MS14-P1 Crystal structure behaviour in the La(Pr)AlO_3–$TbAlO_3$ systems.

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In order to study the phase and structural behaviour in the La(Pr)AlO_3–$TbAlO_3$ pseudo-binary systems series of $La(Pr)_{1-x}Tb_xAlO_3$ samples with x in the range of 0.1 – 0.9 were prepared from the oxides La_2O_3, Pr_6O_{11}, Tb_4O_7 and Al_2O_3 by a combination of solid state reaction and arc melting in Ar atmosphere. The crystal structures and of the solid solutions $La(Pr)_{1-x}Tb_xAlO_3$ and their thermal behaviour in a wide temperature range of 12–1173 K have been investigated by using high-resolution powder diffraction applying synchrotron radiation (beamline B2, HASYLAB at DESY) and DTA/DSC methods. All crystallographic calculations (refinements of the lattice parameters as well as full profile structure refinements) were performed by means of the Windows version of the Crystal Structure Determination program package WinCSD.

From the results of the XRD phase and crystal structural analysis it was established that two kinds of solid solutions with rhombohedral and orthorhombic structures exist at ambient temperature. A wide immiscibility gap exists between these two perovskite-type phases. All lattice parameters decrease monotonically with increasing Tb content in $La(Pr)_{1-x}Tb_xAlO_3$ and a strong anisotropy in the lattice contraction is observed for the rhombohedral and orthorhombic phase. In agreement with Vegard's law an almost linear dependence is observed for the normalized cell volume.

At elevated temperatures, continuous phase transitions from rhombohedral to cubic structures was observed in the $La_{1-x}Tb_xAlO_3$ and $Pr_{1-x}Tb_xAlO_3$ samples with $x < 0.4$ and $x < 0.2$ correspondinly. Onset of another type of phase transition was detected in the $La_{0.4}Tb_{0.6}AlO_3$ and $La_{0.5}Tb_{0.5}AlO_3$. This phase transition was defined as a first-order transformation from the orthorhombic to a rhombohedral structure, similar to other pseudo-binary system based on $LaAlO_3$ [1].

Low-temperature (LT) examination revealed a sequence of phase transformations in the $Pr_{1-x}Tb_xAlO_3$ samples with $x<0.3$, whereas the solid solutions with $x \geq 0.4$ remain orthorhombic below RT. DTA/DSC and synchrotron powder diffraction experiments revealed a sequence of LT phase transformations R-3c↔Imma↔C2/m phase transitions in the $Pr_{1-x}Tb_xAlO_3$ specimens.

Based on the results of in situ synchrotron powder diffraction examinations and DTA/DSC measurements as well as available literature data, the phase diagram of the pseudo-binary system $LaAlO_3$–$TbAlO_3$ and $PrAlO_3$–$TbAlO_3$ has been constructed.

[1] Basyuk, T. V., Vasylechko, L. O., (2010). *Bull. of Lviv Polytechn. Nat. Univ.* **681**, 3-10.

Keywords: perovskites, crystal structures, phase transitions

MS14-P2 High Pressure Crystallography on the CRISTAL beamline at SOLEIL synchrotron.

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Understanding the pressure effects on condensed matter is a growing field of interest. Pressure adds a new thermodynamic dimension to crystal-structure analyses: exploration of phase diagrams and phase transitions, structure-property relationships, investigation of higher-energy state of biomolecules... Therefore, High Pressure Crystallography (HPC) is a unique and powerful technique to reach a deeper understanding of matter at the atomic scale [1]. A large variety of materials (powders or single crystals) are concerned in fields as diverse as geophysics, biophysics, physics or chemistry. Furthermore, the availability of high brillance synchrotron sources and the development of dedicated setups at diffraction beamlines have allowed one to study more complex samples (e.g. proteins), more smaller samples (few microns), and to reach higher pressure (>100 GPa). In that context, we have recently implemented a HPC setup on the CRISTAL beamline at SOLEIL synchrotron[2].

CRISTAL is a general-purpose crystallography undulator based. One of its three diffractometers can accommodate pneumatic or Membrane Diamond Anvil Cell (MDAC) for powder or single crystal samples. Pressure studies can be realized at ambient temperature and more recently at low temperature, mounting the MDAC to the cold finger of a specially designed helium flux cryostat (T_{min} = 5K). In both case, the pressure is measured *in-situ* (fluorescence of a ruby crystal). Data collection for structure determination (refinement) is possible thanks to the use of 2D detectors (Rayonix SX-165 or XPAD pixel detector[3]) and the implementation of the rotation method for data collection.

Several examples will be presented to illustrate the possibility of the beamline for HPC studies. They demonstrate that although CRISTAL is not specialized in high-pressure studies, HPC can be routinely and successfully performed in conditions analogous to those found at dedicated beamlines in other synchrotron facilities.

[1] E. Boldyreva, P. Dera (2010), 'High-Pressure Crystallography: from fundamental phenomena to technological applications', NATO Science for Peace and Security Series B: Physics and Biophysics, Springer.
[2] http://www.synchrotron-soleil.fr
[3] http://imxpad.com

Keywords: pressure; diffraction; diamond anvil high-pressure apparatus