NEUTRON DIFFRACTION INVESTIGATION OF PRESSURE DEPENDENCE OF $Nd_5Mo_3O_{16+\delta}$ CRYSTAL STRUCTURE

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We have previously studied isomorphic substitutions of neodymium for other rare-earth elements in the $Nd_{5-x}Ln_xMo_3O_{16+\delta}$ series [1, 2]. It was found that the introduction of rare-earth elements with a smaller ionic radius in comparison with neodymium into $Nd_5Mo_3O_{16+\delta}$ molybdate leads to decreasing in the unit cell parameter. When the substitution limit is reached, a morphotropic transition occurs from the cubic phase to the monoclinic one (gp. gr. C2/c). $Ln_5Mo_3O_{16+\delta}$ molybdates have a monoclinic structure for lanthanides with a smaller ionic radius than neodymium and are included in the homogeneity region of Ln_2MoO_6 molybdates. It is possible that this transition of neodymium molybdate will also occur with a decrease in the unit cell parameter caused by high pressure. To establish the effect of pressure on the crystal structure of $Nd_5Mo_3O_{16+\delta}$ molybdate, neutron diffraction experiments were carried out on the DN-6 instrument on IBR-2 pulsed reactor in the pressure range of 0 - 5.9 GPa [3].
Single phase $Nd_5Mo_3O_{16+\delta}$ molybdate with cubic fluorite-related structure (sp.gr. Pn-3n) was prepared by solid state method. Analysis of neutron spectra showed the $Nd_5Mo_3O_{16+\delta}$ neodymium molybdate retains a cubic fluorite-like structure over the entire studied pressure range at room temperature.

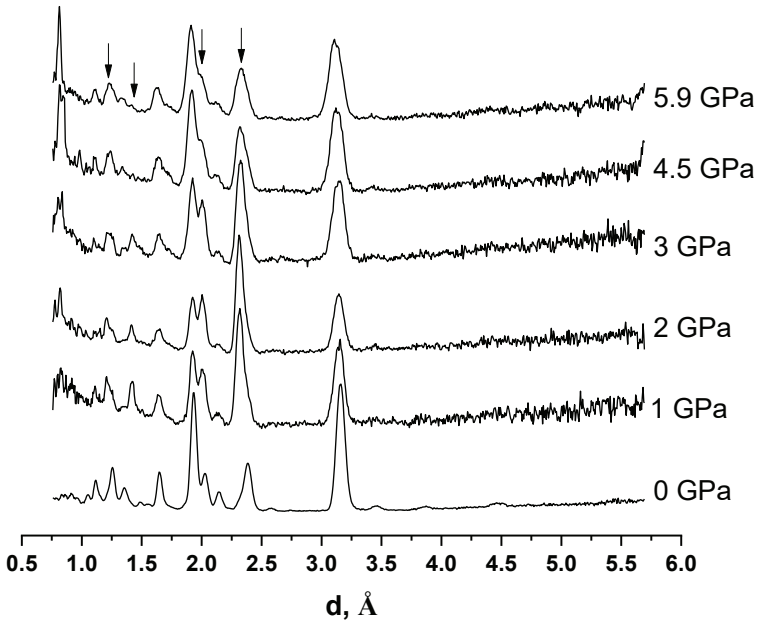

Fig. 1. Neutron diffraction patterns of neodymium molyddate at different pressure (Arrows indicate materials of high pressure equipment)

The unit cell parameters calculated by full profile analysis of neutron diffraction patterns using Rietveld method are shown in fig. 2.

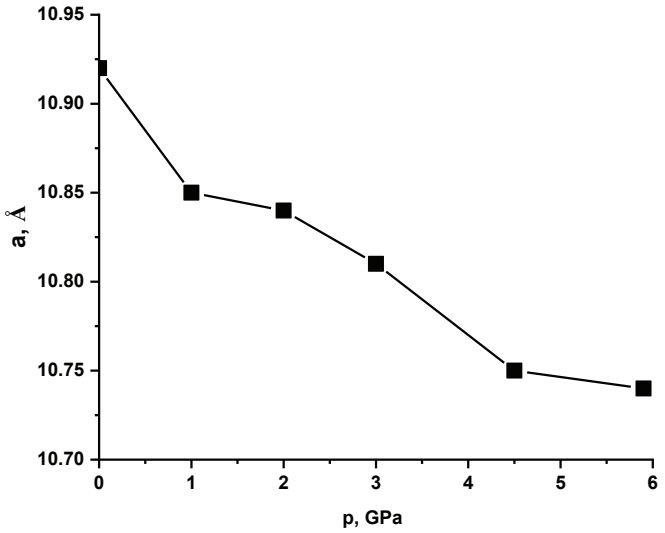

Fig. 2. Dependence of unit cell parameter on pressure value.

An increasing of pressure leads to decreasing in the unit cell parameter of neodymium molybdate without any phase transitions. This can be explained by the fact that, monoclinic phase of $Ln_5Mo_3O_{16+\delta}$ are subtraction solid solutions ($Ln_{5/3}MoO_{16/3+\delta}$) with respect to the compositions of Ln_2MoO_6. Therefore, the transition from the cubic to the monoclinic phase should be accompanied by the formation of vacancies in the sublattice of the rare earth element and oxygen, which is energetically disadvantageous at elevated pressure.

[1] K.A. Chebyshev (2015). Crystal structure and electrical conductivity of $Nd_{5-x}Sm_xMo_3O_{16}$ solid solutions. Inorganic Materials. 51, 1033–1038.
[2] E.I. Get'man (2016). Isomorphous substitutions and conductivity in molybdates $Nd_{5-x}Ln_xMo_3O_{16+y}$ (y~0.5), where Ln = La, Ce, Pr. Journal of Alloys and Compounds. 686, 90-94.
[3] D. Kozlenko (2018). The DN-6 Neutron Diffractometer for High-Pressure Research at Half a Megabar Scale. Crystals. 8, 331.