08-Inorganic and Mineralogical Crystallography

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.

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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 avariety 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 (\sim 3mm thick and \sim 10mm in diameter) were cut out from single domain materials of LiNbO $_3$ and LiTaO $_3$.

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 10 µm-SIZE REAIO3 SINGLE CRYSTALS OBTAINED BY FLUX METHOD: APPLICATION OF A UNIQUE DIFFRACTOMETER USING A CURVED PSPC AND CONVENTIONAL SHIELD TUBE X-RAY SOURCES H.Horiuchi*, S.Nojima, Mineral. Inst., Faculty of Science, Univ. of Tokyo, Hongo, Bunkyo, Tokyo 113, Japan, M.Tanaka, Photon Factory, Nat. Lab. for High Energy Physics, T.Shishido and T.Fukuda, Inst. for Materials Research, Tohoku University, Katahira, Sendai 980, Japan.

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 investigated by a single crystal ata collections method. Data diffraction performed with a curved one dimensional position sensitive proportional counter(PSPC) using a conventional shield tube X-ray sources(CuKa, 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 $0.1mm\phi$. Crystal orientation can be controlled by $_{\omega}$, 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 Software systems for data collection 2θ angles. were developed in this investigation. structures of REAlO3(RE=Dy-Lu) belo Crystal belong to 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 $10\mu\text{m}\phi$ X-ray beams. This work was financially supported by Nihon-Itagarasu and Ohkura Kazuchika Foundations.

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 $LaAlO_3$ has been widely used as the base material of the superconducting thin film and it has caused great interest. The pure and Th-doped $LaAlO_3$ crystals were investigated by neutron scattering and X-ray diffraction respectively.

High purity (99.99%) La_2O_3 and Al_2O_3 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 $LaAlO_3$. The single crystals of $LaAlO_3$ 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 $Cu_{K\alpha 1}$ radiation. X-ray diffraction data

were indexed and lattice parameters were refined by least-squares refinement. The results show that the doped $LaAlO_3$ belongs to the cubic system.

The (100) and (210) reflections 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 $LaAlO_3$ crystals will be continued.

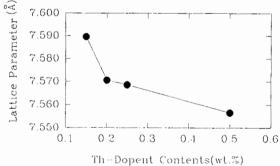


Fig.1 Lattice Parameters of Th-doped LaAlO3.