PS10.04.25 STRUCTURAL PHASE TRANSITIONS IN Rb₂CoCl₃ SINGLE CRYSTAL. Novikova Marina 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) over satellite reflections (R-factors: over main reflections wR=0.088, wR=0.108 over satellite reflections). The results were compared with those of 4-dimentional space group P(Pcmn/ss(-1)) (R-factors: over main reflections wR=0.096 over satellite reflections). Temperature dependence of the q vector shows a 5 K histeresis under ferroelectric phase transition. The ferroelectric phase was refined at T=177 K in space group P(Pc2₁n/x(-1y(-1))) (R-factors: over main reflections wR=0.088, wR=0.108 over satellite samples were cut in such a way that the slide plane - (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 transformations 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 polyhedral structures the examples of 2H->12R->3C, 9R->6H->3C, 3C'-3C" transformations were demonstrated. The structure after deformation is characterized as an intermediate combination of polytypes with sphalerite - 3C. The possible mechanisms of transformation are discussed.

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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 atomic structure of the polyhedral structure undergoes to single crystal sphalerite. Also it proved to be real the transitions 4H ->3C, 6H. The samples were cut in such a way that the slide plane - (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 transformations 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 polyhedral structures the examples of 2H->12R->3C, 9R->6H->3C, 3C'-3C" transformations were demonstrated. The structure after deformation is characterized as an intermediate combination of polytypes with sphalerite - 3C. The possible mechanisms of transformation are discussed.

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PS10.04.27 PECULIARITIES OF QUASICONTINUOUS MEDIUMS. V. A. Sosnovsky, Technical University of Moldova, bul. Shefian 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, =m, =m, =m, =m).

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 3,5/2,2. They take place in the all classes QM except centrosymmetrical point groups and provide optical activity. Such property possess the symmetry point groups 5/2,2,5.

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

The absolute value of spontaneous polarization Pₓ (m3m,m35,5m2) and spontaneous magnetization Iₓ (5/m,5) change.


The structure of IT-TaS₂ 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 6/13 x 6/13 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 P₃ for 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.