PS-08.04.15 THE POLARITY OF THERMAL CONDUCTIVITY IN LiNbO₃ AND LiTaO₃. By M.Tokonami*, O.Tachikawa, Y.Ono and T.Shinozaki, Mineralogical Inst., Faculty of Sci., Univ. of Tokyo, Japan, and S.Kan, Daiso Co.,LTD., Japan, and K.Yamamoto and J.Hikita, R&D Center,Toshiba Ceramics Co.,LTD., Japan.

Thermal conductivity is believed to be a property of second-rank symmetrical tensor and then to have no difference between any given direction and the reverse. We have studied the hypothesis that the conductivity might reflect the polarity of the materials (Tokonami,M. et.al.,(1992), Abstract of AsCA'92, Singapore, 15R-18). We measured thermal diffusivity of polar crystals by laser flash method and observed significant differences between (+) and (-) directions along polar c-axis . Frn a variety of polar crystals, LiNbO₃ and LiTaO₃ are chosen since their polarity is hard to be reversed at room temperature, and synthesized crystals with good homogeneity are readily obtained.
The oriented specimen were prepared: The single crystals are made by the CZ techniques and carefully taken poling procedure. The discs (∼ 3mm thick and ∼10mm in diameter) were cut out from single domain materials of LiNbO₃ and LiTaO₃.
Thermal diffusivity were measured by ULVAC TC-3000 flash-type thermal constant analyzer.
The diffusivity with the (+) direction is significantly larger than one with the (-) direction and the difference of the diffusivity in LiTaO₃ larger than that of LiNbO₃. Finally, the thermal conductivity, which is product of the diffusivity, the specific heat and the density, is also concluded to be one of the polar properties.

PS-08.04.16 CRYSTAL STRUCTURE ANALYSES OF 10μm-SIZE REAlO3 SINGLE CRYSTALS OBTAINED BY FLUX METHOD: APPLICATION OF A UNIQUE DIFFRACTOMETER USING A CURVED PSPC AND CONVENTIONAL SHIELD TUBE X-RAY SOURCES
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10μm size single crystals of REAlO3(RE=Dy-Lu) were synthesized using KF-flux in air at around 1000C and at ambient pressure. The crystal structures were investigated by a single crystal X-ray diffraction method. Data collections were performed with a curved one dimensional position sensitive proportional counter(PSPC) using a conventional shield tube X-ray sources(CuKα, 35KV, 25mA, with Ni-filter) (Horiuchi et al.,AsCA'92, 15Q-09, Singapore, Nov.,1992). The distance from X-ray source through the specimen to detector is 310mm and X-ray beam was collimated by hole of 0.1mmφ. Crystal orientation can be controlled by ω, χ and φ axes as for a four-circle goniometer but with a completetly different hardware system (DX-MAP2/JEOL). PSPC can cover 0-140 degrees for 2θ angles. Software systems for data collection were developed in this investigation. Crystal structures of REAlO3(RE=Dy-Lu) belong to a perovskite-type structure with space group, Pbnm, as reported by Dernier and Maines(Dernier & Maines, Mat. Res. Bull.,6,433-440,1971). The atomic parameters were refined based on the collected intensities. The system can also be applied to analyze crystallographic orientation

relationship among the phases which comprize mineral textures using 10μmφ X-ray beams.

PS-08.04.18 INVESTIGATION OF PURE AND Th-DOPED LaAlO₃ CRYSTAL STRUCTURE. BY Yu Yude*, Chang Yingchuan, Xie Sishen, Hou Desen Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P.R.China. H. Boysen Institüt für Kristallogie und Min. der München Univsität, 8000 München 2, F. R. G.

In recent years LaAlO₃ has been widely used as the base material of the superconducting thin film and it has caused great interest. The pure and Th-doped LaAlO₃ crystals were investigated by neutron scattering and X-ray diffraction respectively.

High purity(99.99%) La₂O₃ and Al₂O₃ were mixed and pressed into pellets. Slowly heated up to 1350°C for two days and then pure LaAlO₃ was obtained. The neutron powder scattering measurement was made at the Grenloben neuclear reactor with incident wavelength 1.594 Å. The Rietveld profile refinements of LaAlO₃ were carried out and space group R$\bar{3}$c is determined. The structural parameter was listed in Table 1. It is obvious that only the oxygen atoms are slightly displaced from idea position. From the projection onto the X-Y plane, it can be found that the oxygen atoms rotate around the center of the octahedron and it is possible to be the real reason to cause the rhombic symmetry for the pure LaAlO₃. The single crystals of LaAlO₃ doped with Th(0.15, 0.2, 0.25, 0.5 wt%) were grown by the Czochralski method. X-ray powder measurements were made by rotated target X-ray diffractometer with Cu$_{Kα1}$ radiation. X-ray diffraction data were indexed and lattice parameters were refined by least-squares refinement. The results show that the doped LaAlO₃ belongs to the cubic system.

The (100) and (210) reflecxions were observed and no extinction condition was found. The possible space group might be $Pm\bar{3}m$, $P432$, $P\bar{4}3m$. The relation between the lattice parameters and dopent content is plotted in Fig. 1. More detail study of Th-doped LaAlO₃ crystals will be continued.
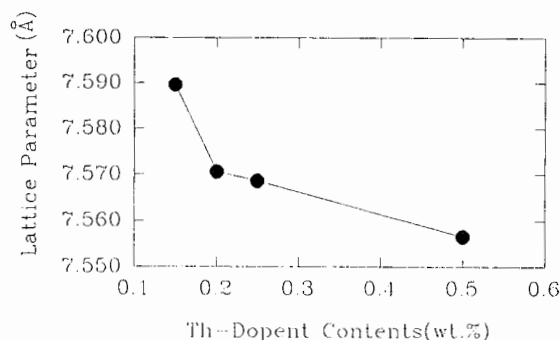

Fig.1 Lattice Parameters of Th-doped LaAlO₃.

ATOM	POSITION	X	Y	Z	N	B[$\AA^2$]
La	6a	0	0	0.25	1.0	0.25(2)
Al	6b	0	0	0	1.0	0.43(5)
O	18e	0.474(1)	0	0.25	1.0	0.57(2)

Table 1 Structural parameters of $LaAlO_3$.

PS-08.04.19 A SINGLE-CRYSTAL X-RAY-DIFFRACTION STUDY OF THE ORTHORHOMBIC Al_3Mn PHASE. By N.C.Shi[†], X.Z.Li[‡], Z.S.Ma[†] and K.H.Kuo[‡], † X-Ray Laboratory, China University of Geosciences, Beijing 100083, China. ‡ Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O.Box 2724, Beijing, China.

Al_3Mn (with a stoichiometrical composition $Al_{29}Mn_{10}$), M_r=1331.8, orthorhombic, $Pn2_1a$, a=14.837(4), b=12.457(2), c=12.505(2)$\AA$, V=2311.4(8)$\AA^3$, Z=4, D_x=3.56, Mo Kα=0.71069$\AA$, μ=5.62mm^{-1}, F(000)=2355.02, T=room temperature, R=0.068 for 1550 reflections. About 2/3 Mn atoms have icosahedral coordination. In a repeat unit b, there are 4 interlocked icosahedra (two Mn and two Al) consisting of 1 pentagonal prism and 4 antiprisms. The icosahedral subunits form a network on (010) constituting a layer structure, consisting of an almost "flat" layer F sandwiched between two puckered P and p layers in the sequence of PFpP'F'p'..., where P'F'p' is rotated from PFp by 180° around the layer normal. A similar layer structure has also been found in the π-AlMnM (M=Ni,Cu,Zn) phases. Both these two crystalline structures can be obtained from that of the Al-Mn decagonal quasicrystal with a periodicity of 12.4$\AA$ along the tenfold axis by substituting a rational ratio of two consecutive Fibonacci numbers F_{n+1}/F_n for the irrational τ=(1+√5)/2 in two quasiperiodic directions on the plane normal to the tenfold axis.

PS-08.04.20 SYNTHESIS AND CRYSTAL STRUCTURE OF $RNb_3(Se_2)_6$, WITH R=In,Sb. By S.Q. Deng, H.H. Zhuang, J.S. Huang and J.L. Huang, State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Academia Sinica, Fuzhou(350002), PRC.

In recent years, a number of intriguing physical phenomena related to the charge density wave (CDW) have been observed in some low dimensional materials. Because most of these materials were found to be of the early transition metal chalcogenides, we have studied the ternary system R-Nb-Se (R=In,Sb).

$InNb_3(Se_2)_6$ was synthesized by the reaction of Nb_2Se_9 and In with approximately stoichiometric proportions at 773-873K.

The preparation of $SbNb_3(Se_2)_6$ succeeded by an analogous procedure with the stoichiometric elements as the starting reactants at 973k.

The structures are determined by single crystal X-ray diffraction method. The results showed that $InNb_3(Se_2)_6$ (a=9.450(1), c=19.068(9)A, P4/mnc,z=4) and $SbNb_3(Se_2)_6$ (a=9.466(2), c=19.075(3)A, P4/mnc,z=4) are very similar in structural parameters. Both of the structures are composed of the one dimensional infinite chains [$Nb_3(Se_2)_6$]$_\infty$ along the c axis with the third component R (R=In,Sb) intercalated between them. In one [$Nb_3(Se_2)_6$]$_\infty$ chain, the distances between the niobium atoms are arranged in a periodic sequence of ···Nb-3.037-Nb-3.248-Nb -3.248A-Nb··· for $InNb_3(Se_2)_6$. According to the Nb-Nb distances

in the sequence, the $Nb_3(Se_2)_6$ unit can be formally viewed as the building block of a chain. In comparison with the Nb-Nb bond lengths in (MX$_4$)nY(Gressier, Meerschaut, Guemas,Rouxel & Monceau, J. Solid State Chem., 1984, 51, 141) and α-NbI$_4$ (Dahl & Wampler,Acta Cryst.,1962,15,903), the Nb-Nb distances in the above sequence should also involve chemical bonding. Therefore the $Nb_3(Se_2)_6$ units in one chain may be viewed as combined together by the bridging $(Se_2)^{2-}$ ligands as well as the Nb-Nb bonding. Considering the long distance (6.69A) between the center lines of different chains, the metal-metal interaction is very anisotropic and typical of the one dimensional character. The bond lengths of Nb-Se (2.558(1)~2.721 (2)A) and Se-Se (2.325(2)~2.356(2)A) are all in agreement with those in other known niobium selenides such as NbSe$_3$ (Hodeau,et al.,J. Phys. C.,11, 4117). The In atoms located in the one dimensional channels between different chains form the tetragonal pyramid coordination geometry with four equidistant Se atoms from four different chains. The height of the tetragonal pyramid, which shows the position of the intercalated atom in the channel, for InSe$_4$ is 0.364A, and which reveals the main difference between the structures of $InNb_3(Se_2)_6$ and $SbNb_3(Se_2)_6$ (0.589A for SbSe$_4$). The large distance of In···Se (3.233(1),3.263(3)A for Sb···Se) suggests that the In(Sb) atoms are inserted as in $In_{~3}Mo_{15}Se_{19}$ (Gruttner & Yvon, Acta Cryst.,1979,B35,285). Unusual high values of U_{33}/U_{11} (2.42 and 4.51 for In and Sb, respectively) are indicative of the large thermal vibrations of the intercalated atoms along the c axis. Electrical resistivity measurements indicate that $InNb_3(Se_2)_6$: ρ_a=19.2(3), ρ_b=19.4(4), ρ_c=0.74(1)Ω cm (298K); $SbNb_3(Se_2)_6$: ρ_a=26.0(5), ρ_b=25.5(5), ρ_c=0.11(2)Ω cm (298K) and the dash rises of ρ_c at ~165 and 64K for $InNb_3(Se_2)_6$; ~185, 70 and 30K for $SbNb_3(Se_2)_6$ in the range of 289K-298K.

PS-08.04.21 A PATTERSON SYNTHESIS WITH PROFILES OF DIFFRACTION INTENSITIES. By Y.Ono* and M.Tokonami, Mineralogical Institute, Faculty of Science, University of Tokyo, Japan.

It has been shown previously (Kaplow, R., Rowe, T.A. & Averbach, B.L.(1968). Phys. Rev. 168, 1068-1079) that the 'Coupling coefficient' of atomic interaction to be defined in study of a radial distribution function of hexagonal selenium by the powder method. As for single crystals, with a conventional structure analysis by integrated diffraction intensities, we can only obtain average atomic interactions, such as thermal atomic vibration, of all unit cells in the crystal. In this work, to obtain the coefficients also in single crystals, a 'direct' Patterson synthesis which is unusually calculated with a data set of profiled intensities collected by step-scan is investigated. The sample was a monoclinic α-selenium crystal and the intensity data have been collected in the range of $2\theta < 45°$ with wave length of 0.7Å. The scan width and step width of the peak profile data were +0.5° and 0.01° in ω and total data of hkl used were 778. In the Patterson map with profiled intensity data, the periodicity of unit cells have disappeared:Remarking the origin peak, usually 'equivalent' peaks' height and widths become the lower and the broader as far from the origin. This means that the stronger interactions of