Low Temperature XRD Study of Cu Doped FeSe Based Superconductor

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Superconducting Fe_{1.01}Se shows a tetragonal-toorthorhombic phase transition at 90K [1]. In this work, temperature dependence of crystal structure on Cu doped FeSe was investigated by low temperature XRD measurements. Chemical doping has been proved a valuable way to induce phase transformation and create new superconductors with interesting superconducting and magnetic properties [2-3]. Here we studied the evolution of crystal structure of FeSe under Cu doping (up to 12%). The powdered samples were loaded in capillaries, sealed and attached to a cryostat. The XRD measurements were performed at BL01C2 beamline. Normalized XRD patterns of 1% Cu doped FeSe at various temperatures are shown in Fig. 1. By comparing with the simulated diffraction patterns of crystal phases of FeSe in the literature (Orthorhombic: ICSD#163555 and Tetragonal: ICSD#420379), the 1% Cu doped FeSe samples have dominant orthorhombic structure at 300K, 150K and 20K. There might be some overlapping between tetragonal (002) and orthorhombic (002) indicating coexistence of both phases. The relative intensity of reflections at (002) decreases with decreasing temperature from 300K to 150K and remains unchanged when further cooling to 20K.

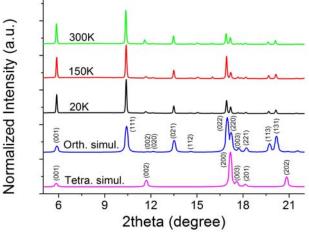


Fig. 1: XRD patterns at 300K, 150K and 20K showing temperature dependence of diffraction patterns of 1% Cu doped FeSe. The simulated XRD patterns of orthorhombic and tetragonal FeSe are also plotted. Photon energy: 22 keV.

With increasing Cu doping, the XRD patterns of Cu doped FeSe show increasing damping of (002) peaks of both orthorhombic and tetragonal structure. In addition,

at all doping levels, temperature dependence is not observed, especially between 150K and 20K. At the highest Cu level (12%), as shown in Fig. 2, the (002) reflection peaks eventually vanish indicating the absence of tetragonal phase.

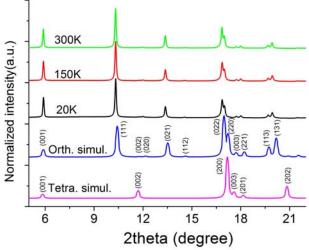


Fig. 2: XRD patterns at 300K, 150K and 20K showing temperature dependence of diffraction patterns of 12% Cu doped FeSe. The simulated XRD patterns of orthorhombic and tetragonal FeSe are also plotted. Photon energy: 22 keV.

The absence of no low temperature structural modification is unexpected and is also inconsistent with the phase transition as for nondoped FeSe superconductor. Upon appropriate chemical substitution, superconducting transition temperature might be tuned based on temperature dependence of crystal structure as demonstrated for Te doped FeSe superconductor [2, 3]. A correlation study of Cu doping on phase transition, superconductivity and magnetic ordering is underway. Analysis of temperature dependence of lattice parameters allows discussion on influence of Cu doping on transport and magnetic properties of FeSe.

References

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