Experimental report

09/02/2016

Proposal: **4-04-475** **Council:** 4/2015

Title: Magnetic excitation and ground-state doublet splitting in Nd2Ir2O7 and Nd2Hf2O7

Research area: Physics

This proposal is a new proposal

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Samples: Nd2Ir2O7
Nd2Hf2O7

Instrument	Requested days	Allocated days	From	To
IN6	7	10	25/11/2015	01/12/2015
			04/12/2015	08/12/2015
IN5	7	0		

Abstract:

Recent neutron measurements revealed that Nd2Ir2O7 has a long-rang ordered antiferromagnetic structure below ~20 K, and the Kramers ground-state doublet of Nd3+ splits below its metal-to-insulator transition (MIT) temperature. In our recent polarized neutron scattering experiments at DNS at MLZ, long-range magnetic order at low temperatures have been observed in both Nd2Ir2O7 and Nd2Hf2O7. Since Hf4+ in Nd2Hf2O7 is expected to be nonmagnetic, it would be of high interest to verify whether a similar ground-state doublet splitting also occurs in Nd2Hf2O7 via inelastic neutron scattering (INS). However, such INS investigations have not been reported so far. We propose to investigate low-energy magnetic excitations and possible ground-state doublet splitting on two similar Nd-based pyrochlore compounds Nd2Ir2O7 and Nd2Hf2O7 at the cold-neutron time-of-flight spectrometer IN5 or IN6. we request in total 7 days of beamtime at IN5 (can be reduced to 4 days if necessary) or IN6 for the proposed two samples. The proposed experiment is complementary to our proposed IN4 experiment, and would form an important part of the PhD studying of the main proposer.

Quantum Fluctuation in magnetic Weyl semimetal candidate $Nd_2Ir_2O_7$

Scientific background

Weyl semimetals are a class of novel materials that can be regarded as three dimensional analogs of grapheme upon breaking time-reversal or inversion symmetry. Exotic massless quasi-particle Weyl fermions can emerge in Weyl semimetals. The surface state of a Weyl semimetal displays pairs of entangled Fermi arcs at two opposite surfaces. [1] Recently, the experimental realization of a Weyl semimetal has been achieved on TaAs and other related binary transition-metal pnictide compounds, which is intrinsically diamagnetic and its lattice doesn't have space inversion symmetry, by observing Fermi arcs formed by its surface states using angle-resolved photo-emission spectroscopy (ARPES). [2,3,4] Pyrochlore iridates ($A_2Ir_2O_7$, A=rare earth and Y) are magnetic Weyl-semimetal candidates due to the time-reversal symmetry broken caused by Ir^{4+} magnetic ordering, meanwhile metal-to-semimetal transition takes place. [1,5] For example, optical conductivity studies give evidence that $Eu_2Ir_2O_7$ has Weyl semimetal state below T_N=110K. [6] Although band structure studies of Pr2Ir2O7 show a quadratic Fermi node near Fermi surface, $Pr_2Ir_2O_7$ cannot be Weyl semimetal due to its metallic nature. [7] Nevertheless, our polarized neutron scattering studies of $Nd_2Ir_2O_7$ provide the direct evidence of magnetic ordering of Ir^{4+} below T_{MI} =36K, (see Fig1b) implying that $Nd_2Ir_2O_7$ is possibly the best candidate of a magnetic Weyl semimetal. Unfortunately, the direct observation of band structure of $Nd_2Ir_2O_7$ has not been obtained yet due to the absence of single crystal. Moreover, the effect of the Fermi node on magnetic excitation in $Nd_2Ir_2O_7$ is still unknown.

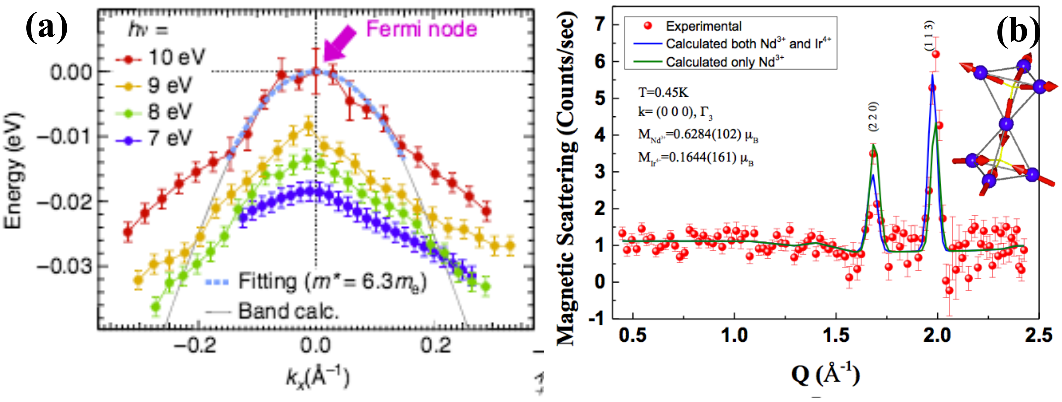

Figure 1. (a) ARPES spectra revealing a quadratic Fermi node in the 3D band of Pr2Ir2O7.[7] (b) magnetic scattering of $Nd_2Ir_2O_7$ at T=0.45 K and 'all-in-all-out' configuration [8,9].

Previous results

Polarized neutron scattering studies of $Nd_2Ir_2O_7$ have been performed on DNS at MLZ. Both Nd^{3+} and Ir^{4+} show 'All-In-All-Out' (AIAO) magnetic long-range order below T_{MI}=36K. The temperature dependence of $Nd_2Ir_2O_7$ behaves induced ordering, meaning the ordering parameter doesn't saturate even at 0.1K. Its akin compound $Nd_2Hf_2O_7$ within nonmagnetic ion Hf^{4+} has sharp AIAO magnetic order transition at 0.5K. The magnetic diffuse scattering of $Nd_2Hf_2O_7$ above T_N=0.5K indicates short-range spin correlation. (see Fig. 2a) However, the inelastic neutron scattering

(INS) of $Nd_2Hf_2O_7$ (performed on IN6 in last year, proposal number # 4-04-475) shows no quasielastic or inelastic scattering at 0.6K within instrumental resolution. (see Fig. 2b) This implies spin freezing process, which takes place in classical spin ice $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$. [10] However, due to the instrument resolution limit, the low energy feature is still unknown. Moreover, the INS measurement of $Nd_2Ir_2O_7$ has not been undertaken due to limited beamtime.

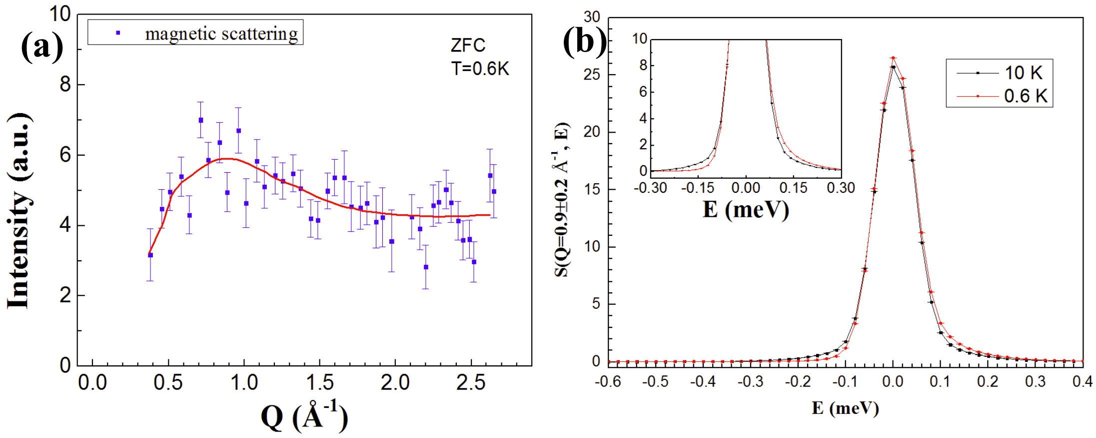

Figure 2. (a) Magnetic diffuse scattering of $Nd_2Hf_2O_7$ at T=0.6K taken on DNS @ MLZ; [8] (b) Qcut of INS of $Nd_2Hf_2O_7$.taken at IN6 @ ILL. [8]

Aims and details of the proposed experiment

We propose to investigate the quantum fluctuation in Weyl semimetal candidate $Nd_2Ir_2O_7$ by the inelastic neutron scattering at the cold-neutron time-of-flight spectrometer IN5 due to its high energy resolution and high incident beam flux. The low-lying excitation of $Nd_2Hf_2O_7$ is also expected to accomplish by changing an instrument with higher resolution. Both of samples are already loaded in annulus-type sample cans with optimal thickness. A dilution insert with standard orange cryostat would be requested for the measurement of $Nd_2Ir_2O_7$ since the order parameter doesn't saturate at 0.1K. [6] Optimal Ei and chopper frequency will be chosen to cover a reasonable energy transfer range and to provide a sufficient energy resolution. Based on our experience, we would need at least 1 day for the setting up of the dilution refrigerator and for the cooling to the base temperature. The INS data will be collected at the base temperature, 0.6K, 10K and 40K. We request 3 days of beamtime for measurements of $Nd_2Ir_2O_7$ due to its strong neutron absorption. Additionally, 2 more days are expect for further investigation of $Nd_2Hf_2O_7$, so that we can accomplish the low-lying excitation investigation of $Nd_2Hf_2O_7$ by changing instrument resolution. Therefore, we request in total 6 days of beamtime at IN5 for the proposed two samples.

Refernces:

[1] X. Wan, *et.al.*, Phys. Rev. B. **83**, 205101 (2011).

[2] B. Q. Lv, *et.al.*, Phys. Rev. X. **5**, 031013 (2015).

[3] S. Y. Xu. *et.al.*, Science. **349,** 6248, pp613 (2015).

[4] Y. Liu, *et.al.*, doi:10.1016/j.jmmm.2016.01.100

[5] K. Matsuhira, *et al.*, J. Phys. Soc. Jpn. **80**, 094701 (2011).

[6] A. Sushkov, *et.al.*, Phys. Rev. B, **92**, 241108(R) (2015)

[7] T. Kondo, *et.al.*, Nat. Commun., **6**, 10042 (2015)

[8] E. Feng, *et.al.*, ICM 2015 abstract, unpublished.

[9] V. K. Anand, et.al., Phys. Rev. B, **92**, 184418 (2015).

[10] J. P. Clancy, et.al., Phys. Rev. B, **79**, 014408 (2009).