Poster Presentation

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X-Ray Diffraction Study of Oxygen-Conducting Compounds $Ln_2Mo_2O_9$ (Ln = La, Pr)

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Lanthanum molibdate $La_2Mo_2O_9$ (LM) and the compounds on its basis (LAMOX) attract much attention because of the high oxygen conductivity ($6x10^{-2}$ Sm/cm), which were found by Lacorre group. LM has the first-order phase transition at about 580°C and two phases: low-temperature monoclinic α-phase ($P2_1$) and high-temperature β-phase ($P2_13$) [1]. In the present work single crystals $Ln_2Mo_2O_9$ (Ln = La, Pr) were obtained by spontaneous flux crystallization in the Ln_2O_3—MoO_3 oxide systems. The LM and PM single crystals are studied by precision X-ray diffraction and high-resolution transmission microscopy. A cubic cell with a = 7.155(1) and 7.155(1) Å was chosen for two LM samples (LM_I and LM_II, respectively). More than 90% (LM_I) and 60% (LM_II) of the reflections measured were indexed in this cell. The unit cell parameter of the PM compound is slightly shorter: a = 7.087(1) and 7.089(1) Å for the PM_I and PM_II samples, respectively. More than 90% of the reflections measured were indexed for both PM crystals. It was found that the LM_II crystal consists of two cubic components grown together; a ≈ 7.155 Å for both components. The crystal structures for two LM and two PM samples are determined in space group $P2_13$. It is found that La and Pr atoms, as well as Mo1 and O1 atoms, are located in the vicinity of 3-fold axes rather than on the axes like in the high-temperature cubic phase. In both structures, the O2 and O3 positions are partially occupied. The coexistence of different configurations of the Mo coordination environment facilitates the oxygen ion migration in the structure. Based on the X-ray data, activation energies of oxygen atoms are calculated and migration paths of oxygen ions in the structures are analyzed. The conductivity of PM crystals is close to that of LM crystals. Oxygen atoms O2 and O3 make main contributions to ion conductivity of LM and PM. This study was supported in part by part by the Russian Foundation for Basic Research (project no. 14-02-00531).

[1] *P. Lacorre , F. Goutenoire , O. Bohnke, R. Retoux, Y. Laligant, Nature, 2000, 104, 856*

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