Magnetic order in pyrochlore iridate $Nd_2Ir_2O_7$ probed by employing muon spin relaxation†

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Pyrochlore iridates are highly suitable to investigate novel topological phases based on the network of corner-sharing tetrahedra structures and the relatively large spin-orbit coupling (SOC) inherent in Ir 5d electrons.[1)] The interplay between SOC and electron-electron correlations (U) produces characteristic electronic states. A series of $R_2Ir_2O_7$ (R-227, R = Nd-Ho) compounds exhibit metallic or semi-metallic behavior and undergo metal-insulator transitions (MITs) at a temperature T_{MI}[2)] while Pr-227 shows metallic behavior down to 0.3 K.[3)]

In this study, we focus on Nd-227, which shows metallic behavior at high temperatures and undergoes a MIT at T_{MI} of about 30 K, and the magnetic susceptibility shows the bifurcation below T_{MI} in zero-field-cooling (ZFC) and field-cooling (FC) conditions.[2)] Muon spin precession is observed below T_{MI}, and the spectra were fitted using the following function:

$$A(t) = A_1 e^{-\lambda_1 t} + A_2 \cos(\gamma_\mu H_{int} t + \varphi) e^{-\lambda_2 t} \qquad (1)$$

where H_{int} is the internal field at the muon site, λ_1 is the muon spin-lattice relaxation rate, and λ_2 and φ are the damping rate and initial phase of the muon spin precession, respectively.

The temperature dependence of the extracted parameters is shown in Fig. 1. H_{int} begins to increase below T_{MI}, following the Brillouin-type ordering and tends to saturate below about 20 K to a value of about 350 G. Below about 10 K, H_{int} increases again. λ_2 continues to decrease below T_{MI} and increases again from the same temperature at which H_{int} exhibits an increase. ¿From the inset of Fig. 1(a), it can be seen that λ_1 increases monotonically with decreasing temperature, reflecting the slowing down of the magnetic moments. A small increase is observed around T_{MI}. However, no critical slowing down behavior is observed, as shown in Fig. 1(b). λ_1 continues to increase below T_{MI} and shows a broad peak at around 10 K.

The increase in H_{int} below about 10 K is consistent with the results of the neutron scattering experiment that shows the ordering of Nd^{3+} moments, so it is attributed to the ordering of Nd^{3+} moments from our muon spin relaxation (μSR) experiment. The decrease in λ_1 below about 10 K is then accounted for by the freezing out of the magnetic fluctuations, and the increase in λ_2 suggests that the distribution of the internal field becomes larger at the vicinity of the magnetic ordering. The ordering below T_{MI} is then attributed to the ordering of the Ir^{4+} moments, suggesting its close relationship with the MIT.

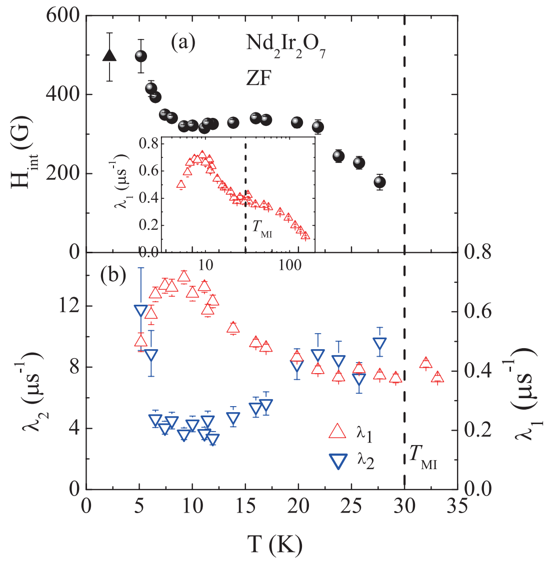

Fig. 1. Temperature dependence of the extracted parameters from our fits to Eq. (1). (a) The internal field at the muon site. (b) The damping rate of muon spin precession and the muon spin-lattice relaxation rate. The inset in (a) shows the whole temperature range of λ_1.

According to a local spin-density approximation calculation including U and SOC, the magnetic structure of the Ir sublattice is the all-in/all-out type, which does not break the lattice periodicity; therefore, the Slater transition is ruled out to account for the relationship between the MIT and the magnetic transition. On the other hand, the Lifshitz-like transition in which the hole band and electron band are moved downward and upward, respectively, due to the specific magnetic structure and the large SOC of Ir 5d electrons may explain the mechanism of MIT.

The saturated internal field from the ordered Ir^{4+} moments is found to be much smaller than that in the case of the other pyrochlore iridates with a magnetic insulating ground state. This implies a stronger hybridization between the Ir 5d and the O 2p electronic orbitals in Nd-227.

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References
1) X. Wan *et al.*, Phys. Rev. B 20, 205101 (2011).
2) K. Matsuhira *et al.*, J. Phys. Soc. Jpn. 80, 094701 (2011).
3) S. Nakatsuji *et al.*, Phys. Rev. Lett. 96, 087204 (2006).