Temperature dependence of $\sqrt{2} \times \sqrt{2}$ phase in superconducting $K_{0.8}Fe_{1.6}Se_2$ single crystal

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ABSTRACT

We report the structural phase transition properties of the newly discovered $K_{0.8}Fe_{1.6}Se_2$ superconductor ($T_c = 31.8$ K) using synchrotron single crystal x-ray diffraction. The basic structure of the sample at room temperature is found to be tetragonal $ThCr_2Si_2$ -type, modulated by a vacancy ordering induced superlattice structure together with a coexisting minority phase having a $\sqrt{2} \times \sqrt{2}$ ordering. At 520 K, the reflections corresponding to the $\sqrt{2} \times \sqrt{2}$ phase merge with the parent tetragonal phase. The super-lattice peaks corresponding to the vacancy ordering disappears at 580 K, indicating an order-disorder phase transition at this temperature.

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Introduction – The discovery of iron based superconductors (FeSC) has triggered renewed interest in the field of high temperature superconductivity [1,2]. After an intensive study of more than five years, several families of compounds are discovered, of which the latest one with general formula $A_xFe_{2-y}Se_2$ [$A = K$ [3,4], Cs [5,6], Rb [7], (Ti,Rb) [8], has triggered a new storm [9] in the field. Most striking common feature of the FeSC is the appearance of a common active layer of $FePn$ or $FeCh$ (Pn : pnictogen and Ch : chalcogen) edge sharing tetrahedrons [2]. The new $A_xFe_{2-y}Se_2$ family is also no exception to this. However, these compounds display a host of interesting properties, and add a brand new family of compounds to the 25 year old high-temperature superconductors [10]. The most distinguishing feature of this new family compared to the other FeSC is the presence of a Fe -square lattice decorated by regular array of vacancies [11-15] arranged in a complex phase separation scenario [15,16]. Unlike most of the FeSC, where the pairing mechanism is thought to be of “S” type, with the Fermi surface nesting condition seems to be satisfied, in $A_xFe_{2-y}Se_2$ family, it seems to be not an important criteria [17-19]. For the construction of realistic models, the most relevant input needed is the precise crystal structure information. Room temperature structure of the

$A_xFe_{2-y}Se_2$ systems are established from the structural model refinements of the diffraction data [11,12]. Temperature dependent neutron diffraction studies revealed the structural and magnetic phase transitions related with the vacancy ordering in this system [11,14]. Here we present a systematic temperature dependent single-crystal x-ray diffraction study of the $K_{0.8}Fe_{1.6}Se_2$ superconductor ($T_c=31.8$ K) to follow the structural dynamics of the system. The system undergoes an order-disorder transition at 580K, as evidenced by the disappearance of the super-lattice peaks due to the vacancy ordering. The superlattice peaks intensities follow the same behavior upon heating and cooling, thus indicating the temperature hysteresis associated with the transition to be < 3 K. Unlike the earlier diffraction studies using bulk samples [11], our high resolution single crystal x-ray diffraction data show the occurrence of yet another phase transition in $K_{0.8}Fe_{1.6}Se_2$ at 520 K, about 60 K lower than the vacancy ordering temperature, indicating the co-existence of a minority phase. Careful analysis of the minority phase further show the appearance of yet another component at around 300 K, but with a very low volume percentage.

Experiment - Single crystals of nominal composition $K_{0.8}Fe_{1.6}Se_2$ were prepared following

the method described in [4]. The resistivity and magnetization studies showed the presence of a sharp superconducting transition at about 31.8 K (T_c onset 33 K) [4]. The x-ray diffraction (XRD) data on the single crystal samples were collected at the XRD1 beamline at ELETTRA synchrotron radiation facility in Trieste. The samples were oriented by means of a four-circle diffractometer with a motorized goniometric head and a Mar-Research 165 mm CCD camera. The data were collected in the K geometry, with a photon energy of 20 keV ($\lambda = 0.61992$ Å), selected from the source by a double-crystal Si(111) monochromator. The scattered beams (haloes and/or Debye rings) reached a 2D CCD detector (MAR-Research), kept at a distance around 70 mm from the sample. Data from a LaB_6 standard is also collected for calibration. Measurements were conducted between 80 and 600 K with a temperature step of 3 K for the heating (80 to 600 K) and 2 K for the cooling (600 to 80 K) runs. For the measurements between 80 and 300 K, sample temperature was varied and controlled by means of a cryo-cooler (700 series Oxford Cryosystems). For measurements between 300 and 600 K, a heat blower facility (Oxford Danfysik gas blower, DGB-0002) was used. In both cases, the temperature control was better than ± 1 K. All the images measured by the single crystal x-ray diffraction were properly processed using FIT2D program. The processed images were analyzed using a *matlab*[®] based software-package developed in-house.

Figure 1: Central panel shows the single crystal XRD pattern at 300 K. The measurements were done in transmission geometry, with aligned plane along the crystallographic ab . The right panels show the evolution of the super-lattice

peaks around the beam center during the heating cycle.

Results – The main panel of figure 1 shows the single crystal XRD pattern at 300 K. A systematic transmission electron microscopy (TEM) study on the superconducting $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ identified the superlattice peaks corresponding to the Fe-vacancy ordering at $(1/5, 3/5, 0)$ and $(1/4, 3/4, 0)$ in the notation of the tetragonal 122 unit-cell. Careful observation of the pattern reveals that the overlapping superlattice peaks forms group of eight reflections around the main peaks (which are allowed by the tetragonal symmetry), identical to the pattern reported for similar systems at room temperature [14]. The room temperature pattern including the super-lattice reflections can be indexed with a $\sqrt{2} \times \sqrt{2} \times 1$ expanded unit-cell (symmetry $I4/m$) of the basic ThCr_2Si_2 structure [11-15]. An estimation of the lattice parameter $a=b=8.9$ Å, agrees reasonably well with the lattice parameters calculated from the powder diffraction. The right panels of figure 1 show the reflections around the beam-center for selected four temperatures. At 600 K, except for the direct beam, there are no other features. However, pattern for 525 K clearly shows small bright spots on the top and bottom of the central beam spot. With a bit of image contrast adjustments, one can clearly identify a group of eight. These group of spots can be identified as the sum of two families of satellites with geometry $\sqrt{5} \times \sqrt{5}$ and $\sqrt{2} \times \sqrt{2}$ [14]. Cooling down 580K the first class of superlattice peaks disappear and at 520K the $\sqrt{2} \times \sqrt{2}$ class vanished too. $\sqrt{5} \times \sqrt{5}$ superstructure phase was earlier described for the $\text{TlFe}_{2-x}\text{Se}_2$ system by Haggstrom et al. [20].

In figure 2, we present the temperature dependence of the $\sqrt{5} \times \sqrt{5}$ intensity between 400 K and 600 K. The peak intensity disappear around 580 K. Such a behavior confirms perfectly the results coming from neutron diffraction study [11], as evident from a perfect overlap between the two set of data (see figure 2). During cooling from 600 K, the superlattice peaks start to reappear at around 580 K, the same temperature where it disappeared during the heating run. In other words, the temperature dependence of the peak intensity variation seems to be identical in the heating and cooling runs. This means the temperature hysteresis associated with this transition is less than 3 K, the temperature step used in the heating run.

Figure 2: The figure shows the evolution of the $\sqrt{5} \times \sqrt{5}$ superlattice peak intensity (empty blue circles) during the heating run, from 400 to 600 K. The data collected are in very good agreement with the neutron diffraction results [11] (red empty crosses).

The Figure 3 panel A shows the temperature evolution of the (3 3 0) Bragg spot during the heating runs from 80 to 600 K. At 84 K, the peak have two low intensity sub-peaks indicative of the presence of co-existing compressive lattices. The smallest phase (phase B) correspond to $\sqrt{2} \times \sqrt{2} \times 1$ is merging in the second non-magnetic minority phase (phase A) at around 300 K. Ones merged, both together merge to the main phase $\sqrt{5} \times \sqrt{5} \times 1$ at 520 K, as shown in Figure 3 panel B, where the intensity evolution phases A and B is plotted as a function of temperature. The non-magnetic phase A is almost the 22% respect to the total but at 301 K when the phase B appears its intensity drops of almost 3.8%, corresponding to the fraction that represent the phase B. Figure 3 panel C presents the temperature evolution of the in-plane lattice parameters, evidencing a totally unexpected multiple phase separation scenario in $K_{0.8}Fe_{1.6}Se_2$ in which the phases A and B with compressed lattice appear at 520 K and 301 K respectively. It should be stressed that the new phase B appearing at around 300 K is only having a very low volume percentage, and is not easily distinguishable from the phase A. Obviously, it is not associated to the sample degradation, as the diffraction pattern of the partially damaged $K_{0.8}Fe_{1.6}Se_2$ are easily identifiable [21].

Figure 3: Panel A: Temperature evolution of (3 3 0) Bragg reflection at six selected temperatures. Going from 600K to room temperature the main peak splits into two phases (original and phase A). Continue cooling down to 80K, the phase A further splits in two (designated as phases A and B). Panel B: Normalized Intensity of phase A and B as a function of temperature. The phase separation temperature is calculated to be 520K and 301K for the phases A and B respectively. The already well known non-magnetic phase A is almost the 22% respect to the total but at 301K when the phase B appears its intensity drop by almost 3.8% exactly the fraction that represent phase B. Panel C: Temperature evolution of the in-plane lattice parameters, two non-magnetic phase, A and B appears at 520K and 301K respectively.

Discussion – We first discuss the transition associated with the superlattice peaks. The first thing to notice is that the temperature evolution of the $\sqrt{5} \times \sqrt{5}$ superlattice peaks perfectly coincide with the structural phase transition observed in the neutron diffraction studies [11] on similar systems (figure 2). The Neel temperature estimated from the neutron diffraction studies is around 560 K, below the order-disorder transition observed at 590 K [11], thus, presenting a close analogy between the structural and magnetic transition observed in “1111” family of FeSCs [1,2,22-24] and the new $A_xFe_{2-y}Se_2$ systems. Interestingly, the magnetic and structural transitions are concurrent in the structurally identical “122” pnictides [1,2,25].

Before discussing the phase separation occurring at 520 K in this $K_{0.8}Fe_{1.6}Se_2$ system, let us comment about the second transition we identified at around 300 K. Earlier structural

studies using bulk samples [11] did not reveal such a transition mostly due to the tiny volume fraction of this phase. However, several studies looking into the superconducting properties of these system have identified a minority superconducting phase with transition temperatures above 40 K [26,27]. This phase can be one possible candidate for such an exotic state. Another possible candidate is a different co-existing magnetically ordered state.

Coming back to phase separation occurring at 520 K in $K_{0.8}Fe_{1.6}Se_2$ system, the first point to be underlined is the input from the local structural studies which showed the importance of local inhomogeneities in determining the superconducting properties of the doped chalcogenides [28]. A ^{57}Fe Mössbauer study on $K_xFe_{2-y}Se_2$ system revealed abrupt changes in the magnetic fraction of the sample about a similar temperature [29] as the second phase transition observed here. An earlier Mössbauer study [20,30] on $TiFe_{2-y}Se_2$ and $RbFe_{2-y}Se_2$ showed that at lower temperature, the anti-ferromagnetic (AFM) and paramagnetic fractions co-exist with the majority phase to be of AFM nature. But, above 450 K, the AFM fraction decreases to zero, with a concurrent increase in the paramagnetic fraction. The temperature evolution of the magnetic fraction observed in the Mössbauer studies of $K_xFe_{2-y}Se_2$ is also of similar nature. These results clearly indicate the existence of two components in the low temperature region of the $K_xFe_{2-y}Se_2$. The phase transition we observe at 520K in $K_xFe_{2-y}Se_2$ should be associated with such a change in the magnetic ground-state of the system. Differential scanning calorimetric measurements on superconducting $Cs_xFe_{2-y}Se_2$ show two distinct heat-flow peaks, larger one at a higher temperature and a weaker one at lower temperature [14], further supporting two possible phase transitions in superconducting $K_xFe_{2-y}Se_2$. In this context, it is to be recalled that the single crystal studies can provide more insights into the phase transition properties, as revealed in the case of “1111” FeSCs [23, 31, 32].

Given the many questions surrounding the magnetic ordering of the iron moments in the $A_yFe_{2-x}Se_2$ system, our observation of a second phase transition which coincide with the changes observed in the magnetic fraction adds new input to theories dealing with the magnetic properties [33] of this system. Although the ^{57}Fe Mössbauer spectroscopy in $K_xFe_{2-y}Se_2$ could not be used to determine magnetic structures directly, the

observation of a single, well-split magnetic component prompted the authors to rule out any structure in which the iron sub-lattice is further subdivided into multiple, in-equivalent sites [29]. However, the development of a paramagnetic component that coexists with the magnetically ordered phase and that grows at its expense on heating prompted the authors to conclude that such a magnetic transition should be first order in nature and associate with changes in the crystal structure [29]. The present observation of multiple phase transitions with the co-existence of a minority phases seems to suggest the importance of inhomogeneities in the $A_xFe_{2-y}Se_2$ systems, similar to that observed in the $FeSe_{1-x}Te_x$ [28]. The $K_xFe_{2-y}Se_2$ system with a large local disorder [34] and interesting temperature dependent vacancy ordering and coexisting phases [15,16] calls for parallels with the oxygen ordering effects on the superconductivity of cuprates [35,36].

Conclusions - We report the structural phase transition properties of the newly discovered $K_{0.8}Fe_{1.6}Se_2$ superconductor using synchrotron single crystal x-ray diffraction. The basic structure of the sample at room temperature is found to be tetragonal $ThCr_2Si_2$ -type, modulated by a vacancy ordering induced super-lattice structure together with two coexisting minority phases. Below 300 K, we identify the presence of a minority phase (phase A) with a very low volume fraction co-existing with the $\sqrt{2}\times\sqrt{2}\times 1$ phase (phase B). Above 300 K, the phases A and B merge to be a single $\sqrt{2}\times\sqrt{2}\times 1$ phase. At 520 K, the $\sqrt{2}\times\sqrt{2}\times 1$ phase merge with the parent tetragonal phase. The superlattice peaks corresponding to the magnetic ordering disappears at 580 K. All of these results strongly support the existence of a multiscale phase separation scenario in the $A_xFe_{2-y}Se_2$ systems driven by lattice misfit strain [37,38] indicating the importance of local lattice inhomogeneities [28,34], particularly the presence of competing ground states in determining the functional properties of these systems.

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