

CHEMICAL STRAIN IN PEROVSKITE-LIKE MATERIALS

Andrey Zuev, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia
andrey.zuev@urfu.ru

Vladimir Sereda, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

Ivan Ivanov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

Dmitry Malyshkin, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

Dmitry Tsvetkov, Institute of Natural Sciences and Mathematics, Ural Federal University, Russia

Key Words: perovskite, double perovskite, chemical strain, defect structure, preferable coordination.

Pseudo-cubic perovskites based upon substituted oxides $\text{RBO}_{3-\delta}$ as well as double perovskites $\text{RBaB}_2\text{O}_{6-\delta}$ and Sr_2BMoO_6 , where R=rare-earth element and B=3d-transition metal, with A-site and B-site, respectively, cation ordering are very promising materials for a variety of different devices for moderate high temperature applications. The unique feature of the oxides is their ability to undergo both thermal strain and that induced by the defects of oxygen nonstoichiometry in the oxide crystal lattice. The latter is called as chemical or defect-induced strain, which is extremely sensitive to the defect structure of the oxide material. This property was shown recently to be isotropic for pseudo-cubic perovskites unlike that of double perovskites. The crystal lattice of a double perovskite expands along **a**-axis and simultaneously contracts along **c**-axis with the decreasing lattice oxygen content. The model of the oxide lattice chemical strain based on a change of mean ionic radius due to reduction of most reducible cation has been recently developed by us. In this work we introduced the new feature in the model such as change of preferable coordination of cations caused by change of oxygen content in the oxide.

The modified model was shown to enable correct prediction of chemical expansion upon increasing oxygen nonstoichiometry along **a**-axis for both pseudo-cubic and double perovskite oxides and simultaneous lattice contraction along **c**-axis in double perovskites. Thus most important finding is that simultaneous lattice contraction along **c**-axis in double perovskites is caused by aforementioned change of preferable coordination.