

*Polymorphism and structure of Ion conducting rare-earth molybdates*Alexander Antipin¹, Olga Alekseeva², Natalia Sorokina², Alexander Dudka², Valentina Voronkova³¹National Research Center Kurchatov Institute, Moscow, Russian Federation, ²Shubnikov Institute of Crystallography of Federal Scientific Research Centre "Crystallography and Photonics" of Russian Academy of Sciences, Moscow, Russian Federation,³Lomonosov Moscow State University, Moscow, Russian Federation

E-mail: antipin@physics.msu.ru

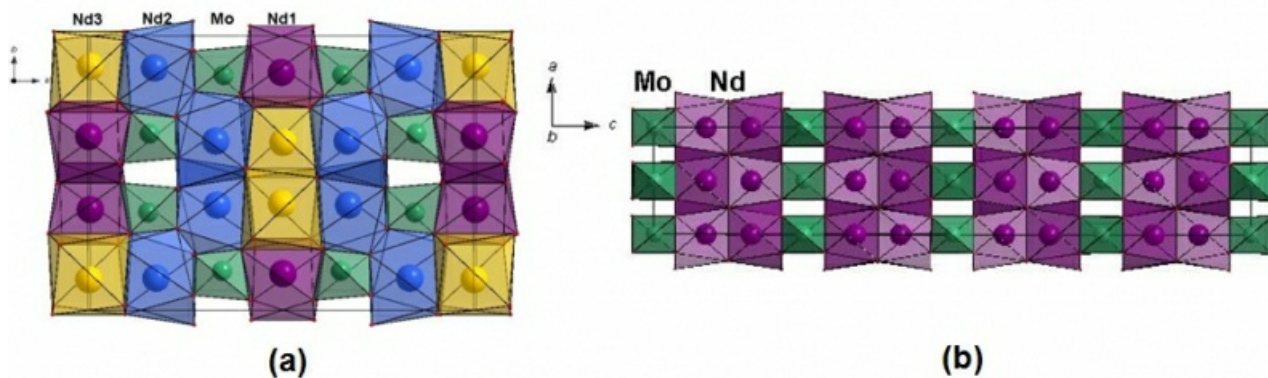
Rare-earth molybdates with a range of unique physical properties can be obtained in the oxide system Ln₂O₃-MoO₃. Scientific interest in this system has increased after the opening of the high ionic conductivity in 2000 [1]. Crystalline materials with different composition and properties can be synthesized depending on the ratio of oxides in the system. The Ln₂MoO₆ compounds, so-called oxymolybdates, can be obtained with all the rare-earth elements and attract the attention due to their chemical resistance, high refractive index, luminescence intensity. Earlier it was found [2,3] that these molybdates have a tetragonal structure of La₂MoO₆-type or a monoclinic structure of Nd₂WO₆-type depending on the ionic radius of the rare earth element. In the case of large cations (La, Pr, Nd) the oxymolybdates synthesized at above 1000 °C have a tetragonal structure. Earlier the Nd₂MoO₆ monoclinic phase was obtained for the first time under annealing at 900°C. This phase has the irreversible phase transition at 1010°C into the tetragonal phase. The purpose of the present work was growth, study of polymorphism and structure of Ln₂MoO₆ (Ln=Pr, Nd) single crystals. The tetragonal single crystals were obtained by crystallization from a molten solution at a maximum temperature of 1250°C; the monoclinic Ln₂MoO₆ single crystals were obtained by slow melt at 800 °C temperature. X-ray diffraction study of Ln₂MoO₆ single crystals were carried out using synchrotron radiation at the SNBL station (ESRF) and using XCalibur S and Smart Apex 2 diffractometers. The local displacement of all the atoms was found for the first time for oxymolybdates. An indirect confirmation of a possible violation of the translational periodicity in the distribution of the Mo and Nd atoms and statistical disorder of oxygen atoms were found. Our structural studies confirmed that oxymolybdates polymorphic transformations occur in an extremely low speed and appears continuously over a wide temperature range. Phase transition from monoclinic to the tetragonal phase occurs by ordering of the cation layers with temperature increasing.

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[2] P.V. Klevtsov et. al // Crystallography reports. 1975. V. 20. № 3. P. 524.

[3] Xue J.S., Antonio M.R., Soderholm L. // Chem. Mater. 1995. V. 7. P. 333.

Crystal structure of monoclinic (a) and tetragonal (b) phases of Nd₂MoO₆ compound.**Keywords:** [Polymorphism](#), [crystal structure](#), [unique properties](#)