08-Inorganic and Mineralogical Crystallography

PS-08.04.04 THE POLARITY OF THERMAL CONDUCTIVITY IN LiInO$_3$ AND LiTaO$_3$ by H. Tokonami*, O. Takikawa, Y. Omo and T. Shinoda, Mineralogical Inst., Faculty of Sci., Univ. of Tokyo, Japan, and K. Yamamoto and J. Kimoto, R&D Center, Toshiba Ceramics Co., Ltd., Japan.

Thermal conductivity is believed to be a property of second-rank asymmetrical 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), Abstr. ASCA'92, Singapore, 158-158). We measured thermal diffusivity of polar crystals by laser flash method and observed significant differences between (+) and (-) directions along polar axes.

For a variety of polar crystals, LiInO$_3$ and LiTaO$_3$ 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 crystal were made by the Cz techniques and carefully taken polishing procedure. The discs (-3 mm thick and ~10 mm in diameter) were cut out from single domain materials of LiInO$_3$ and LiTaO$_3$.

Thermal diffusivity was measured by ULVAC TCI-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 LiTaO$_3$ larger than that of LiInO$_3$. 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.


10μm-size single crystals of PSAO3(RE= Dy-Lu) were synthesized by the horizontal flux method at around 1000°C and at ambient pressure. The crystal structures were investigated by a single crystal X-ray diffractometer using a conventional curved GP tube X-ray source (CuKα, 35 K, 25 mA, with Ni filter) (Horiiuchi et al., ASCA'92, 158-158, Singapore, Nov., 1991). The distance from the X-ray source through the specimen to detector is 310 mm and the X-ray beam was collimated by a 0.1 mm Cystal orientation can be controlled by a 1° x and z axes thus for a four-circle goniometer but with a completely different hardware system (IX-MAP/2EDL). FPSG can cover 0-140 degrees for 2θ angles. Software systems for data collection were developed in this investigation. Crystal structures of PSAO3(RE= Dy-Lu) belong to a perovskite-type structure with space group Pm̅n, as reported by Dierick and Maisner (Dierick & Maisner, Mat. Res. Bull. 11. 8, 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 comprise mineral textures using 10μm X-ray beams. This work was financially supported by Nimon-Itagaya and the Kure Kusukida Foundations.

PS-08.04.18 INVESTIGATION OF PURE AND TH-DOPED LaAlO$_3$ CRYSTAL STRUCTURE. BY Y. Yade*, Chang Yi, Tianmin, Xie Sihe, Hou Qiaoning, China H. Boyen Institut für Kristallografie und Min. der München Universität, 8053 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%) LaAlO$_3$ and Al$_2$O$_3$ were mixed and pressed into pellets. Slowly heated up to 1350°C for two days and then pure LaAlO$_3$ was obtained. The neutron powder scattering measurement was made at the Grenoble reactor using incident wavelength 1.594 Å. The Rietveld profile refinement of LaAlO$_3$ was carried out and space group R3c is determined. The structural parameters are listed in Table 1. It is obvious that only the oxygen atoms are slightly displaced from initial 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 rhombohedral symmetry for the pure LaAlO$_3$. The single crystals of LaAlO$_3$ doped with Th(0.15, 0.25, 0.5, 1.0%) were grown by the Czochralski method. X-ray powder measurements were made by the two target X-ray diffractometer with CuKα$_1$ 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 Pn̅3m, P4̅32, P4̅3m. The relation between the lattice parameters and dopant content is plotted in Fig. 1. More detail study of Th-doped LaAlO$_3$ crystals will be continued.
Table 1 Structural parameters of LaAlO₃.

<table>
<thead>
<tr>
<th>Atom</th>
<th>Position X</th>
<th>Y</th>
<th>Z</th>
<th>N</th>
<th>B [Å²]</th>
</tr>
</thead>
<tbody>
<tr>
<td>La</td>
<td>6a</td>
<td>0</td>
<td>0</td>
<td>0.25</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>6b</td>
<td>0</td>
<td>0</td>
<td>0.43</td>
<td>1.0</td>
</tr>
<tr>
<td>O</td>
<td>18e</td>
<td>0</td>
<td>0.476(1)</td>
<td>0.25</td>
<td>1.0</td>
</tr>
</tbody>
</table>

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PS-08.04.29 A SINGLE-CRYSTAL X-RAY-DIFFRACTION STUDY OF THE ORTHORHOMBIC Al₂Mn, Al₃Si₃, and Mn₃Si₃ PHASES. By N.C. Shi, Z.-Y. Lu, Z.-S. Li, and C.-H. Ku, X-Ray Laboratory, China University of Geosciences, Beijing 100083, China. \( \text{X} \) Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, P.O. Box 2724, Beijing, China.

Al₃Si₃ (with a stoichiometric composition Al₃Si₃): M₃=131.8, orthorhombic, \( \text{Pn} \)=2, \( a=14.837(4), b=12.457(2), c=12.585(2) \), \( V=2321.4(4) \), \( Z=2, D_c=3.56, M_{Ko}a=7.1069 \mu m, m=5624 \mu m^3, F(000)=2355 \). The temperature factor \( \tau=0.0946 \) for 1550 reflections. About 2/3 M₃ atoms are in the basal plane coordination. In a repeat unit \( \text{b}, \) there are 4 interlocked isocubates (two M₃ and two Al₂) consisting of 1 pentagonal prism and 4 antiprisms. The isocubate subunits form a network on \( \text{O}_1 \) by forming a layer structure, consisting of an almost "flat" layer \( \text{p} \) sandwiched between two puckered \( \text{p} \) layers in the sequence of \( \text{p}^3\text{p}^3\text{p} \), where \( \text{p}^3\text{p} \) is rotated from \( \text{p} \) by 90° around the layer normal. A similar layer structure has also been found in the \( \text{KAlMnO}_6 \) (M=Na, K) phases. Both these \( \text{p}^3\text{p} \) structures can be obtained from that of the Al₂M₃ (Al₂M₃, Cu₃M₃) phases. All these \( \text{p}^3\text{p} \) structures are stable under high pressure and have been observed in low dimensional materials. Because most of these materials were found to be of the transition metal chalcogenides, we have studied the ternary system K-Mn-Se (K-In-Se).

InK₃Se₃ was synthesized by the reaction of K₃Se and In with stoichiometric compositions at 773-873K. The preparation of \( \text{InMnSe}_3 \) succeeded by an analogous procedure with the stoichiometric compositions at 773-873K.

PS-08.04.20 SYNTHESIS AND CRYSTAL STRUCTURE OF NH₄Se\( \_n \). WITH R-In-Se. By S. Ono, H. Ishikawa, J. S. Hwang, J. D. Huang, State Key Laboratory of Structural Chemistry, Peking University, Institute of Research on the Structure of Matter, Academia Sinica, Beijing (030002), PRC.

In recent years, a number of interesting 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 transition metal chalcogenides, we have studied the ternary system K-Mn-Se (K-In-Se).

\( \text{InMnSe}_3 \) was synthesized by the reaction of \( \text{InMnSe}_3 \) and In with stoichiometric compositions at 773-873K. The preparation of \( \text{InMnSe}_3 \) succeeded by an analogous procedure with the stoichiometric compositions at 773-873K.

PS-08.04.21 A PATTERSON SYNTHESIS WITH PROFILES OF DIFFRACTION INTENSITIES. By S. Inoue, M. Kononov, Mineralogical Institute, Faculty of Science, University of Tokyo, Japan.

It has been shown previously (Kaplow, R., Rowe, T.A. & Auerbach, B.L., 1965, Phys. Rev. A6, 1698-1707) that the "coupling coefficients" 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 structural 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 crystal, a "direct" Patterson synthesis which is usually calculated with a data set of profile intensities collected by step-scan is investigated. The sample was a monoclinic selenium crystal and the intensity data have been collected in the range of 2θ=45° with wave length of 0.72. The scan width and step width of the peak profile data were 0.3° and 0.1° in 2θ and total data of hkl used were 178.

In the Patterson map with profiled intensity data, the periodicity of unit cells have disappeared: Remarkable the origin peak, usually "equivalent" peaks' height and width become the lower and the broader as far from the origin. This means that the stronger interactions of