The 21 Century COE Project

Exploring New Science by Bridging Particle-Matter Hierarchy

Short-term Foreign Researchers

Research Report

Name: Hong Ding

Affiliation: Boston College

Host Researcher in Tohoku University: Tahashi Takahashi

Your Stay Period in Japan: From Jan 10, 2004 to Jan 17, 2004

Title of Research in Japan:

ARPES study on novel superconducting material NaxCoO2

This joint project is to study the evolution of electronic structure of Na_xCoO_2 for different Na doping level x by using the experimental technique of angle-resolved photoelectron spectroscopy (ARPES). The recent discovery of superconductivity in $Na_xCoO_2 \cdot yH_2O$ (T_c = 5K) has generated great interests in the condensed matter physics community due to its potential connection to the high-T_c superconductivity and its unusual properties. Over the past 17 years, the phenomenon of the high-T_c superconductivity is only found in copper oxide compounds (cuprates). The unexpected finding of superconductivity in cobalt oxide (cobalates) has raised the hope that it may help to solve the high-T_c problem. The cobalate Na_xCoO_2, having a layered structure, is highly two-dimensional, which is similar to the cuprates. However, unlike the cuprates that have a square lattice, the cabalate has a hexagonal lattice. For the electronic structure, both compounds have unfilled 3d orbitals, which controls low-energy excitations and physics. In cuprates, Cu^{2+} has $3d^9$ configuration, and forms the highest e_g ($d_{x^2-y^2}$) band near-E_F, with a strong hybridization to O $2p$ orbital. In cobalate, the electronic configuration of Co^{4+} is $3d^5$, which occupies the three lower t_{2g} bands, with the topmost band being $A_{1g} = d_{xy}+d_{yz}+d_z$. The hybridization to the O $2p$ is greatly reduced due to the weaker overlap of the triangular bonding.

In addition to these similarities in crystal structure and band orbitals, another important connection among the three materials is that they are all strongly correlated electron systems. Strong on-site Coulomb interactions make the half-filled compounds Mott insulators. It is widely believed that the physics of the high T_c cuprates is that of doped Mott insulator. It is likely that the cobalate is also an electron-doped Mott insulator, since the "parent" compound Na_0CoO_2 is a half-filled insulator. With increasing Na that serves as charge reservoir, Na_xCoO_2 becomes metallic with some exotic properties. At x = 0.5, $Na_{0.5}CoO_2$ is a good thermal electric material at high temperature. The first cobalate superconductor, $Na_{0.35}CoO_2 \cdot yH_2O$ has a 5K transition temperature. It has been found that Tc decreases on both sides of x = 0.35. This is very similar to the phase diagram of the high T_c cuprates.

It is important to first understand the electronic structure of this material in order to fully understand its superconducting and normal state properties. The reason we choose to come to Tohoku University to do ARPES experiments is that Prof. Takahashi's lab has a state-of-the-art ARPES system in the world, with one of the best resolution, photon flux, and low-temperature capability (4K). The one-week experiment was highly efficient and productive. We have successfully measured more than ten samples at three different doping levels. We clearly observed systematical changes in the band structure and Fermi surface topology as Na concentration changes. This result is significant and we plan to report it to Physical Review Letters soon.

We also plan to come back some time in the near future to measure the superconducting gap in this material. With some minor modifications to the existing facility, we should be able to probe the superconducting state. This would be crucial in understanding the novel superconductivity in the cobaltates as well as in the cuprutes.