High Pressure XRD and XAFS Study of FeSe Based Superconductor

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High pressure (HP) treatment and chemical doping to non-superconducting materials have been proved two valuable ways to induce phase transformation and therefore the formation of new superconductors [1-3]. Here we employed synchrotron XRD measurements to reveal the evolution of crystal structure of FeSe under conditions of applying pressure (up to 16 GPa) and Cu doping (up to 12%). As shown in Fig. 1, both samples undergo the tetragonal to hexagonal phase transition starting at pressure about 8 GPa with a wide range of coexistence of both phases during 8 – 15 GPa. This result confirms the pressure-induced phase behaviour as revealed in our recent publication [1]. We also found that phase transition is reversible and at pressure release both samples completely transforms back into the tetragonal phase. Analysis of pressure dependence of lattice parameters allows discussion on influence of Cu doping on transport and magnetic properties of FeSe.

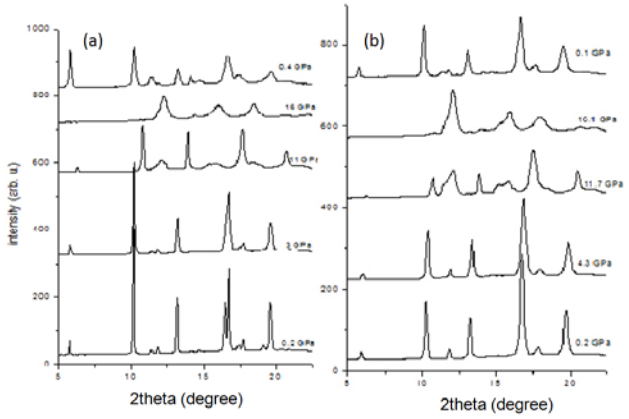

Fig. 1: XRD patterns showing pressure induced evolution of diffraction patterns of pure FeSe (a) and Pressure induced evolution of diffraction patterns of FeSe doped with Cu (b). Photon energy: 22 keV. The spectra corresponding to "pressure release" are labeled as 0.4 GPa and 0.1 GPa, respectively.

Effects of Cu doping on crystal structure of FeSe superconductor are described in Fig. 2. By comparing with the simulated diffraction patterns of crystal phases of FeSe in the literature (Orthorhombic: ICSD#163555; Tetragonal: ICSD#420379; Hexagonal: ICSD#57294) and $FeCuSe_2$ (Tetragonal: ICSD#73376), all the Cu doped FeSe samples have basic orthorhombic structure. It has been reported that non-doped $Fe_{1.01}Se$ superconductor exists in a tetragonal phase at room temperature and has an orthorhombic distortion [4]. However, the situation is opposite when FeSe superconductor was doped with copper because the dominant phase is orthorhombic and with a tetragonal distortion. For the lowest Cu level, tetragonal (002) and orthorhombic (002) overlaps evidently. Similar overlapping is observed between tetragonal (200) and orthorhombic (220). Also note that the extent of coupling between orthorhombic and tetragonal phase degrades with increasing Cu doping. With increasing Cu amount, separations between orthorhombic (002) and (020) decrease and contribution from the tetragonal phase diminish accordingly. In addition, all the reflection peaks increasingly shift collectively to those corresponding to tetragonal $FeCuSe_2$. At the highest Cu level, tetragonal phase almost plays no role.

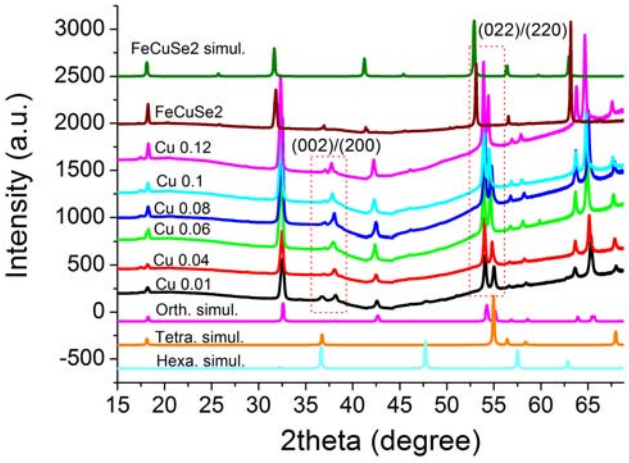

Fig. 2: XRD patterns showing dependence of crystal structure on Cu doping. Photon energy: 7.12 keV. The red rectangulars highlight the evolution of two sets of reflection planes ((002)/(200) and (022)/(220)) as a function of Cu concentration.

Both NEXAFS and EXAFS analysis on both Cu and Se K-edges indicate that, at all Cu level, the local atomic environments around Cu and Se are very similar and definitely differentiate themselves from metallic Fe and Se. A correlation study of Cu doping on long- and short- range order structure, superconductivity and magnetic ordering is underway.

References

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