Experimental report

06/09/2018

Proposal:	**5-32-853**	**Council:**	4/2017
Title:	Neutron diffraction study of Sr2FeCoO6, SrLaFeCoO6 and La2FeCoO6		
Research area:	Materials		

This proposal is a new proposal

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Samples: La2FeCoO6
SrLaFeCoO6
Srt2FeCoO6

Instrument	Requested days	Allocated days	From	To
D7	7	3	15/06/2018	18/06/2018

Abstract:

Double perovskites are a fascinating material class with a lot of functional properties. Multiferroicity, magneotcapacitance, magnetoresistance, different magnetic ground states including spin-glass and three dimensional quantum magnetism have been either experimentally observed or theoretically proposed for these materials. We propose to do polarized neutron diffraction study on the double perovskites Sr2FeCoO6, SrLaFeCoO6 and La2FeCoO6 as a function of temperature in the range 1.5 – 300 K in fine temperature steps. The XYZ polarization analysis available on the polarized diffractometer D7 will enable us to separate magnetic and nuclear scattering absolutely essential in order to interpret the data properly. We request 7 days of neutron beam time on D7 for this.

Polarized neutron diffraction study of Sr_2FeCoO_6, $SrLaFeCoO_6$ and La_2FeCoO_6

Introduction:

Double perovskites are a fascinating material class with a lot of functional properties. Multiferroicity, magneotcapacitance, magnetoresistance, different magnetic ground states including spin-glass and three dimensional quantum magnetism have been either experimentally observed or theoretically proposed for these materials. One of the famous double perovskite discovered is the Sr_2FeMoO_6, where high magnetoresistance (MR) was reported [1]. A strong correlation between the observed MR and the inherent crystallographic *antisite* disorder was proposed in that compound. The *antisite* disorder – where the transition metal atoms occupy the crystallographic positions interchangeably – is found to be an ubiquitous presence in most of the double perovskite compounds and plays an important role in the magnetism of these materials. Theoretically proposed (using the Goodenough-Kanamori rules) to behave as long-range ordered magnets, the double perovskites often display strong signs of disordered magnetism or short-range magnetic order primarily due to the presence of *antisite* disorder. Following the work on Sr_2FeMoO_6, we extended our research to related compounds Sr_2FeCoO_6, $SrLaFeCoO_6$ and La_2FeCoO_6 [2-4].

In order to achieve a better understanding of the disorder effect and spin states of Fe and Co, a suitable non magnetic doping at the *A* site can be done. *A*-site doping in double perovskites have shown that *antisite* defect have a role to play [5]. Since Fe and Co have a similar x-ray scattering factor, it is necessary to do neutron diffraction analysis to determine the amount of *antisite* disorder. Also, it has been known that the degree of disorder can be understood better by analyzing the variation of anisotropic thermal parameters with respect to temperature [6]. Substituting La at Sr-site in Sr_2FeCoO_6 modifies the magnetic and transport properties. An interesting change is that, while Sr_2FeCoO_6 showed a clear spin-glass nature in dynamic susceptibility studies such a behavior is not observed in $SrLaFeCoO_6$. Though there is irreversibility seen in dc magnetization, no frequency dependence of the transition is observed in ac susceptibility. Another remarkable fact is the hysteresis observed in the real part of ac susceptibility. Though the MR gets reduced by 10%, a hysteretic nature in MR is observed at 5 K, which seems to vanish at 50 K. The magnetization is found to increase with La substitution, which is quite the opposite that has been found in Sr_2FeMoO_6.

On the other extreme, when Sr is completely replaced by La it shows no magnetoresistance or spin-glass behaviour. Interestingly, at room temperature, La_2FeCoO_6 crystallizes in rhombohedral *R-3c* space group. As the temperature decreases, it is seen to develop a mixed-phase consisting of *R-3c* and orthorhombic *Pnma*. The presence of this structural mixed-phase reflects in magnetic measurement as a thermal hysteresis. Further, a broad magnetic phase transition is seen to occur at temperatures very close to 300 K.

Experimental results:

We have done the polarized neutron diffraction experiment on D7 on the double perovskites. In the limited allocated neutron beam time of only three days allocated by the subcommittee we could measure only two compounds; out of these La_2FeCoO_6 which was suspected to order magnetically, was measured rather well for two and half days and the other magnetic glass compound $SrLaFeCoO_6$ could be measured only partially for half a day. The interesting canonical spin-glass compound Sr_2FeCoO_6 could not be measured at all. We have done XYZ polarization analysis of the neutron diffraction intensities and separated them into nuclear coherent, nuclear spin incoherent, spin flip magnetic and non-spin flip magnetic parts. Here we have considered only the average magnetic intensities in the following results.

Fig. 1 (a) shows 011 magnetic peaks at several temperatures of La_2FeCoO_6 that appear at about $Q = 1.4$ Å^{-1} below about $T_N = 220$ K. We have fitted these peaks with a Gaussian function. Fig 1(b) shows the temperature variation of intensity of 011 reflection and its power-law fit. The fit gives $T_N = 250$ +- 17 K and exponent $\beta = 0.44$ +- 0.07. The appearance of 011 magnetic peak below $T_N = 250$ K suggests G-type magnetic ordering at lower temperatures.

For $SrLaFeCoO_6$ we have observed no magnetic Bragg peaks. But we have observed diffuse magnetic scattering close to $Q = 1.4$ Å^{-1} and $Q = 1.6$ Å^{-1}. Fig. 2 (a) shows the magnetic diffuse scattering observed in the Q range 1 – 2 Å^{-1}. We have fitted two Loretzian functions for the two peaks. The peaks at Q = 1.4 and 1.6 Å^{-1} represents spin fluctuations. We are still analyzing the data to understand its implications. We have also observed temperature dependence of the background close to Q = 0 shown in Fig. 2 (b). The higher background at low temperatures may signify ferromagnetic correlation at Q = 0. The data for $SrLaFeCoO_6$, are preliminary only. To do any definite conclusions about the short-range correlation and its temperature dependence we need to measure this sample with much higher counting statistics.

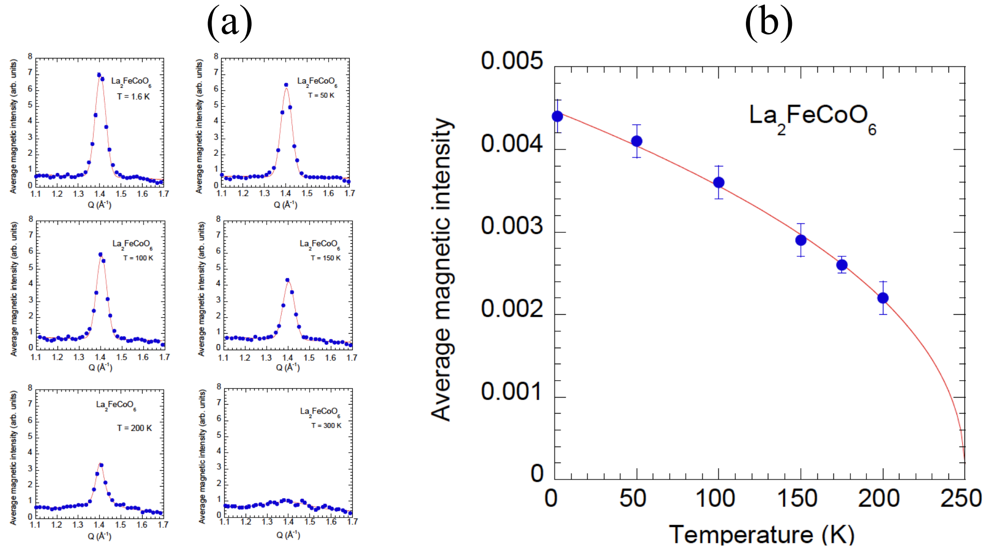

Fig. 1 (a) The 011 magnetic peaks at several temperatures of La_2FeCoO_6 that appear at about Q = 1.4 Å^{-1} below about T_N = 220 K . We have fitted these peaks with a Gaussian function. (b) Temperature variation of intensity of 011 reflection and its power-law fit. The fit gives T_N = 250 +- 17 K and exponent β = 0.44 +- 0.07.

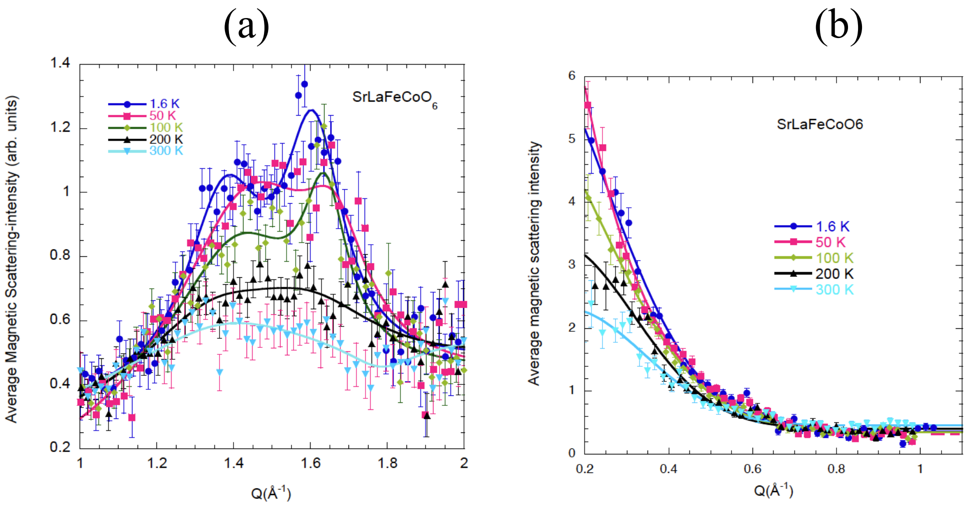

Fig. 2 – (a) Magnetic diffuse scattering from $SrLaFeCoO_6$. We have apparently two magnetic broad peaks which we fitted with two Lorentzians. The widths of these peaks are much larger than the resolution width of the instrument. These broad peaks indicate short range magnetic order. (b) Temperature variation of the background of from $SrLaFeCoO_6$ close to Q = 0. The higher background at low temperatures may signify ferromagnetic correlation at Q = 0.

References:

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