## **2 Geometrical Correlation Project**

Quest for the origin of heavy fermion behavior in
*d*-electron systems –

# 2-1 Strongly anisotropic muon-Mn hyperfine interaction in *d*-electron heavy-fermion metal $Y_{1-x}Sc_xMn_2$

Geometrical frustration in the electronic degrees of freedom such as spin, charge, and orbit, which is often realized on the stages of highly symmetric crystals, has been one of the major topics in the field of condensed matter physics. In particular, the heavy fermion (HF) behavior in  $Y(Sc)Mn_2$ [1] and  $LiV_2O_4$  [2] has attracted broad interest, where such a local electronic correlation specific to the highly symmetric pyrochlore structure may be of direct relevance to the formation of the heavy quasiparticle (QP) state. However, despite decades of studies, the microscopic mechanism of how such a *local* correlation is transmuted into the heavy QP mass of *itinerant d*-electrons in those compounds remains controversial.

We have been focusing on  $Y_{1-x}Sc_xMn_2$  in recent years to clarify the relation between spin dynamics and the HF behavior.  $Y_{1-x}Sc_xMn_2$  is an inter-metallic compound with the cubic C15 Laves phase structure [space group  $Fd^{-}3m$ , as shown in Fig. 1], where the Mn atoms form a three-dimensional (3D) network of corner-sharing tetrahedra called pyrochlore lattice. While it falls into an antiferromagnetically ordered state with a helical spin structure below  $T_N$ = 100 K, substitution of Y by Sc leads to the HF behavior upon suppression of the magnetic order for *x*>0.03.

In FY2013, we reported the result of muon Knight shift measurements in a sample of  $Y_{1-x}Sc_xMn_2$  with x = 0.05, where the development of unexpectedly strong line broadening was observed at lower temperatures (<150 K) [3]. Such a broadening of  $\mu$ SR line shape was strikingly similar to another HF-like compound, LiV<sub>2</sub>O<sub>4</sub> [4], suggesting an

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additional link regarding the origin of HF behavior between those two compounds.

The internal field distribution in  $Y_{0.95}Sc_{0.05}Mn_2$ probed by muons at 2 K was not reproduced by the powder pattern for isotropic hyperfine interaction, suggesting that there might be a strong anisotropy in the local spin susceptibility due to the crystal field and/or spin-orbit coupling even in this kind of metallic compound.

Meanwhile, there remain a number of possibilities why the observed line broadening might have been of extrinsic origin. For example, it is known that the compound would exhibit instability to the spin-glass state for smaller Sc content, and thereby muons might have been probing the slowing down of staggered Mn moments at lower temperatures. Another possibility is the influence of crystallographic randomness introduced by Sc substitution that might have induced modulation of



**Fig. 1:** Crystal structure of  $YMn_2$ , where Y and Mn atoms are indicated by green and red spheres, respectively. The network of corner-shared Mn tetrahedra comprises the pyrochlore lattice. The muon site is situated at the 16c site (center of a hexagon consisting of Mn at its corners).

hyperfine interactions.

In order to clarify the origin of the line broadening, we have extended the muon Knight shift measurement on  $Y_{1-x}Sc_xMn_2$  to greater Sc content (x = 0.05, 0.07, and 0.09). A µSR experiment was performed using the HiTime µSR spectrometer on the M15 beamline of TRIUMF. The result is summarized in Fig. 2(a), where the Fourier transform (FT) of µSR spectra measured at 2 K under TF = 6 T is shown for samples with three different *x*. The FT-µSR spectra commonly exhibit asymmetric broadening, showing least dependence on the Sc content *x*. Thus, these spectra demonstrate that the line broadening is intrinsic to  $Y_{1-x}Sc_xMn_2$ .

The observed field distribution  $P(B_{int})$  is explained by a uniaxial powder pattern with easy plane magnetic anisotropy. In Fig. 2(b), a time spectrum at 2 K is shown together with the



**Fig. 2:** (a) Fourier-transformed  $\mu$ SR spectra observed at 2 K in Y<sub>1-x</sub>Sc<sub>x</sub>Mn<sub>2</sub> samples with *x* = 0.05, 0.07, and 0.09. (b)  $\mu$ SR time spectra at 2 K (shown on a rotating reference frame). The solid curve shows the result of simulation based on a model of field distribution (inset) described in the text.

simulated curve calculated from  $P(B_{int})$  assuming that the staggered Mn moments are allowed to develop within the [111] plane. The model seems to reasonably reproduce the observed line shape, suggesting that local interaction such as the Dzyaloshinsky-Moriya interaction and/or spin-orbit interaction may play an important role in inducing anisotropy of the local susceptibility.

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