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Synthesis and Characterization of $\text{FeSe}_{1-x}\text{Te}_x$ ($x=0, 0.5, 1$) Superconductors

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Abstract. In this study, $\text{FeTe}_{1-x}\text{Se}_x$ ($x=0,0.5,1$) samples were prepared by conventional solid state reaction method and investigated by powder XRD, SEM, Raman and resistivity measurement techniques to reveal the effect of tellurium (Te) substitution in FeSe matrix. Rietveld analysis was performed on room temperature recorded, X-ray diffraction (XRD) patterns of pure FeSe, FeTe and $\text{FeSe}_{0.5}\text{Te}_{0.5}$ which shows that all the compounds are crystallized in a tetragonal structure. SEM images show the dense surface morphology. Raman spectra recorded in the range from 100 to 700 cm^{-1} at ambient temperature has been interpreted by P4/nmm space group of the lattice. The variation in intensity and shift in peak positions of some phonon modes has been discussed on the basis of variation in crystalline field effect by substituting Te in FeSe lattice. The resistivity versus temperature curves reveals that FeSe becomes superconductor at 7 K and $\text{FeSe}_{0.5}\text{Te}_{0.5}$ shows superconductivity below 14 K while FeTe is non-superconducting compound.

INTRODUCTION

Today one of the most active areas of research in condensed matter physics is iron-based high critical temperature (T_c) superconductivity. In particular the superconductivity of Fe-doped LaFeAsO with $T_c \sim 26$ K [1] had presented a remarkable achievement in the study of competing magnetism and superconductivity and had opened an interesting and promising era for new research topics in the field of superconductivity. PbO type FeSe is a typical example of iron chalcogenides with $T_c \sim 8$ K [2] which is recently the subject of intensive research, covering the tentative mechanism behind superconductivity and magnetism and has similar structure than the pnictides. The T_c of FeSe is increased to 15 K either by partial substituent of chalcogenides (Te or S) for Se, or even by applying pressure of 1.4 GPa that drastically enhances $T_c = 37$ K [3,4]. It has attracted world wide attention due to its simple structure, non-toxic nature and higher upper critical magnetic field that makes this material useful for superconducting wires and tapes [5,6].

Nuclear magnetic resonance (NMR) and density function calculations studies reported that doped FeSe has a nonconventional superconducting nature that is mediated by antiferromagnetic spin fluctuations and it is not an electron phonon superconductor [7,8]. Since electron phonon coupling was found to be weak to produce a superconductivity state in FeSe(Te), so in this matter Raman Spectroscopy provides an important information about superconducting state in this system [9].

In this paper we present a very simple and low cost process for the synthesis of Fe-based superconducting samples. We discussed in detail the synthesis, phase formation and physical properties of Te doped FeSe in the following sections.

EXPERIMENTAL

Samples $\text{FeTe}_{1-x}\text{Se}_x$ ($x=0, 0.5, 1$) were synthesized through standard solid state reaction route. The stoichiometric ratio of highly pure ($> 3N$) Fe, Se, and Te are ground, pelletized and then encapsulated in an evacuated (10^{-3} Torr) quartz tube. The encapsulated tube is then heated at 750°C for 12 hours and slowly cooled to room temperature. The X-ray diffraction (XRD) are taken on *Rigaku* diffractometer with $\text{Cu } K_\alpha$ ($\lambda = 1.54 \text{ \AA}$). The surface morphological information was derived by using scanning electron microscope (SEM, Leo-440, UK) for recording micrographs. Micro Raman spectrometer (RAM HR 800, Horiba J.Y.) having 632.8 nm laser source was used for recording Raman spectra of these samples (100-700) region. Resistivity measurement was done on physical property measurement system (PPMS).

RESULTS AND DISCUSSION

XRD Studies

Figure.1 shows the room temperature X-ray diffraction (XRD) patterns of $\text{FeSe}_{1-x}\text{Te}_x$ samples with $x=0, 0.5$ and 1. All the three samples show tetragonal crystal structure with space group $P4/nmm$, along with preferential orientation (101) plane. The calculated lattice parameters a and c are respectively 3.76 \AA and 5.53 \AA for FeSe, 3.781 and 5.97 for $\text{FeSe}_{0.5}\text{Te}_{0.5}$ and 3.81 and 6.28 for FeTe these results are in good agreement with earlier reported paper [10]. In $\text{FeTe}_{1-x}\text{Se}_x$ system both a and c were found increased corresponding to ionic radii of Te [11, 12].

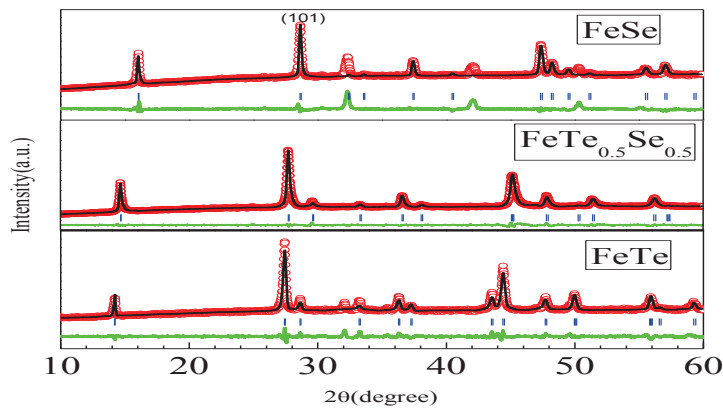


Figure 1. XRD patterns of FeSe, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ and FeTe Samples

SEM Studies

SEM micrographs of FeTe, FeSe and $\text{FeSe}_{0.5}\text{Te}_{0.5}$ are presented in Fig. 2(a,b,c) respectively. These images exhibit the dense surface morphology with layered structure arranged in block form with scattered small fragments. The structure becomes more uniform and rearranged on substituting Te in FeSe.

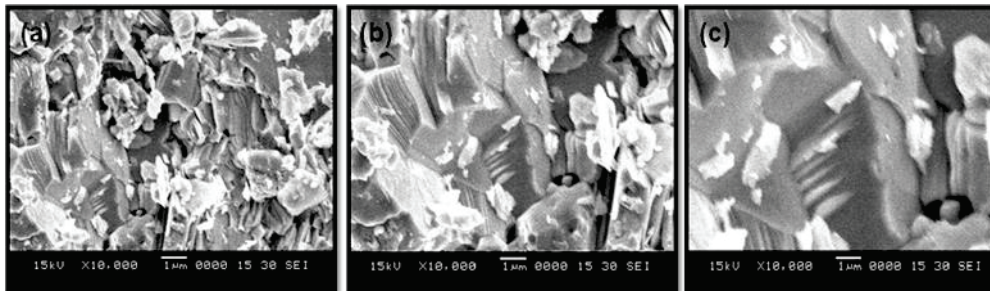


Figure 2. SEM micrographs of (a) FeSe (b) $\text{FeSe}_{0.5}\text{Te}_{0.5}$ and (c) FeTe

Raman Analysis

These spectra were analysed by using the tetragonal phase of space group $P4/nmm$, with Fe-based planar sublattice layered structures. There are four Raman active phonon modes having irreducible representations $A_{1g} + B_{1g} + 2E_g$ for FeSe and FeTe in $100 - 400 \text{ cm}^{-1}$ region modes. Figure 3 shows the five Raman-active modes in 100 to 400 cm^{-1} region for all the three samples with maxima at $120, 139, 217, 279$ and 392 cm^{-1} . These peaks are tentatively assigned to phonon peaks pertaining to $A_{1g}(\text{Te}), E_g(\text{Te}), E_g(\text{Fe}), B_{1g}(\text{Fe})$ and FeSe at room temperature. The variation in the intensity and shift in peak positions of some bands are observed due to the lattice distortion in $\text{FeSe}_{0.5}\text{Te}_{0.5}$ lattice network [13] with a small fraction of FeSe hexagonal phase. The intensity of $A_{1g}(\text{Te})$ and $E_g(\text{Te})$ phonon modes reduces on doping Te in FeSe as compared to pure FeTe. The strengthening intensity of $E_g(\text{Fe}), B_{1g}(\text{Fe})$ and FeSe phonon modes is observed through the improvement in intensity with more stabilized structure on doping Te in FeSe lattice.

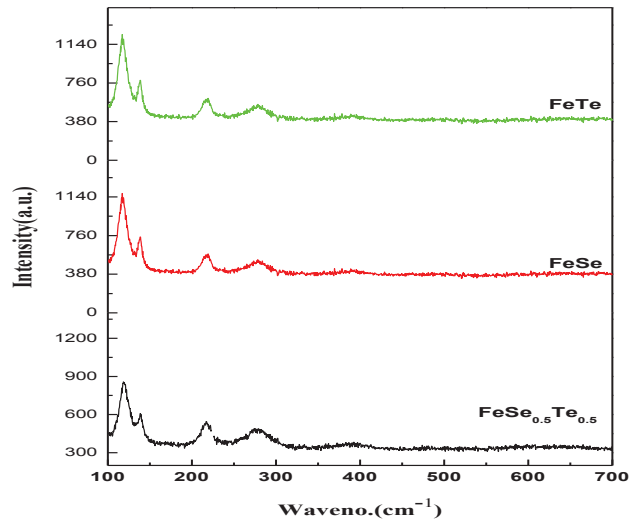


Figure 3. Raman Spectra of FeTe, FeSe and $\text{FeSe}_{0.5}\text{Te}_{0.5}$ samples

Resistivity Measurements

Figure 4 shows the temperature dependence of resistivity $\rho(T)$ of the $\text{FeSe}_{1-x}\text{Te}_x$ samples, the resistivity of sample decreases abruptly on the emergence of superconductivity in FeSe at 7K and enhancement of T_c infact sharpfall transition has been found in $\text{FeSe}_{0.5}\text{Te}_{0.5}$ sample at 13K while in FeTe superconductivity disappeared and rigid anomaly due to structural phase transition occurred around 78 K [12].

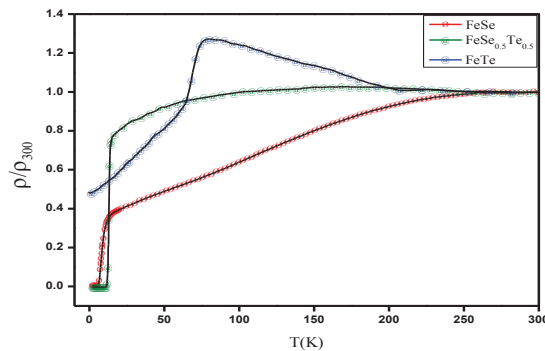


Figure 4. Resistivity vs. Temperature of FeSe, $\text{FeSe}_{0.5}\text{Te}_{0.5}$ Superconductors and FeTe

CONCLUSION

FeSe_{1-x}Te_x (x = 0, 0.5, 1) compounds were prepared by solid state reaction and its structural, Raman and resistivity verses temperature studies were carried to reveal the effect of Te doping in FeSe matrix. The XRD and SEM shows that the polycrystalline nature with dense surface and agglomeration of particles. The resistivity measurement confirms that FeSe and FeSe_{0.5}Te_{0.5} are superconductors with enhancement of T_c after Te substitution such property was absent in FeTe. All Raman active phonon modes are identified and tentatively assigned. The presence of multiple peaks has been attributed to the presence of different Fe-Se, Fe-Te and Se-Fe-Te modes.

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