20.3–7 POLYTYPISM IN MELT-GROWN CRYSTALS OF CdI_2, PbI_2 and $CdBr_2$. By G. C. Trigunayat and S. K. Chaudhary, Department of Physics, University of Delhi, Delhi-7, India.

Single crystals of the polytypic materials CdI_2, PbI_2, and $CdBr_2$ have been grown and purified by the method of zone-refining. The experimental set-up used for the purpose has been described. The crystals have been investigated by x-ray diffraction to know how the impurities influence the growth and polytypism of the crystals. Only the most stable small period polytypes have been found to exist in the three materials. The x-ray photographs have been found free from streaking and arcing, revealing absence of both random and ordered stacking faults in the crystals. Significant structural transformations have been observed in the PbI_2 crystals at room temperature. The results have been discussed in terms of creation and expansion of stacking faults.

20.3–8 POLYTYPISM AND PHASE TRANSFORMATION ZINC BLENDE-WURTZITE. By G.Steger, H.Jagodzinski and F.Frey, Universität München, W-Germany

The zinc blende-wurtzite transformation occuring between 1200-1300 K was studied by X-ray experiments on powders and single crystals of different origin in order to investigate the dependence on various parameters (grain size, chemical purity, temperature, temperature-time-treatment) and to clarify the connection with polytypic and disordered structural variants. We found that the original degree of disorder, but not the chemical purity is of essential influence. Well ordered single crystals transform hardly into the wurtzite polymorph, but polytypic variants occur as function of the individual T-T-treatment. Polytype arrangements extend over more than 1000 Å, the volume ratio is greatly determined by the original crystal quality. Polytypes do not act as "nuclei" for the transformation, this role play more probably disordered structural variants. A quantitative analysis of the degree of disorder in frame of 1-d disorder models could only be performed by several assumptions due to an inhomogeneous sample behaviour. Obviously polytypic and disordered sequences are results of rearrangement processes frozen in for kinetic reasons. We conclude that polytypes in ZnS are no stable phases in a strict sense. Statistical fluctuations are responsible for the transformation which has more the character of a solid state reaction. The transformation is due to a nucleus formation process, the activation energy of which being affected by defects, strains,.. A growth process of any kind completes the transformation: new wurtzite crystals with different orientations occur

20.4–1 ИСКАЖЕНИЕ СОДАЛИТОВОГО КАРКАСА В СТРУКТУРЕ ТРИКЛИННОГО ЛАЗУРИТА (ТЛ)

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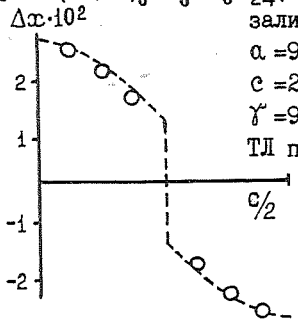
Лазурит Малобыстринского месторождения Прибайкалья представлен как изотропными, так и в различной степени анизотропными разновидностями. Монокристаллы максимально анизотропного минерала $(Na,Ca)_8Al_6Si_6O_{24}(SO_4,S,CO_3,Cl)_2 \cdot nH_2O$ оказались триклинной сингонии: $a = 9.071$, $b = 12.905$ ($\approx a\sqrt{2}$), $c = 25.734$ ($\approx 2a\sqrt{2}$) Å, $\alpha = \beta = 90°$, $\gamma = 90.207°$. Основу структуры ТЛ представляет искаженный содалитовый каркас, (Al,Si)-O=1.63-1.71 Å. Тетраэдры в структуре ТЛ закономерно смещены по оси x из положений содалитовой структуры. Величина смещений атомов Al, Si при y=const удовлетворительно описывается уравнением $\Delta x = 12.5(\cos 2\pi z + \cos 2\pi z / |\cos 2\pi z|)$. На рис. пунктирной линией изображена вычисленная кривая изменения Δx и нанесены средние экспериментальные смещения атомов Al,Si



20.4–2 ON MODULATED CRYSTAL OPTICS. By B.W.H. van Beest and A. Janner, Institute for Theoretical Physics, University of Nymegen, Nijmegen, The Netherlands.

Ewald's foundation of crystal optics is based in an essential way on the lattice translational invariance of perfect crystals (Ewald, Ann. der Physik (1916) 49, 1). The existence of incommensurate crystals missing such a symmetry asks for a proper extension of Ewald's theory. Furthermore, one is interested in knowing how the superspace group symmetry (De Wolff, Janssen and Janner, Acta Cryst. (1981) A37, 625) of incommensurate crystals is reflected in the optical properties.

Following Ewald, a plane electromagnetic wave propagating through the crystal is the result of a superposition of spherical waves radiating from oscillating dipoles located at the atomic positions, each dipole being excited by the fields of all the other ones. The case of a modulated crystal is considered and the Hertz-potential of the dipole assembly is evaluated in terms of (modulated) lattice sums (Van Beest and Janner, Physica 122A (1983) 263). Those expressions indeed have the right symmetry properties required by the superspace group of the crystal.

Work is in progress in deriving optical dispersion in modulated (incommensurate) crystals. The merits of a group theoretical approach of the electromagnetic excitations in crystals, similar to the one used with lattice vibrations, are investigated.