Phonon dynamics of iron-based superconductors

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Since the discovery of Fe-based superconductors with superconducting transition temperatures (Tc) of up to 55 K, intensive studies have been conducted to clarify the mechanism of Cooper pair formation. For example, the possibility of phonon-mediated superconductivity has been studied intensively. Calculations using the density functional perturbation theory, however, revealed very weak electron-phonon coupling constants, suggesting that, within those simplified models, conventional phonon-mediated superconductivity is unlikely. Nevertheless, a mechanism involving phonons remains possible. Studies on phonon dynamics using single crystals are essential for elucidating the role of phonons in the appearance of superconductivity in Fe-based superconductors.

We found that phonon softening occurs under K doping in Ba1-xKxFe2As2 using inelastic X-ray scattering technique [1]. To clarify whether this softening is a universal phenomenon in Fe-based superconductors, it is essential to study in other samples. In this study, therefore, we measured phonon dynamics of Ba(Fe1-xCox)2As2 using inelastic neutron scattering technique.

Neutron scattering measurements were carried out using a triple-axis spectrometer, TOPAN at the JRR-3 reactor of JAEA at Tokai. The final neutron energy was fixed at Ef=14.8 meV using a pyrolytic graphite (PG) monochromator and analyzer. The sequences of horizontal collimators were 40′-60′-S-60′-B where S denotes the sample position. A single crystal of Ba(Fe1-xCox)2As2 was grown by the self-flux method using excess FeAs. All measurements were conducted at room temperature.

We measured phonon dispersion along [100] and [110] directions. Phonon dispersion was analyzed using a Born-von Karman force-constant model. The longitudinal and transverse force constants of 11 atomic pairs were chosen as fitting parameters, and the calculated energies were fitted to the measured data. As results we could not find any difference between non-doped BaFe2As2 and superconducting Ba(Fe1-xCox)2As2. The softening can be observed only in K doping samples. This suggests that the softening in Ba1-xKxFe2As2 is due to reduction of interatomic force constants around (Ba,K) sites caused by substitution of divalent Ba by monovalent K ions.

[1] C. H. Lee et al., J. Phys. Soc. Jpn. 79, 014714 (2010).