Experimental report

20/01/2021

Proposal: **EASY-544** **Council:** 4/2019

Title: Determination of cation order in the high pressure Mn2LiReO6 double perovskite and double corundum polymorphs.

Research area: Materials

This proposal is a new proposal

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Experimental team:

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Samples: Mn2LiReO6_DPv / Mn2LiReO6_DC

Instrument	Requested days	Allocated days	From	To
D20	8	8	25/01/2020	26/01/2020

Abstract:

Mn2LiReO6 double perovskite (DPv) and double corundum (DC) metastable high pressure polymorphs have recently been measured in D20 using 42 degrees take off angle and 2.41 A wavelength at low temperatures to study their magnetic behaviour. This is ruled by only short-range correlations in the case of the DC and the presence of two different propagation vectors ([0 0 0] and [0 0 0.5]) in the case of the DPv. The degradation of the samples motivated the collection of data in different experiments (2015 and 2019). The comparison of both data sets reveal different proportion of magnetic phase fractions in the DPv, which could be due to different degree of cation disorder. In both cases, the presence of broad peaks prevents the accurate determination of the cation order (note both Li and Mn have negative neutron scattering lenghts).

Further data are needed to solve the accurate nuclear structures and thus be able to solve/explain their magnetic structure/behaviour (DPv/DC). For this reason and provided the potential degradation of the samples while stored at the ILL, room temperature high resolution scans are requested using the 1.54 A wavelength at 90 degree take off angle.

Determination of cation order in the high pressure Mn_2LiReO_6 double perovskite and double corundum polymorphs.

Compounds of general formula ABO_3 have been widely studied in the last decades as they are versatile, accepting a wide range of compositions in both A and B sites and giving rise to several structures in competition and an extensive range of possible properties. For instance, the spintronic perovskite $MnVO_3$-II [1] or the multiferroic $MnTiO_3$-II with LiNbO3-type structure.[2]In particular, combining different transition metals into either A or B to originate cation order is a common technique to prepare new functional materials.[3] Among such $A_2BB'O_6$ compounds, high-pressure (HP) A-site manganites have attracted much attention due to the spin, charge and orbital degrees of freedom of Mn.

HP_Mn_2BReO_6 compounds show a *P*2$_1$*/n* double perovskite structure (DPv) for B = Mn^{2+}, Fe^{3+}, Co^{2+} and Ni^{2+}. [4,5,6,7] We have recently prepared two new polymorphs of Mn_2LiReO_6. The introduction of Li^+ cations introduces a new playground in these systems, allowing for Re^{7+} instead of Re^{6+} or Re^{5+} as before. This has enabled the preparation of not only the isostructural DPv compound but also a double corundum (DC) polymorph, never observed before for B' = Re. It is notable that this features only the second HP_$Mn_2BB'O_6$ system showing DPv/DC polymorphism, only observed before for B' = Sb^{5+}. [8,9,10,11]

We have recently measured both DPv and DC_Mn_2LiReO_6 compounds in D20 using the 42° take-off angle and 2.41 Å wavelength at low temperatures to study their magnetic behaviour. They seem to be ruled by only short-range correlations in the case of the DC and the presence of two different propagation vectors ([0 0 0] and [0 0 0.5]) in the case of the DPv. The degradation of the samples motivated the collection of data in different experiments (2015 and 2019). The comparison of both data sets reveal different proportion of magnetic phase fractions in the DPv, which could be due to different degree of cation disorder. In both cases, the presence of broad peaks prevented the accurate determination of the cation order (note both Li and Mn have negative neutron scattering lengths).

Further data have been collected in this EASY experiment at room temperature in the high resolution mode using the 1.54 Å wavelength at 90° take-off angle. The collection of very long scans together with a long scan of the empty cryostat for a reliable background noise subtraction, have enabled full determination of the nuclear structures and identification of minor secondary phases in the DPv (~2% MnO, responsible for the magnetic peaks initially assigned to a possible [0 0 0.5] propagation vector). The real magnetic structure of the AFM DPv_Mn_2LiReO_6 can therefore be refined from the previous data collected at low temperature with k = [0 0 0] as deduced from the results of this experiment.

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