Experimental report

20/12/2021

Proposal: 5-31-2691 **Council:** 4/2019

Title: Nature of magnetic transitions in Sr2FeMoO6-d

Research area: Physics

This proposal is a new proposal

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Samples: Sr2FeMoO6
La0.5Ba0.5CoO2.75

Instrument	Requested days	Allocated days	From	To
D2B	3	3	05/03/2021	08/03/2021

Abstract:

Goal of experiment is the investigation of the magnetic disorder at the micro- and nano level in the Sr2FeMoO6-d crystal structure below and above the Curie temperature, depending on the antristructural defects and concentration of oxygen vacancies. They influence the formation of various antiferromagnetic clusters of Fe2+-O2--Fe2+, Fe3+- O2--Fe3+ or Mo5+-O2--Mo5+ cations. These investigations will enrich materials science with new knowledge about the crystal structure peculiarities and the background of enhanced physical properties of the double perovskite ferrimagnetics for the effective applications in spintronics

$Sr_2FeMoO_{6-\delta}$ (SFMO) compounds attract attention of researchers to their high values of the Curie temperature (T_c = 400 – 600 K), large values of the negative magnetoresistance (MR) at low temperatures (~ 30-90%), and practically 100% spin polarization of the conduction electrons [1 - 4]. The SFMO has a ferrimagnetic structure as a result of the ordering of electron spins of Fe^{3+} and Mo^{5+} cations, which possesses the superstructural ordering Fe/Mo [2, 4]. The presence of point antistructural defects of the Fe_{Mo}, Mo_{Fe} type, and anionic vacancies in the SFMO structure promotes the formation of antiferromagnetic clusters, and lowers the probability of a formation of the long-range ferrimagnetic ordering, considerably decreasing the magnetoresistance (MR) value of the SFMO [3]. More detailed investigations of the magnetic disorder at the micro- and nanolevel at low temperatures, depending on the antistructural defects and concentration of oxygen vacancies, should realize a control of Fe and Mo cations spin states, which could have large prospects for spintronic applications of the SFMO.

The use of partially recovered precursors for the synthesis of SFMO samples in the studies of the influence of antistructural defects and oxygen vacancies on galvanomagnetic properties has made it possible to realize there a different value of Fe^{3+} and Mo^{5+} cations superstructural ordering (P) [4,5]. With that, the anion vacancies, which promote a redistribution of electronic density between Fe^{3+} and Mo^{5+} cations are formed in the SFMO crystal lattice. From the temperature dependences of the magnetization (M) it has been determined that the SFMO samples with P=64% are ferrimagnetics with the same phase transition temperature (418 K). The behaviour of M(T) dependences given in Fig.a are caused by a transition of the part of Fe cations being in the high spin state $Fe^{3+}(t_{2g}^3 e_g^2)$ to the intermediate spin state $Fe^{2+}(t_{2g}^4 e_g^2)$ or to the low spin state $Fe^{1+}(t_{2g}^6 e_g^0)$. Such transition increases the probability of a formation of Fe^{2+}-O^{2-}-Fe^{2+}, Fe^{3+}-O^{2-}-Fe^{3+} or Mo^{5+}-O^{2-}-Mo^{5+} antiferromagnetic clusters. Magnetoresistive characteristics of the SFMO samples at low temperatures indicate their magnetically-inhomogeneous state. In this case, the magnetoresistance (MR) value at low temperatures increases up to 14% at 8 T and 15 K. The magnetic homogeneity of the SFMO is improved with increasing superstructural ordering of the Fe/Mo cations.

We have performed neutron diffraction experiments of 3 Sr_2FeMoO_6 samples with different amount of antisite disordering using D2B spectrometer in a wide temperature region. A structure, distances and angles of Fe-O-Fe, Mo-O-Mo bonds have been calculated as well as a magnetic structure has been refined.

Fig.1 and Fig.2 show a Rietveld refinement of Sr_2FeMoO_6 at lowest temperature 2K and highest 500K.

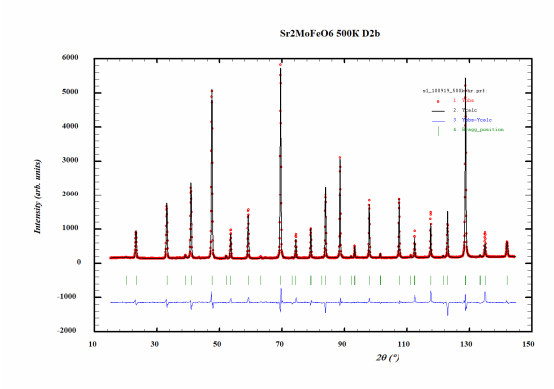

Fig.1. Sr_2FeMoO_6 at 600K.

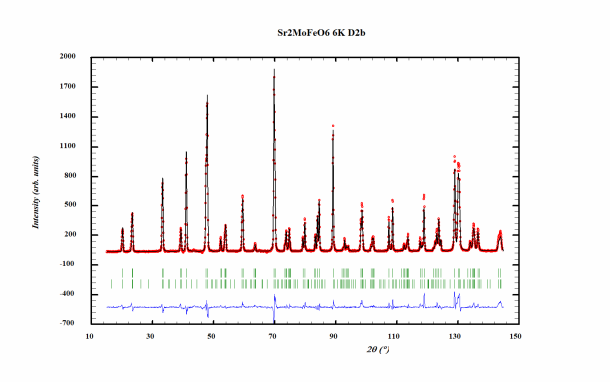

Fig.2. Sr_2FeMoO_6 at 2 K. Both structure and magnetic structure ar shown

Fig.3 shows magnetic structure of the Sr_2FeMoO_6 at low temperature.

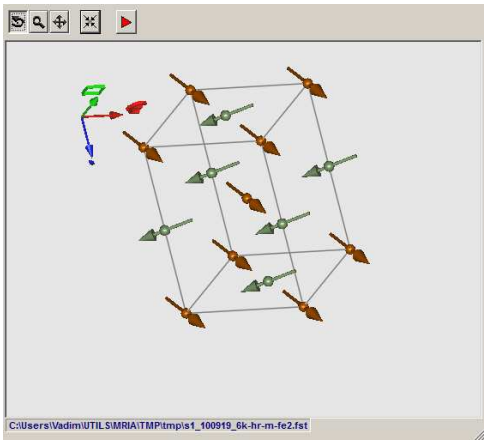

Fig.3 Magnetic structure of Sr_2FeMoO_6 . Only positions of magnetic ions Fe and Mo are shown.

Superstuctural ordering observed for the Sr_2FeMoO_6 causes a decrease in the unit cell volume, which is accompanied by a reduction in the length of the Mo/Fe-O bonds, located in the basal plane of oxygen octahedra.

References

[1] M.K.Chung, P.J. Huang, W.-H. Li, et al., Physica B **385** (2006) 418

[2] J.Rager, M.Zipperle, A.Sharma, et al., J. Am. Ceram. Soc., **87** (2004) 1330

[3] N.A. Kalanda, L.V. Kovalev, M.V.Yarmolich, et al., SAM **7** (2015) 446

[4] M.Yarmolich, N.Kalanda, H.Terryn, et al., Beilstein J. Nanotechnol., **7** (2016) 1202

[5] M.Yarmolich, N.Kalanda, N.A.Sobolev et al., Phys. Status Solidi, B **253** (2016) 2160