

I series existed at RT in polar orthorhombic phase are isostructural to BW at  $0 < x < 0.6$  and BM at  $0.7 < x < 1$ . Part of solid solutions at  $0 < x < 0.3$  and  $0.8 < x < 1$  transforms into monoclinic phase through intermediate unpolar orthorhombic phase. The transition temperatures depended considerably on doping level and heating rate. The only reconstructive transition into monoclinic phase without intermediate phase was observed at  $0.4 < x < 0.7$ . The restricted solid solutions in series II with the polar BW structure ( $0 < x < 0.3$ ) have also exhibited two transitions. The monoclinic phase based on BM exists in series II at  $x > 0.3$ . Obtained results have shown that the BW and BM compounds, which existed in polar phase at RT, at heating are similar in respect of numbers and sequences of their transition phases.

Keywords: phase transitions, Aurivillius phases, solid solutions

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#### Structural investigations of crystallization processes in amorphous rare earth borates

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Calcite, vaterite and aragonite phases are well known for rare earth borate system. As a rule, different phases in thermodynamic equilibrium states are observed for different rare earth elements. For example,  $\text{YBO}_3$ ,  $\text{YbBO}_3$  and  $\text{GdBO}_3$  are crystallized in vaterite phase while  $\text{ScBO}_3$  is crystallized in calcite phase only. At the same time  $\text{LuBO}_3$  could be crystallized in the both calcite and vaterite phases. Our studies showed that the structures, which do not exist in equilibrium phase diagram, can be obtained during the crystallization of amorphous borates in non-equilibrium conditions. By non-equilibrium conditions a quick heating up to high temperature and subsequent quench is implied. Moreover by means of this method we have produced the x-phase for  $\text{ScBO}_3$  with so far unknown structural type. Two methods have been used for amorphous borate synthesis. These are thermolysis of the solution-melt and precipitation from the solution. We found that the synthesis method influences considerably on the phase states of the material upon further treatment. Considering this feature we have undertaken the studies of the borate phase crystallization from different starting material under different crystallization conditions such as starting temperature, heat rate, annealing time at final temperature. By this report crystal structure data of the obtained phases and possible routes of the x-phase-vaterite-calcite transformations will be presented.

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#### Structures and transitions in praseodymium at high pressure

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The trivalent lanthanide elements exhibit a range of different close-packed structures as a function of increasing 4f occupancy (hcp  $\rightarrow$  Sm-type  $\rightarrow$  dhcp  $\rightarrow$  fcc) [1]. The same series of structures is also accessible in individual lanthanides by the application of pressure. Two further phases can also be accessed on compression. The first, the distorted fcc phase (d-fcc), has a structure that is closely related to the fcc structure, while the second phase, with the alpha-Uranium structure, arises from the delocalisation of the 4f electrons and marks the end of the sequence of close-packed structures. Despite numerous X-ray diffraction studies dating back 30 years, the structure of the d-fcc phase remains ambiguous. Here we present details of our own structural studies of d-fcc Pr made using powder diffraction methods. In Pr, the d-fcc phase, previously reported to be stable between 9 and  $\sim 20$  GPa, is found to comprise two different structures. Between 9 and 14 GPa, we find the structure to be rhombohedral [2], and can rule out previous reports of a C-centred monoclinic structure. At 14 GPa, we find a structural transition to a second phase, the structure of which does not agree with that reported recently [3]. Further studies reveal that this second phase also exists in Nd, suggesting that there may be a new high-pressure phase in the general lanthanide phase-transition sequence.

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#### Phase transformations induced by point defects studied by group-subgroup relationships

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Symmetry determination for new compounds, structural relations between crystal structures, phase transition paths and new phases generated by point defects, are some of the structural aspects that can be performed by mean of group-subgroup relationships. This work is focused in the analysis of phase transformations induced by point defects *v.gr.* vacancies, interstitial or substitutional impurities. For instance, in monoclinic hydroxylapatite ( $P112_1/b$ , No.14) defects are created in the Wyckoff position  $6h$  for phosphorus substituting the  $\text{PO}_4^{3-}$  by  $\text{CO}_3^{2-}$ ; and the symmetry changes to give the hexagonal hydroxylapatite ( $P6_3/m$ , No.176). Since direct structural relations cannot be established in going from  $P112_1/b$  to  $P6_3/m$ , a common subgroup between these two space groups was considered, *i.e.* the non-centrosymmetric space group  $P2_1$  (No.4) reported for monoclinic chlorapatite under the action of a weak electric field [1]. In the phase transformation from  $\text{YPO}_4$  ( $P4_1/amd$ , No.141) to  $\text{YPO}_4$  ( $Fddd$ , No.70), the orthorhombic phase is induced by  $\text{Li}_2\text{CO}_3$  during the reaction process, its transformation can be described by a translationengleiche subgroup of index 2. The last case considered, was the  $\alpha$ -quartz type germanium oxide ( $P3_221$ , No.154), which phase transformation to  $\text{GeO}_2$  stishovite type ( $P4_2/mnm$ , No.136) was promoted, doping the phase with vanadium. In this phase