

[3] Different sets of stacking vectors give non-congruent sets of interatomic distances which yield almost the same Patterson function and hence similar diffraction patterns.

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Keywords: thermoelectrics; homometry; tellurium compounds¹

FA2-MS04-P08

Temperature- and Concentration-induced Structural Transitions in $\text{Pr}_{1-x}\text{R}_x\text{AlO}_3$. Leonid Vasylechko^a, Tetyana Basyuk^a, Anatoliy Senyshyn^{a,b}, Dmytro Trots^b, Rainer Niewa^c, Stefan Hoffmann^d. ^a*Department of Semiconductor Electronics, Lviv Polytechnic National University, Lviv, Ukraine.* ^b*TU Darmstadt, Germany.* ^c*TU Munich, Germany.* ^d*MPI CPfS, Dresden, Germany.*
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The pseudo-binary systems PrAlO_3 – RAIO_3 (R = rare earth metals) display complex phase and structural behaviours. Seven different types of crystal structures ranging from the ideal cubic perovskite to its triclinic derivative are found among $\text{Pr}_{1-x}\text{R}_x\text{AlO}_3$ solid solutions, depending on composition and temperature [1]. In this work, the influence of both “chemical pressure” and temperature on the crystal structures of PrAlO_3 -based perovskites and on the character of structural phase transformations occurring in the pseudo-binary systems PrAlO_3 – RAIO_3 is discussed on the basis of *in situ* high resolution powder diffraction applying synchrotron radiation and differential thermal analysis.

At room temperature (RT), continuous solid solutions $\text{Pr}_{1-x}\text{R}_x\text{AlO}_3$ with rhombohedral perovskite structures are formed in the La and Nd systems, whereas in the systems with Sm, Eu and Gd, the phase separation in two solid solutions with LaAlO_3 and GdFeO_3 types of structures occurs. One more kind of solid solution with orthorhombic structure (*Imma*) at RT has been observed in the systems with Ho–Er and Y. At elevated temperatures, orthorhombic and rhombohedral PrAlO_3 -based perovskites undergo structural phase transitions *Pbnm*–*R-3c* and *R-3c*–*Pm-3m*, respectively. Similar to the “pure” aluminates, both transitions can be parameterized in the terms of Goldschmidt tolerance factor. The transition temperatures increase linearly with decreasing average R-cation radii in $\text{Pr}_{1-x}\text{R}_x\text{AlO}_3$ solid solutions.

Much intricate relationship was observed between the cationic substitution and low-temperature (LT) structural transformations *R-3c*–*Imma* and *Imma*–*I2/m* in the PrAlO_3 – RAIO_3 systems. In the systems with La and Nd, the temperatures of both transitions decrease with decreasing Pr content, whereas in the systems with Sm–Tm and Y a decrease of the *Imma*–*I2/m* and an increase of the *R-3c*–*Imma* transition temperatures are observed. The range of existence of the orthorhombic (*Imma*) phase expands in these systems with decreasing Pr content, thus explaining an appearance of this phase in the Ho–Er and Y systems

at RT. Unexpectedly, in the PrAlO_3 – NdAlO_3 system a rare triclinic structure has been found below 70 K, which is the first representative among the perovskites with a single B-cation.

A complicated character of electron-phonon and phonon-phonon coupling is evidently the reason of the anomalous thermal behaviour recently observed in the majority of RAIO_3 perovskites (R=Eu–Dy, Er, Tm, Y) [1]. However, in contrast to PrAlO_3 and CeAlO_3 , in which such a coupling leads to the change of crystal structures at LT, the present anomalies are reflected in the different deviations of the lattice expansion from the “normal” trends.

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Keywords: perovskite oxides; structural transitions; phase diagrams

FA2-MS04-P09

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The structure and phase transformation behaviour of promising hydrogen storage materials has been investigated by neutron powder diffraction. In this contribution, we report on measurements carried out at the high-resolution neutron powder diffractometer SPODI (FRM II / Garching n. Munich, Germany) [1]. The instrument provides diffraction patterns with excellent profile shape and high resolution over a wide 2 θ scattering angular range. Thus it suited for structure refinement on complex systems, in particular phase mixtures. On the other hand, the stepwise movement of the detector array limits the possibilities for kinetic studies.

Fully deuterated samples of the system LiD/Mg(ND)_2 have been studied after desorption and re-deuteration at 220 °C and different pressures up to 70 bar to analyse the phase transformation behaviour. The measurements were carried out using a wavelength of 2.536 Å. The analysis of diffraction patterns collected at different deuterium pressure levels revealed that the deuteration occurs via intermediate reaction steps. Corresponding intermediate phases could be identified and analysed by Rietveld refinement.

A sample of $\text{Li}_4(\text{NH}_2)_3(\text{BD}_4)$ was studied at ambient conditions using a wavelength of 1.548 Å. The compound was synthesized by mixing a 1:3 stoichiometric ratio of