

## STUDY ON CRYSTAL STRUCTURE AND GROWTH OF PYROELECTRIC

TRIC PHASE OF TRIGLYCINE SULPHATE. By X. Solans, M. Font-Altaba C. Miravittles and M. Aguiló. Dept. de Cristallografia, Univ. Barcelona, Granvia 585, (Barcelona-11); Instituto Jaime Almera, CSIC-Barcelona, and Facultat de Química, Tarragona.

Franco et al. has shown the inhibition of ferroelectric switching, when TGS crystals are treated during 1000 hours with an electric potential. In order to determine whether the inhibition may be explained in terms of the structure, we have determined the crystal structure of a switching fatigued crystal. The results obtained are:

$C_6H_{17}N_3O_{10}S$ . Monoclinic,  $P2_1$ ,  $a=9.152(2)$ ,  $b=12.640(2)$ ,  $c=5.768(1)$ ,  $\beta=105.5(2)^\circ$ ,  $Z=2$ . The structure was solved by direct methods with the MULTAN system of computer programs and refined by full-matrix least squares. R final 0.066 (Rw=0.072).

The main difference among the crystal structure of the virgin TGS and the switching fatigued, are the cell parameters. The glycine I is twisted about  $180^\circ$  around the a-axis and  $44.8^\circ$  around the b-axis with respect to the position of these groups in the virgin crystal, and the sulphate ion is twisted only  $44.8^\circ$  around the b-axis; these rotations produce a non-simple movement in glycine II and III.

05.2-28 ELECTRICAL CONDUCTIVITY AND DIELECTRIC CONSTANT OF PURE AND DOPED TRIGLYCINE SULPHATE SINGLE CRYSTALS. By M. Gaffar and A. Abu El-Fadi Physics Department, Faculty of Science, Assiut University, Assiut, Egypt.

The dielectric constant and both the A.C. and D.C. electrical conductivity of pure and doped single crystals of TGS are investigated in the temperature range 300-450°K. The influence of Ni, Cu, Co, Cr and Fe ions on the type of conduction, type of transition, transition temperature, Curie Weiss constants and the dielectric constant are studied. The effect of sample thickness and pressure contact on the electrical conductivity is also discussed. Some interesting features of the correlation between the valency and ionic radii of the dopant is presented.

05.2-29 GROWTH AND PROPERTIES OF FERROELECTRIC SINGLE CRYSTALS OF TETRAGONAL TUNGSTEN BRONZE STRUCTURE TYPE. By Ju. I. Kopylov, V. B. Kraychenko, A. T. Sobolev, Institute of Radio-engineering and Electronics, Academy of Sciences of the USSR, K. Marx av. 18, Moscow, GSP-3, 103907, USSR.

Crystal-chemical stability analysis is made for tetragonal tungsten-bronze structure type  $A_4A_2C_4B_8B_2O_{30}$  (where  $A$  and  $A'$  are large cations in five- and four-sided channels of the structure,  $C$  are cations in three-sided channels,  $B'$  and  $B''$  are multi-valent cations in two types of octahedra) in case when  $A$  are cations of alkaline and alkaline-earth metals. Single crystals of some solid solutions of this type are grown. The stability field of ferroelectric crystals having this structure type is determined for  $(Ba, Sr, Ca)Nb_2O_6$  system. This field is shown to be much broader than for ceramic samples studied earlier (G. A. Smolensky et al., Fizika tverdogo tela, Moscow-Leningrad, 1959, v. 2, p. 244). Dielectric, optical and electrooptical properties of  $(Ba, Sr, Ca)Nb_2O_6$  single crystals are studied.

Curie temperatures and half-wave voltage values increase and dielectric constant at room temperature  $\epsilon'_c$ , widths of  $\epsilon'_c(T)$  maxima and extent of broadening of ferroelectric phase transition decrease with increasing Ba contents in the crystals. Line widths of  $Gd^{3+}$  ESR spectra in the crystals increase with increasing of phase transition broadening. Structural reasons of this are given.

05.2-30 RELATIONS BETWEEN THE STRUCTURE, MORPHOLOGY AND PHYSICAL PROPERTIES OF TRIGONAL AND MONOCLINIC  $TRAl_3[BO_3]_4$  CRYSTALS. L. I. Leonyuk and N. I. Leonyuk, Department of Geology, Moscow State University, Moscow, USSR.

Two structural types of  $TRAl_3[BO_3]_4$  crystals are known. The one, possessing a R32 space group (structural type of huntite) is more stable. It exists in the entire series of rare-earth-aluminium orthoborates. At temperatures exceeding 1270 K, TR-Pr-Eu compounds are crystallized according to the C 2/c space group as well.

There is a direct relationship between the development of hkl faces and the experimentally observed total intensity of X-rays reflected from the corresponding atomic lattices (e.g.  $I_{001} + I_{002} + I_{003} + \dots + I_{00l}$ ). Faces  $\{110\}$ ,  $\{\bar{1}10\}$  and  $\{010\}$  of monoclinic crystals correspond to two trigonal prisms  $\{1120\}$  and  $\{2\bar{1}10\}$  in huntite-structured crystals. The base-pinnacoid  $\{001\}$  conforms to that having the same index in the trigonal crystal. The huntite rhombohedron  $\{1011\}$  of the monoclinic crystal is represented by a rhombic prism  $\{111\}$  and pinacoid  $\{202\}$ . The violated significance of the faces in monoclinic crystals as compared with the trigonal ones is due to the peculiarities of their internal structure.

$TRAl_3[BO_3]_4$  crystals possess piezoelectric and nonlinear-optical properties. These properties vanish in the phase transition into the monoclinic modification.