論文の内容の要旨

論文題目 Electronic Transport and Angle-resolved Photoemission Studies of Iron-based Superconductors

(電子輸送および角度分解光電子分光による鉄系超伝導体の研究)

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Almost all of the parent compounds of iron-based superconductors (FeSCs) harbor metallic antiferromagnetic (AFM) ground states. The AFM transition is either accompanied or preceded in temperature by a structural transition that breaks a fourfold rotational symmetry of the tetragonal high-temperature lattice. Due to the proximity of the AFM phase to the superconducting phase, many efforts have been done, especially in the most studied "122" family of compounds (for example BaFe₂As₂), to investigate its electronic nature with the broken fourfold rotational symmetry. However, several important controversies on the experimental results such as the origin of the remarkable resistivity anisotropy and the Fermi surfaces (FSs) in the AFM state still exist. In this thesis, we mainly focused on the effects of atom substitution in the metallic AFM state of the "122" iron pnictides and the "11" iron chalcogenides through transport and angle-resolved photoemission spectroscopy (ARPES) measurements.

In the "11" compounds, we first studied the effect of unavoidably preexisting excess Fe ions via transport measurements in the parent compound $Fe_{1+x}Te$. Our results showed the evolution of the temperature dependence of resistivity upon increasing excess Fe content, which corresponds to the change of the magneto-structural phase tuned by the excess Fe content. It was revealed that excess Fe ions exhibit strong scattering effects in both AFM and paramagnetic-tetragonal phases. The in-plane

resistivity anisotropy was investigated in single crystals detwinned by applying uniaxial pressure. No anisotropy was observed well above T_s , while a clear anisotropy appeared when the temperature was decreased below T_s . Notably, ρ_a was higher than ρ_b , opposite to the anisotropy observed in the iron pnictides. It was found that the resistivity anisotropy was mostly determined by the anisotropy in the residual resistivity component. Further studies of Cu-substituted Fe_{1+x}Te found that the magnitude of resistivity anisotropy increased with a larger amount of impurity (excess Fe and/or Cu) ions while the AFM order was correspondingly suppressed. This is suggestive of the generic applicability of the impurity-induced-anisotropy scenario for explaining the origin of resistivity anisotropy observed in the iron-based materials.

In the "122" system, it was surprisingly shown that Ru substitution for Fe atoms exhibited a much weaker effect on increasing residual resistivity in the AFM state, compared with electron doping via 3d transition-metal (e.g., Co) substitution. ARPES measurements on detwinned crystals of Ba(Fe₁. $_x$ Ru_x)₂As₂ (x = 0.04) were performed to reveal the intrinsic anisotropic electronic structures. Three types of FS pockets were revealed: isotropic hole pockets located at the Brillouin zone center, Diraccone-like tiny electron pockets along the Z-X direction which originate from the band crossing at 20 meV below E_F , and another relatively larger electron pocket along the Z-Y direction, which arises from the band folding and consequent band reconstruction. The most anisotropic feature in the band dispersions was the d_{xz} - d_{yz} band splitting around the 2-Fe Brillouin-zone corner, similar to that reported for Ba(Fe_{1-x}Co_x)₂As₂, where the electron doping had a relatively large effect on the suppression of the electronic anisotropy compared to the structural modification induced by 4d Ru substitution. Moreover, our results presented a strong three dimensional character both in the hole pocket and in the energy scale related to the band splitting.

Besides, the existence of line nodes has been strongly suggested in the Ru-substituted BaFe₂As₂ like in the isovalent P-substituted BaFe₂As₂. Our ARPES studies of Ba(Fe_{1-x}Ru_x)₂As₂ (x = 0.35) found that the superconducting (SC) gaps both on the hole FSs and the electron FSs are isotropic in the k_x - k_y plane, suggesting the inexistence of "vertical" line nodes. It was also revealed that the SC gaps on the hole FSs showed a strong k_z dependence, namely, the gap minimum appears around the Z point, implying the possible existence of "horizontal" line nodes near Z. The resemblance in the SC-gap structure of P- and Ru-substituted 122 compounds suggests an important role of pnictogen height in tuning the SC-gap structures of iron-based superconductors.