Designing perovskite AMO3 phases by controlling the oxygen pressure and temperature during synthesis for a given combination of A and M ions.

A. Baszczuk[a], B. Dabrowski[b], M. Avdeev[c] and M. Jasiorski[a]

[a] Wroclaw University of Technology, Department of Mechanics, Materials Science and Engineering, Smoluchowskiego 25, 50-370 Wroclaw, Poland
[b] Department of Physics, Northern Illinois University, DeKalb, IL 60115, USA
[c] Bragg Institute, Australian Nuclear Science and Technology Organization, Menai, NSW 2234, Australia

The AMO_3 perovskite structure is common among ternary metal oxides, with many derived compositions and structures based on chemical substitutions at the A or M sites, or variations in the oxygen content. The interest in compounds belonging to this family arise in the large variety of magnetic and electric properties and consequently in their great industrial importance.

The stability of perovskite structure is described by a ratio of A-O and M-O bond lengths expressed by tolerance factor $t = (r_a+r_o)/\ \sqrt{2}(r_b+r_o)$ (where r_a, r_b and r_o are ionic radius of A, B and O ions). AMO_3 compounds with low t (below 0.75) are not stable but it's reported that using special techniques as high pressure and high temperature synthesis, chemical composition ranges can be considerably extended.

Here we present the structural properties of the greatly distorted orthorhombic perovskite $PrInO_3$ measured by high-resolution neutron-powder diffraction in the temperature range 303 - 1123 K. By comparing $PrInO_3$ with other AMO_3 perovskites containing fixed-oxidation ions on the A and M crystal sites we show that possibility of designing and obtaining perovskite phases by controlling the oxygen pressure, global pressure and temperature during synthesis is limited in the group of $A^{+3}B^{+3}O_3$ compounds. This limitation results from the slow thermal change of $(r_a+r_o)/\ \sqrt{2}(r_b+r_o)$ ratio with temperature and pressure.

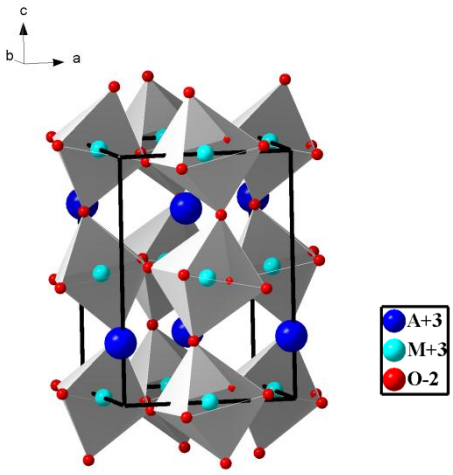

Figure 1 The crystal structure of strongly distorted AMO_3 perovskite.

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