

INTERACTION OF COMPONENTS IN PrAlO₃- AND LaAlO₃-BASED SYSTEMS

T. Basyuk¹, L. Vasylechko¹, S. Fadeev¹, V. Berezovets², D. Trots³, R. Niewa⁴

¹Lviv Polytechnic National University, Lviv, Ukraine

²Karpenko Physico-Mechanical Institute, Lviv, Ukraine

³HASYLAB at DESY, Hamburg, Germany

⁴Technische Universität München, München, Germany

E-mail: tanya.basyuk@gmail.com

In order to study crystal structures, thermal expansion and phase transitions in the PrAlO₃-RAlO₃ and LaAlO₃-RAlO₃ (R = Nd-Lu, Y) pseudo-binary systems, series of samples have been synthesized by a combination of solid state reactions in air and arc-melting in Ar atmosphere. The ICP-OES method was used for the determination of cationic composition of selected specimens. It was established, that at room temperature continuous solid solutions with rhombohedral LaAlO₃-type of structure are present in the systems PrAlO₃-RAlO₃ and LaAlO₃-RAlO₃ (R = La, Pr, Nd). However, in the other systems two or three kinds of solid solutions with rhombohedral and orthorhombic (*Pbnm* and *Imma*) structures with immiscibility gaps between the different perovskite-type phases are formed. Lattice parameters and cell volumes of Pr_{1-x}R_xAlO₃ and La_{1-x}R_xAlO₃ solid solutions decrease monotonically with decreasing R content.

Study of structural and thermal behaviour of the the solid solutions performed by means of *in situ* high-resolution powder diffraction technique applying synchrotron radiation (beamline B2, HASYLAB at DESY) and thermal analysis revealed several kinds of phase transformations. The La_{1-x}Nd_xAlO₃ solid solutions undergo only phase transition from a rhombohedral to the cubic structure. Continuous phase transition $R\bar{3}c \leftrightarrow Pm\bar{3}m$ and a first-order transformation $Pbmn \leftrightarrow R\bar{3}c$ are observed in the systems LaAlO₃-RAlO₃ (R = Sm-Lu, Y). Both transitions are induced by a structural deformation and its temperatures increase with decreasing R-cation radius and tolerance factor. Besides above-mentioned high-temperature phase transitions, a number of low-temperature phase transformations $R\bar{3}c \leftrightarrow Imma$, $Imma \leftrightarrow I2/m$, $I2/m \leftrightarrow I4/mcm$, $R\bar{3}c \leftrightarrow I2/m$ and $R\bar{3}c \leftrightarrow I\bar{1}$ has been detected in the PrAlO₃-RAlO₃ pseudo-binary systems. The low-temperature transitions in PrAlO₃-based systems are caused by electronic effects and for the most part its temperatures decrease with decreasing Pr content. Substitution of RE cations allow to tune the desired structural properties of LaAlO₃ and PrAlO₃-based perovskites in a wide temperature range in order to use theirs as substrate materials for diverse epitaxial applications.

Based on the results of *in situ* synchrotron powder diffraction examinations and DTA/DSC measurements, as well as available literature data, the structural phase diagram of the pseudo-binary systems PrAlO₃-RAlO₃ and LaAlO₃-RAlO₃ have been constructed.