Title	Studies on Iron Chalcogenide by Mossbauer Spectroscopy and Nuclear Resonant Inelastic Scattering(Digest_要約)
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Citation	Kyoto University (京都大学)
Issue Date	2014-03-24
URL	http://dx.doi.org/10.14989/doctor.k18067
Right	学位規則第9条第2項により要約公開; 許諾条件により要約は2014-06-01に公開
Type	Thesis or Dissertation
Textversion	none

Studies on Iron Chalcogenide by Mössbauer Spectroscopy and Nuclear Resonant Inelastic Scattering

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For the study of high T_c iron-based superconductors, Mössbauer spectroscopy and nuclear resonant inelastic scattering spectroscopy using synchrotron radiation were performed. These methods offer element-specific information and, therefore, are effective to reveal the properties of the respective atoms in the superconductor; information of electronic states from Mössbauer measurement and lattice vibrational states from nuclear resonant inelastic scattering measurement can be obtained. Iron chalcogenide superconductor $FeTe_{0.5}Se_{0.5}$ and its parent compound $Fe_{1.1}Te$ were adopted as the research objects because these compounds contain Fe and Te atoms, for which measurement with ^{57}Fe and ^{125}Te Mössbauer spectroscopy and ^{57}Fe and ^{125}Te nuclear resonant inelastic scattering spectroscopy using synchrotron radiation is possible. Moreover, they have the simplest crystal structure among the iron-based superconductors; iron chalcogenides $FeTe_{1-x}Se_x$ have only conducting layers of Fe tetrahedron surrounded by Te or Se, even though the typical iron-based superconductors have conducting and blocking layers.

To measure ^{125}Te Mössbauer spectra, ^{125}Te synchrotron radiation based Mössbauer spectroscopy was developed, and the validity of this method was confirmed using MS̈sbauer spectroscopy with a radioisotope source. Using the developed method, ^{125}Te Mössbauer spectra of iron chalcogenides were measured for the first time. From the result of ^{125}Te Mössbauer spectroscopic measurement, the hyperfine field of Te in the antifantiferromagnetic phase of $Fe_{1.1}Te$ at 20 K was evaluated to be 4(1) T. The evaluated value of the hyperfine field was comparatively large, and this implies the strong correlation with Fe magnetic moment. In fact, the temperature dependence of the observed hyperfine fields of Te is similar to that of Fe obtained previously and, therefore, the dominant contribution to the hyperfine field of Te is considered to be due to the transferred hyperfine field through the band hybridization between Te and Fe. As for the superconductor $FeTe_{0.5}Se_{0.5}$, no remarkable change of the Mössbauer parameters (isomer shift and quadrupole splitting) below and above the superconducting transition temperature was observed, and this indicates that the change of the electronic state of Te was little.

As for the lattice vibrational states, measurement of ^{57}Fe and ^{125}Te nuclear resonant inelastic scattering of synchrotron radiation was performed. From the observed nuclear resonant inelastic scattering spectra, element-specific phonon densities of states (PDOSs) were extracted. Although electron-phonon coupling is known to result in a large phonon line-width, the Fe-PDOSs of $FeTe_{0.5}Se_{0.5}$ did not show any observable change below and above the superconducting transition temperature of approximately 14 K. The superconducting transition temperature was estimated from the Debye temperature obtained from the Fe-PDOSs using the McMillan formula based on the phonon mediated Bardeen-Cooper-Schrieffer (BCS) theory. The estimated superconducting transition temperature is approximately 0.02 K and is much lower than the experimental value. As for the parent compound $Fe_{1.1}Te$, although the phonon spectra were expected to be affected by the structural phase transition around the Néel temperatures, any significant change in the Fe-PDOSs above and below the transition temperature was not observed. The lack of change in the Fe-PDOSs could be attributed to the minute variations in lattice constants and/or distortion in $FeTe_4$ tetrahedron through the structural transition. These spectra of PDOSs were reproduced by the *ab initio* calculations based on density functional theory. On the other hand, measured spectrum of ^{125}Te nuclear resonant inelastic scattering shows slight discrepancy with the reported results of Raman scattering measurement, but more precise measurement is thought to be required to obtain conclusive result.

From the results of nuclear resonant inelastic scattering measurement, it is implied that the phonon interaction may not be the main mechanism contributing to superconductivity in $FeTe_{1-x}Se_x$. On the other hand, the transferred hyperfine field through the band hybridization was observed by ^{125}Te Mössbauer spectroscopy for parent compound $Fe_{1.1}Te$, and this is compatible with that the magnetic fluctuations have an important role for the occurrence of the superconductivity. Therefore, these ascertain that beyond phonon-mediated BCS mechanism, e.g., the spin fluctuation is required to explain the superconductivity in $FeTe_{0.5}Se_{0.5}$.