Relationship between crystal structure and superconductivity in iron-based superconductors

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Recent discovery of superconductivity in LaFeAsO1-xFx at superconducting temperature of Tc=26K has triggered the energetic study of searching a new superconductor. Soon, it has been found that fluorine-free LnFeAsO1-y (Ln=lanthanoid) samples show superconductivity with maximum Tc=55K. As the Tc is very high, their cooper pairing mechanism could not be explained by the conventional BCS theory. To elucidate the mechanism, their crystal structure should be determined.

The crystal structure of LnFeAsO is characterized by two kinds of stacking layers LnO and FeAs. The Fe atom is surrounded by four As atoms in the FeAs layer forming a FeAs4 tetrahedron. Charges are transferred from LnO to FeAs layers by substitution or introduction of defect of oxygen atoms. 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=La, Ce, Pr, Nd, Tb and Dy) were used for the measurements.

We have clarified the superconducting phase diagram of LaFeAsO1-y and NdFeAsO1-y by estimating the oxygen content. Both systems show superconductivity above y˜0.06. But, doping dependence of Tc is different. In LaFeAsO1-y, Tc attains maximum values at around y=0.12 and decreases with increasing y. Whereas in NdFeAsO1-y, Tc increases till y=0.26. It seems that there is no universal relationship between Tc and carrier concentration.

Figure 1 shows As-Fe-As bond angle as a function of Tc in various pnictide superconductors [1]. The parameters of the samples showing almost maximum Tc in each system are selected to eliminate the effect of carrier doping. The obtained lanthanoid dependence of crystal structure parameters in LnFeAsO1-y system shows that FeAs4-tetrahedrons form a regular shape around NdFeAsO1-y. Obviously, Tc becomes maximum when FeAs4-tetrahedrons form a regular shape, indicating that there is a strong correlation between crystal structure and superconductivity.

[1] C. H. Lee et al., J. Phys. Soc. Jpn. 77, 083704 (2008).
[2] C. H. Lee et al., J. Phys. Soc. Jpn. 77, 44 (2008) Suppl. C.

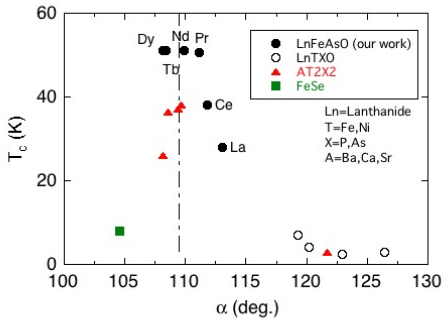

Fig. 1. Tc vs As-Fe-As bond angle α for various pnictide superconductors. Crystal structure parameters of samples exhibiting maximum Tc in each system are plotted. The vertical dashed line indicates the bond angle of a regular tetrahedron (α = 109.47).