Single crystals of Na_2SO_4III are grown by metastable nucleation from aqueous solutions at $50^{\circ}C$. This phase is orthorhombic with space group Cmcm and cell constants a = 5.607A°, b = 8.96A°, c = 6.967A°, Z = 4. The structure is refined to R = 4.5%. The structure consists of tetrahedral and octahedral framework. The thermal vibrations of most of the atoms are large along c-axis (Zeit. Krist. - in Press). Single crystals of this phase III (fig. 3a: Weissenberg Photograph O-layer) on heating upto phase I and cooling, show oriented domains of phase III and phase II in the same crystals (fig. 3b: Weissenberg photograph O-layer).
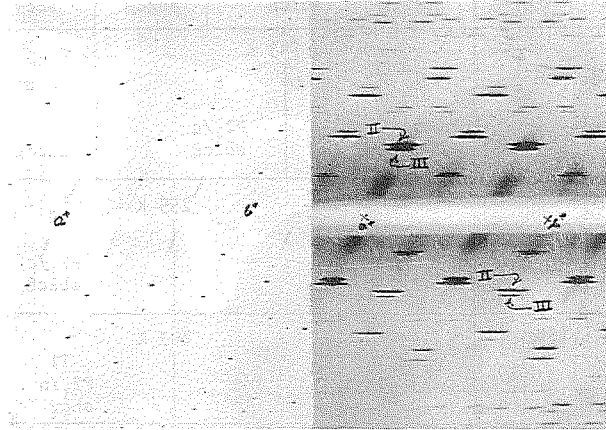

Fig. 3a   Fig. 3b

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05.1-36   ON THE LOW TEMPERATURE PHASE TRANSITION IN $(NH_4)_2SO_4$. By Y.A. Badr, G. Said, M. Mikhail and S. Awad, Faculty of Science, Cairo University, Cairo, Egypt.

An ultracryostat of type KT"90S" and multidecameter (NF-Dekameter type WTW) provided with a special cell were used to determine the temperature dependence of the dielectric constant and dielectric loss over a wide range of frequencies of polycrystalline ammonium sulphate in the region of the low temperature phase transition. A sharp increase was observed in the values of ε' & ε'' at about $-50^{\circ}C$. Besides, a dielectric dispersion was detected and it was found to be more pronounced in the higher temperature phase of $(NH_4)_2SO_4$. This dispersion was attributed to piezoelectric resonance (Badr, et al, Physica status solidi (a)53,K51(1979)).
The observed sudden increase in the values of the dielectric constant and dielectric loss below $-50^{\circ}C$ was inferred to the ferroelectric behaviour of phase II of $(NH_4)_2SO_4$.
DTA studies showed that also a sharp peak at $-50^{\circ}C$ which indicated that the phase transition occurring in ammonium sulphate at $-50^{\circ}C$ was of the first order type. TMA thermograms showed that this transition was associated with a rapid increase in the expansion coefficient. Such increase in the lattice parameter might be attributed to the enhanced rotation of electric dipoles associated with the deformed $SO_4^{=}$ ions. The deformation of the $SO_4^{=}$ ions, in addition to their orientational motion, are thought to be responsible for the ferroelectric behaviour of $(NH_4)_2SO_4$ below $-50^{\circ}C$.

05.1-37   CRYSTAL STRUCTURE CHANGES AND PRINCIPAL DEFECTS IN IRRADIATED CRYSTALS. By E.V. Kolontsova, A.E. Korneyev, V.F. Lutsenko. Moscow State University, Karpov Institute of Physics and Chemistry, Moscow, USSR.

Under the influence of radiation the crystals of Ca_2SiO_4, $CaAlO_3$, $BaTiO_3$, $PbZrO_3$, ZrO_2, $KNbO_3$, $CsNO_3$ and SiO_2 (quartz, cristobalite) transform into the structural states, which are close to the high-temperature phases of unirradiated crystals. The investigation of radiation defects and comparison of crystal structure changes under the influence of irradiation and heating are important for the determination of such transformation mechanism.
By using X-ray diffuse scattering and X-ray crystal structure analysis it was shown that in neutron-irradiated quartz (E $\geqslant$ 0.5 Mev; 3 - 6$\times 10^{19}$ncm^{-2}; $T_{irrad} \sim 100^{\circ}C$) structural states intermediate between α and β-quartz are formed (E.V. Kolontsova, A.E. Korneyev, V.P. Lutsenko. Dokl. Akad. Nauk SSSR (1979), 247,80). The dose dependences of these changes are qualitatively analogous to those in unirradiated crystals at about the $\alpha - \beta$ phase transition temperature. The investigation of diffuse X-ray scattering intensity (I_d) dependence of q (q-distance between reciprocal space point and the next nearest reciprocal lattice node) showed, that I_d falls off like q^{-2}. $I_d \sim q^{-2}$ means (P.H. Dederichs. J. Phys. (1973), F3,471), that isolated point defects are principal defects in neutron-irradiated quartz and therefore they are responsible for the new structural states.
The changes of diffraction pattern from single crystal and powder $CsNO_3$ during heating and X and γ-irradiation (0.1 - 3.0$\times 10^9$R; E= 1.3 Mev; $T_{irrad} \leqslant 40^{\circ}C$) were also studied.
Analysis of these experimental results allows to make a conclusion, that radiation-induced transformation of crystal structure is realized without forming of displacement spikes.
According to the analysis of our and literature data one can conclude that it is possible to consider isolated point defects concentration as an instability parameter under the influence of radiation for some compounds (such as α-SiO_2, $BaTiO_3$, $CsNO_3$, and maybe $KNbO_3$, $PbZrO_3$).