PS10.04.25 STRUCTURAL PHASE TRANSITIONS IN Rb_2CoCl_4 SINGLE CRYSTAL. Novikova Maria Sergeevna, Tamazyan Rafael Arshamovich, Institute of Crystallography RAS, Leninskiy prospekt, 59 Moscow Russia

Temperature dependence of unit cell parameters, q modulation vector and intensities of satellite reflections in the temperature interval 120-305 K were measured and phase transitions from high-temperature phase to incommensurate and from incommensurate to ferroelectric phase established. X-ray diffraction experiments were carried out at the temperature of 348, 294, 202, 177 K. The structure of the high-temperature phase was refined at T=348 K (R=0,046;wR=0,034) and T= 294 K (R=0,025;wR=0,017) correspondingly. Atomic structure of the following incommensurately modulated phase was refined under T=203 K using 4-dimentional space group P(Pcmn/ss(-1)) (R-factors R=0,04;wR=0,046 over main reflections and R=0,079;wR=0,096 over satellite reflections). Temperature dependence of the q vector shows a 5 K histeresice under ferroelectric phase transition. The ferroelectric phase was refined at T=177 K in space group P(Pc21n/s(-1)(-1)) (R-factors: over main reflections wR=0,088, wR=0,108 over satellite reflections). The results were compared with those of our previous structural studies of Rb_2ZnBr_4. Reasons for different behavior of the q vectors in these two structures were analyzed.

PS10.04.26 POLYTYPE TRANSFORMATIONS INDUCED BY UNIAXIAL LOADING IN ZnS CRYSTALS. V.Sh.Shekhtman, S.S.Khasanov, S.Z.Shmurak, B.Zh.Narymbetov Institute of Solid State Physics, 142432 Chernogolovka, Russia.

The structural change of atomic layer sequences by mechanical loading resulting in the interswitching of polytype modifications is an interesting feature of ZnS crystals. In preceding experiments it was established that by oriented compression the polysynthetic structure undergoes to syngle crystal sphalerite. Also it proved to be real the transitions 4H ->3C, 6H ->3C. In this connection it was useful to study the experimental parameters are important for these transformations. The results of investigations of plastic deformation effects on wurtzite crystals are presented. It is shown that the uniaxial compression is accompanied by structural transitions from 2H through polytypes 12R, 9R, 6H to sphalerite 3C.

The samples were cut in such a way that the slide plane - active basal (0001)-was at angle 45° to the direction of loading. The initial and final structural states were analysed by X-rays diffraction and Raman scattering technique. We note that the ordered motion of partial dislocations during plastic deformation causes step by step, structural transfomations by interswitching of close packed layers. The structural state to which 2H-wurtzite goes over depends on specific conditions- external shape of specimen, impurity concentration and temperature of deformation. In the series of experiments with various polysynthetic structures the examples of 2H->12R->3C, 9R->6H->3C, 3C'->3C" transformations were demonstrated. The structure after deformation is characterizied as a intermediate combination of polytypes with sphalerite - 3C. The possible mechanisms of transformation are discussed.

This supported by Russian Foundation of Basic Research,RFFI grant #94-02-03277

PS10.04.27 PECULIARITIES OF QUASICONTINUOUS MEDIUMS. V. A. Sosnovsky, Technical University of Moldova, bul. Shtefan chel Mare 168, Kishinev, 277012, Republic of Moldova

The systems with large number of atoms in a cluster form the quasicontinuous mediums (QM). They have the highest symmetry without external actions (the limit groups of symmetry: ∞/mmm, ∞ mm, ∞/∞ 2, ∞/∞/mmm, ∞/m, ∞/∞mm).

Spontaneous magnetization can take place in the mediums with symmetry point groups 5/m,m,5. Torsional directions in the QM have the symmetry point groups 3,5,5/2. They take place in the all classes QM except centrecymmetrical point groups and provide optical activity. Such property possess the symmetry point groups 532,5/2,5.

The spontaneous polarization increase which is proportional to the temperature changing is known as pyroelectric effect. Pyroelectric classes of QM are 5,532,5m,5/m.

The absolute value of spontaneous polarization P_s (m5m,m35,5m2) and spontaneous magnetization I_s (5/m,5) change.

PS10.04.28 THE INCOMMENSURATE STRUCTURE OF 1T-TaS_2. A. Spijkerman, A. Meetsma, G.A. Wiegers, S. van Smaalen*) and J.L. de Boer. Dept.of Chemical Physics, Nijenborgh 4, 9747 AG Groningen, The Netherlands. *) Lehrstuhl f. Kristallograpie, D-95440, Bayreuth, Germany

The structure of 1T-TaS_2 was studied earlier by several authors and attracted attention for its 'star of David' like clustering of the Ta-atoms (13 in a cluster) in the incommensurate roomtemperature phase. The structure was studied in detail by Brouwer (1978, Thesis) and by Yamamoto (1983, Phys. Rev. B. 27, 7823-7826). The first author used a $\sqrt[a]{13}$ x $\sqrt[a]{13}$ x 3c supercell (equivalent to the commensurate approximation 3/13, 1/13, 1/3 of the q-vector which in reality is 0.245, 0.068, 1/3), both for the intensity measurements as well as for the structure refinement, whereas the second author used Brouwer's intensity data in an incommensurate superspace description. Both authors adopted spacegroup $P\bar{3}$ in the refinements.

There are several unsatisfactory aspects in the just mentioned state. First the intensities of the by the supercell approximated satellite positions were of course not collected at their true positions. Secondly both Brouwer and Yamamoto were aware of the existence of other classes of satellites but these were just not measured; moreover Yamamoto's description of these higher order satellites (6 around each of the 12 'fundamental' satellites) was misplacing 2 of these 6.

We remeasured the structure factors, now associating 84 satellites to each main reflection and refined the data using the program Jana94 (Petricek). Complete results including the choice of spacegroup, together with a comparison with previous structure models, will be presented.