Solubility limit and thermostructural properties of new kagome material

H.S. Rahimi Mosafer [1], F. Aziz [1], R. Minikayev [1], A. Shekhovtsov[2]

1 1Institute of Physics, Polish Academy of Science,02-691 Warsaw,

Poland, 2 Institute for Single Crystals, NAS of Ukraine, 61001 Kharkov, Ukraine

rahimi@ifpan.edu.pl

Kagome-staircase orthovanadates with general formula $M_3V_2O_8$ (M = divalent cations such as Mg, Ni, or Co) constitute an important family of transition-metal oxides exhibiting rich structural, magnetic, and functional properties[1-4]. These compounds crystallize in the orthorhombic $Ni_3(VO_4)_2$-type structure (space group *Cmca*), where the arrangement of edge-sharing MO_6 octahedra and VO_4 tetrahedra forming a kagome-staircase framework. Modification of composition through solid-solution formation has been widely employed to tune the physical properties of these materials, with most previous studies focusing on substitution at the divalent M^{2+} site. In contrast, aliovalent substitution at the pentavalent V^{5+} site remains largely unexplored.

In this presentation, we investigate the structural and thermal properties of the kagome-staircase [5,6], and also solid solution by introducing Nb^{5+} substitution into the tetrahedral framework [6]. X-ray powder diffraction confirms that all compositions crystallize in the orthorhombic *Cmca* structure characteristic of the kagome-staircase $Ni_3(VO_4)_2$-type framework. Rietveld refinements reveal systematic increases in lattice parameters and unit-cell volume with increasing Nb content, and also indicating solubility limit. Non-ambient X-ray diffraction measurements demonstrate anisotropic thermal expansion over a wide temperature range.

These results highlight the thermal stability and anisotropic lattice response of kagome-staircase orthovanadates at non-ambient temperatures and demonstrate that aliovalent substitution at the V site provides an alternative route for tuning the structural and physical properties of the $M_3V_2O_8$ family beyond the commonly explored M^{2+} substitution.

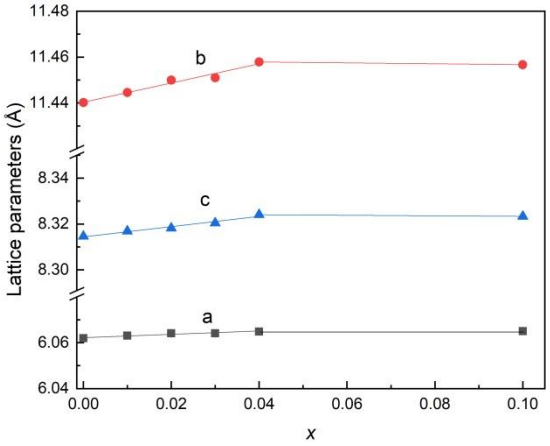


Figure 1. Variation of lattice parameters with Nb substation in Mg3V2(1-x)Nb2xO8 [6]

[1] G. Lawes, et al. "Competing magnetic phases on a Kagomé staircase." Physical review letters 93.24 (2004): 247201.
[2] M. A. Yewale, et al. Materials Letters 338 (2023): 134033.
[3] M. A. Boda, et al. Journal of the American Ceramic Society 106.6 (2023): 3584-3593.
[4] R. A. Kadam, et al. Surfaces and Interfaces 41 (2023): 103267.
[5] F. Aziz, et al. Structural Science 80.6 (2024): 715-723.
[6] H.S. Rahimi Mosafer , et al. J. alloys & compound, submitted Feb 2026