[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.


Keywords: thermoelectrics; homometry; tellurium compounds

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Temperature- and Concentration-induced Structural Transitions in Pr$_{1-x}$R$_x$AlO$_3$, Leonid Vasylechko$^a$, Tetyana Basyuk$^a$, Anatoliy Senyshyn$^{a,b}$, Dmytro Trots$^a$, Rainer Niewa$^a$, Stefan Hoffmann$^a$.

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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 Pr$_{1-x}$R$_x$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 Pr$_{1-x}$R$_x$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–Pmn 3m, respectively. Similar to the “pure” aluminates, both transitions can be parameterized in the terms of Goldschmidt tolerance factor. The transitions temperatures increase linearly with decreasing average R-cation radii in Pr$_{1-x}$R$_x$AlO$_3$ solid solutions.

Much intricate relationship was observed between the cationic substitution and low-temperature (LT) structural transformations R-3c–Imma and Imma–R2/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–R2/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.


Keywords: perovskite oxides; structural transitions; phase diagrams

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Hydrogen Storage Materials Studied at Neutron Powder Diffractometer SPODI, Markus Hoelzel$^a$, Eveline Weidner-Ronnefelder$^b$, Francesco Dolci$^c$, Jianjiang Hu$^c$, Norbert Juenk$^c$, Hartmut Fuess$^c$.

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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 20 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)$_3$ were examined 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 deuteration 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 Li$_2$(NH$_3$)$_3$(BD$_3$) was studied at ambient conditions using a wavelength of 1.548 Å. The compound was synthesized by mixing a 1:3 stoichiometric ratio of