Experimental report

01/06/2020

Proposal: **5-31-2679** **Council:** 4/2019

Title: Charge and magnetic ordering in GaV_2O_5 and the new lacunar spinel oxide GaV_4O_8.

Research area: Materials

This proposal is a new proposal

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Samples: GaV_2O_5
GaV_4O_8

Instrument	Requested days	Allocated days	From	To
D1B	2	2	12/10/2019	14/10/2019

Abstract:

Vanadium oxides have been intriguing substances in solid state physics due to their behavior as strongly correlated electron systems. We have discover a new mixed valent vanadium oxide (GaV_4O_8) with a lacunar spinel structure. We have also prepared the non-studied mixed valent GaV_2O_5. Neutron diffraction is needed in order to elucidate their magnetic structures and possible low temperature charge ordering transitions.

Charge and magnetic ordering in GaV_2O_5 and the new lacunar spinel oxides GaV_4O_8

Vanadium oxides have been intriguing substances in solid state physics due to their behavior as strongly correlated electron systems. Even simple vanadium oxides as VO_2 or V_2O_3 show metal-insulator transition (MIT). Another important characteristic of these oxides is the presence of mixed valence statutes which may be accompanied by charge ordering along with MIT as in V_4O_7.

The ternary system Ga-V-O was reported back on 1981 where it was mentioned the GaV_2O_5 compound[i] purely as the structural characterization, recently on 2018 it has also been reported the GaV_2O_4 spinel[ii] and we have discovered a new GaV4O8 oxide. This novel GaV_4O_8 presents a hexagonal structure *P6₃mc* with a = 5.69474(4) Å and c = 9.38631(3) Å. The magnetic properties of this compound reveal an antiferromagnetic transition at T_N= 40 K with θ = -41.94 K, μ_{eff} = 2.09 μ_B per V which as in the GaV_2O_5 compound, correspond to a mixed valence state, it also presents a second transition at T=78K which from this neutron diffraction measurement was found to be a V_3O_5 impurity. The k vector for this magnetic structure is surprisingly 1/4 1/4 0 with a *Pac* magnetic space group (7.27). On the other side, GaV_2O_5 measurements reveal an absence of magnetic Bragg peaks down to 5 K, and it is probably a spin glass.

About 1 g of GaV_4O_8 and GaV_2O_5 were measured on D1B using a 6 mm V-foil can. Long scans were collected at 5 and 80 K using λ = 2.52 Å. The results, in combination with synchrotron data, allowed the complete structural and magnetic characterization of these samples. The publication of these results is currently under preparation.

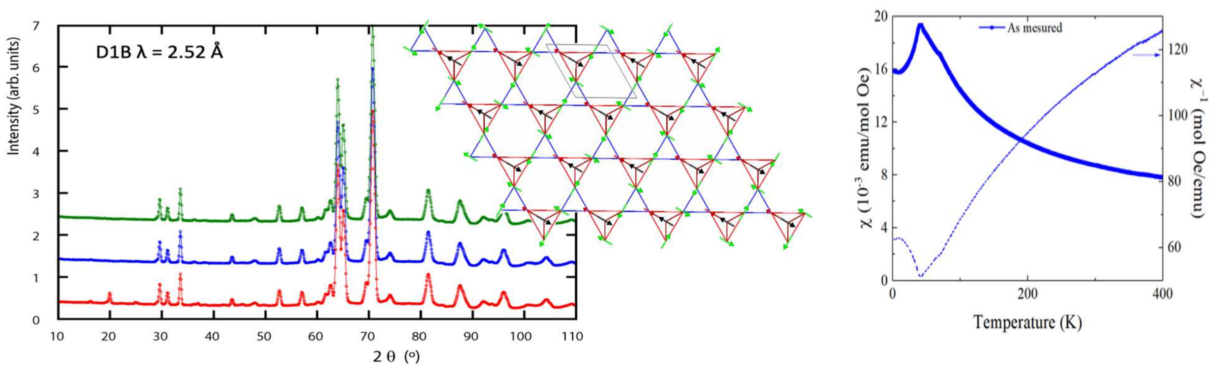

Figure 1. NPD for GaV_4O_8 at 80, 50 and 1.5 K (green, blue, red) collected in D1B. Magnetic structure for GaV_4O_8 (*Pac* magnetic space group). Magnetic susceptibility for GaV_4O_8.

[i] Cros et al., Acta Crystallographica Section B, 1980, vol. 36, no 10, p. 2210-2213.
[ii] Browne, A. J.; Lithgow, C.; Kimber, S. A. J.; Attfield, J. P. *Inorg. Chem.* **2018**, *57* (5), 2815–2822.