Relationship between crystal structure and superconductivity in Fe-based superconductors

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The recent discovery of superconductivity in LaFeAsO1-xFx at the superconducting temperature of Tc = 26 K has triggered an energetic search for new superconductors. The subsequent finding of the high Tc value of 55 K in SmFeAsO1-xFx demonstrates the potential of Fe-based superconductors as beyond the conventional BCS superconductors.

The crystal structure of Fe-based superconductors characteristically consists of two dimensional stacking layers. Commonly, they consist of FeAs-layers that conduct the superconducting current. The Fe atom is surrounded by four As atoms, forming a Fe(Pn,Ch)4-tetrahedron. We focus our attention on crystal structure of FeAs layers, since superconductivity is induced in FeAs layers.

We conducted neutron diffraction measurements at HERMES of the Institute for Materials Research, Tohoku University, installed at the JRR-3 reactor of JAEA at Tokai. The obtained spectra were analyzed by the Rietveld method. Polycrystalline samples of LnFeAsO1-y (Ln=rare-eath), Ca4Al2O6Fe2X2 (X=As,P) were used for the measurements.

We have clarified the superconducting phase diagram of LnFeAsO1-y (Ln=La, Pr, Nd and Tb) by estimating the oxygen content. All samples exhibit superconductivity above y ? 0.04 but the doping dependence of Tc is different. For LaFeAsO1-y, Tc exhibits a flat top at around y = 0.10 and then decreases with increasing y as is usually observed in the overdoped region of a superconducting phase diagram. In contrast, overdoped-like behavior of Tc is not observed for Ln = Pr, Nd, and Tb samples. It seems that there is no universal relationship between Tc and carrier concentration.

The dependence of the bond angle α on the lanthanoid in the LnFeAsO1-y system shows that FeAs4-tetrahedrons form a regular shape around NdFeAsO1-y. Obviously, Tc attains a maximum value when FeAs4-tetrahedrons form a regular shape. This tendency is also observed in other Fe-based superconductors indicating that the relationship between bond angle and superconductivity is a universal one.