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Effect of Lattice Dynamics on Superconductivity in Iron Pnictides

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Recent discovery of superconductivity in LaFeAsO_{1-x} F_x at superconducting temperature of Tc=26K has triggered the energetic study of searching a new superconductor. The fact that T_c of Fe-based superconductors is sensitive to crystal structure [1] implies the importance of lattice dynamics. We, therefore, considered that study on crystal structure as well as phonon dynamics is essential to elucidate the mechanism of superconductivity in Fe-based superconductors.

We conducted inelastic x-ray scattering measurement using the synchrotron radiation x-ray at BL35XU in SPring-8 to study phonon dynamics of $Ba_{1-x}K_xFe_2As_2$ system. Single crystals of $Ba_{1-x}K_xFe_2As_2$ were used for the measurements. We have clarified phonon dispersion of non-doped $BaFe_2As_2$ and superconducting $Ba_{1-x}K_xFe_2As_2$ at room temperature. Comparing both dispersions, we have clarified the difference between non-doped and superconducting samples.

To study crystal structure of LnFeAsO_{1-y} (Ln=La, Ce, Pr, Nd, Tb and Dy), we conducted neutron diffraction measurement using high-resolution powder diffractometer D2B of the ILL in Grenoble, France and 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.

We have clarified the superconducting phase diagram of LaFeAsO_{1-y} and NdFeAsO_{1-y} by estimating the oxygen content. Both systems show superconductivity above y~0.06. But, doping dependence of T_c is different. In LaFeAsO_{1-y}, T_c attains maximum values at around y=0.12 and decreases with increasing y. Whereas in NdFeAsO_{1-y}, T_c increases till y=0.26. It seems that there is no universal relationship between T_c and carrier concentration. The obtained lanthanoid dependence of crystal structure parameters shows that FeAs₄-tetrahedrons form a regular tetrahedron around Ln=Nd.[1] The relationship between the distortion of FeAs₄-tetrahedrons and T_c indicates that T_c attains maximum values when FeAs₄-lattices form a regular tetrahedron. These results suggest the clear relationship between structure and superconductivity.

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

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