Understanding the Mechanism of Superconductivity in $K_{2-x}Fe_{4+y}Se_5$ by Using X-ray Spectroscopic Techniques

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Abstract

Recent discovery of potassium-intercalated iron selenides $K_{2-x}Fe_{4+y}Se_5$ superconductor with T_c ~ 31K introduces new members to this exciting family of Fe-based superconductors. It exhibits peculiar micro-structural properties, like the unique phase separation, Fe vacancy order-disorder and antiferromagnetic order, which distinguish them from other Fe-based superconductor. We have used synchrotron techniques like X-ray absorption near-edge structure (XANES), extended x-ray absorption fine structure (EXAFS) and x-ray emission spectroscopy (XES) to investigate the relationship between electronic and atomic structures in the evolution of superconductor. The high-T_C superconductor, SQ, ($K_{2-x}Fe_{4+y}Se_5$) and non-superconductor, Q, ($K_2Fe_4Se_5$) samples have been synthesized by quenching from various temperatures, 820 ^{0}C (SQ-820 and Q-820) and 750 ^{0}C (SQ-750 and Q-750). The EXAFS spectra at Fe *K*-edge show enhanced local structural disorder around Fe atom in SQ samples as compared to the Q samples. Moreover, this local disorder in SQ-820 is higher than that in SQ-750 at the Fe-Fe bond, and hence strongly associated with the superconductivity by increasing the concentration of Fe atom. According to the Fe $L_{\alpha,\beta}$-edge XES spectra, the SQ-820 sample revealed the lowest resonant ratio factor, I(L_2)/ I(L_3), suggesting an increase in Fe low-spin state which subsequently enhance the superconducting behavior. The Fe $L_{3,2}$-edge XANES suggest that the number of unoccupied Fe 3*d* state in SQ-820 (Q-750) sample is the lowest (highest), whereas, the highest (lowest) number of unoccupied Se 4*p* state in SQ-820 (Q-750) is revealed in the Se *K*-edge XANES. This suggest that the charge transfer effect resulted in the lowest (highest) spin state of Fe in SQ-820 (Q-750). These observations clearly elucidate that the spin state of Fe atom, charge transfer effect and Fe atom structure order-disorder are closely associated with the superconducting behavior in $K_{2-x}Fe_{4+y}Se_5$.