERATURE STRUCTURAL TRANSFORMATIONS IN THE  $Pb_{1-x}Sn_xSe$  SYSTEM. By V.I. Ivanov, V.Sh. Shekhtman, I.M. Shmytko, Solid State Physics Institute of the USSR Academy of Sciences, 142432 Chernogolovka, USSR

A precision investigation has been carried out of the temperature dependence of interplanar spacings of the  $Pb_{1-x}Sn_xSe$  narrow-band semiconductor system ( $x=0,37; 0,42; 0,43$ ) (I.M. Shmytko et. al., Solid State Physics, vol.22, N5, 1384, 1980). Structure transitions of the first order have been observed at 170K and 260K for  $x=0,42$  and  $x=0,43$ , respectively, the hysteresis being 80K. The phase transitions are accompanied with the symmetry decrease,  $F_{cub} \rightarrow P_{ortho}$  and are based on the cubic lattice twinning along the system (010)/(001). The orthorhombic phase unit cell parameters at  $T=255$  K are:  $a=11,694$  A,  $b=4,473$  A,  $c=4,191$  A. The low temperature phase is realized in the form of developed "parquet" systems with the following orientation relations  $[100]_{cub} // [100]_{ortho}$ ;  $[011]_{cub} // [010]_{ortho}$ ;  $[001]_{cub} // [001]_{ortho}$ .

Phase transition for  $x=0,37$  has not been observed. Precision measurements of  $d = d(T)$  have, however, revealed the anomalies in the temperature dependence of the lattice parameter within the temperature range 215-250 K, depending on composition. The anomalies observed are related to the evolution of the narrow-band semiconductor phonon spectrum in the temperature regions corresponding to the valence band-conduction band inversion (L.K. Vodopianov, I.V. Kutcherenko et. al., Letters in JETP, 27, 101, 1978).

05.1-63 THE ROLE OF B SITE CATION DISORDER IN DIFFUSE TRANSITION BEHAVIOUR OF  $Pb(In_{1/2}Nb_{1/2})O_3$  PEROVSKITE FERROELECTRIC By P. Groves and A.M. Glazer, Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, U.K.

In  $Pb(In_{1/2}Nb_{1/2})O_3$  the degree of order of the  $In^{3+}$  and  $Nb^{5+}$  cations in the B sites of the structure can be controlled by suitable thermal annealing. For samples which have been well ordered by annealing for a long time, it is found that single crystals show a first order ferroelectric phase transition from dielectric measurements. With increasing disorder, the crystals exhibit the classical diffuse phase transition typical of a ferroelectric relaxor, with a broad Curie range and strong low-frequency dielectric Debye relaxation in the transition range. Single-crystal X-ray diffraction measurements of the size of the ordered microregions, and of the degree of order are presented for different annealing times. A series of semi-continuous, high-temperature, single-crystal X-ray diffraction photographs, show how the character of the transition changes with prolonged heat treatment. The Curie temperature  $T_c$ , increases with annealing time following an exponential law.

05.1-64 THE CHANGE IN SYMMETRY AT THE I-II PHASE TRANSITION IN DICALCIUM BARIUM PROPIONATE. By S. Singh, Allen Clark Research Centre, Plessey Research Centre, Plessey Research Ltd., Caswell, Towcester, Northants., U.K. and F. R. Wondre, Clarendon Laboratory, Oxford University, Parks Road, Oxford OX1 3PU, U.K.

Dicalcium barium propionate,  $Ca_2Ba(C_2H_3COO)_6$  undergoes two phase transitions at atmospheric pressure: the I-II, first order transition at approximately 267K and the II-III transition at 240K. The symmetry of the low temperature phase II has been characterised by X-ray diffraction methods and has space group Pnma or Pn2<sub>1</sub>a. Powder and single crystal techniques have been used to explain the formation of two kinds of twins, present in phase II, in terms of the phase I lattice. Lattice parameters have been determined in the temperature region of 125K to 300K. The symmetry of phase III was investigated. The relationship between dicalcium barium propionate, DBP and dicalcium barium acrylate, DBA is discussed.