

Origin of weak-ferromagnetism in $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ single crystals

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The filled-skutterudite compounds $\text{YbFe}_4\text{Sb}_{12}$ have showed the various results among the samples prepared so far; some samples show ferromagnetic ordering at low temperatures, and the others remain paramagnetic [1]. As a result of weak-ferromagnetic compounds for $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ single crystals, we reported the magnetization and specific heat results at the previous workshop. For the present time, the exact chemical ratio of Yb, Fe and Sb of these single crystals was determined using the electron-probe micro analyzer (EPMA).

The content of Sb was assumed to be 12, the value of filling ratio of Yb, x , was revealed ranging from 0.875 to 0.910, and the value of chemical ratio of Fe was 4.0 for all samples. It is noted that all the present samples of $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ have no ferromagnetic components at 300 K. As the result, this weak-ferromagnetic behavior of the filled-skutterudite compounds $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ is not due to ferromagnetic impurities such as a small amount of pure Fe metal, but having an intrinsic origin. The filling ratio of Yb is strongly related to the weak-ferromagnetic-transition temperature, T_C , and T_C decreases with increasing x . When x is 0.875, T_C is 20 K, being is the largest for the present experiment, and when x is 0.910, T_C reduces to 6 K. T_C vanishes finally around $x = 0.93$, which is thought to correspond to the quantum critical point (QCP).

Recently Schnelle *et al.*[2] showed that divalent Yb is stable in $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ and that $\text{Yb}_{0.95}\text{Fe}_4\text{Sb}_{12}$ is close to the magnetic instability of the itinerant ferromagnetism. Thus, the weak-ferromagnetism of $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$ is considered to originate from the itinerant 3d electrons of Fe. T_C is, however, tuned by the filling ratio x of Yb atoms. As the electron number per formula unit decreases with decreasing x , the Fermi level lowers when x decreases. Here, we thought that the Fe-3d partial density of states (DOS) at Fermi level is related to the weak-ferromagnetic transition; that is, T_C decreases with decreasing the Fe-3d partial DOS. This idea is consistent with the result of the band-structure calculated by Takegahara *et al.*[3]

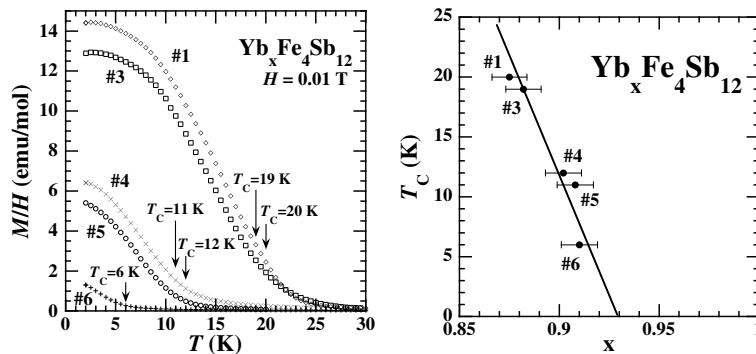


Figure 1: Temperature dependence of the magnetic susceptibility M/H at 0.01 T and phase diagram of T_C dependence of filling ratio x for $\text{Yb}_x\text{Fe}_4\text{Sb}_{12}$.

- (1) I. Tamura *et al.*, J. Phys. Soc. Jpn. **75** (2006) 014707.
- (2) W. Schnelle *et al.*, Phys. Rev. B **72** (2005) 020402R.
- (3) K. Takegahara *et al.*, J. Phys. Soc. Jpn. **71** (2002) Suppl. 240.