

Phonons Dispersion and Lattice Dynamic in FeSe Superconductor

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Recently, superconductivity was observed in α -FeSe_{1-x} with critical temperature ~ 8 K [1]. The crystal lattice of α -FeSe belongs to tetragonal (P4/nmm) symmetry at room temperature and is composed of a stack of edge-sharing FeSe₄-tetrahedra layer by layer [2,3]. The tetragonal phase α -FeSe with PbO-type structure has the same planar sublattice as the layered Fe based quaternary oxypnictides, which is the first system where Fe-element plays the key role to the occurrence of superconductivity [4]. In principle, we have discovered that the phase transition of α -FeSe from tetragonal (P4/nmm) at room temperature and occurs an orthorhombic (CMMA) symmetry around the 105 K. Accompanying the magnetic transition from ferromagnetic to antiferromagnetic, the magnetic ordering plays a quite interesting role in the properties of superconductor and magnetic fluctuation. Moreover, these two factors, structure and magnetic phase transition, should be the major effects for superconducting behavior and to observe the phonon interaction between structure and magnetic fluctuation also should be the key for picture the mechanism of superconducting. It clearly reveals that there is clear separation between in- and out-of-plane vibration, as often happens in layered compound. The phonons dispersion at in-of-plane (G (0 0 0) to M (1/2 1/2 0)) show some specific phonon states near 0 to 15 meV, but there is no clear state at out-of-plane (G (0 0 0) to Z (0 0 1/2)) for the same frequency range. Therefore, we have prepared several single crystals about 1mm diameter in order to investigate the phonon spectrum through the help from inelastic x-ray scattering.

In this experiment using inelastic X-ray scattering, we have successful measure the phonon dispersion for single crystal FeSe and FeTe at room temperature at out-of-plane (G (0 0 0) to Z (0 0 1/2)) and in-of-plane (G (0 0 0) to R (1/2 1/2 0)). The Fig. 1 shows the phonons dispersion along the G (0 0 0) to Z (0 0 1/2). Comparing with the simulation data which was published by Alaska Subedi, et. al., the similar spectrum both on FeSe and FeTe were found from 0-40 meV. The phonons energy for each branch of FeTe was lower then one of FeSe. The phenomena should be caused by the atomic mass difference, which the atomic mass of Te is heavier then one of Se, and the fraction of Te height in the unit cell is higher than on of Se. Moreover, we also have found that the acoustic mode of FeSe and FeTe near the 2-10 meV have higher energy than one of simulation. This energy rising might be caused by magnetic interaction between the Fe-Se or -Te and increasing the magnetic coupling energy. Then, also an additional branch around 5-10 meV

was found especially in FeSe system. This might be caused by the multi-domains or geometry effect in FeSe crystal or really difference in FeSe, FeTe and none-spin involving calculation. So that, in the next step of this experiment, we will keep working on simulating the phonon dispersion spectrum with spin and magnetic approximation at first, also hope to take the phonon spectrum at low temperature phase at next available beam time in order to complete the story and physic explanation of relationship between phonon and superconducting in iron based superconductor.

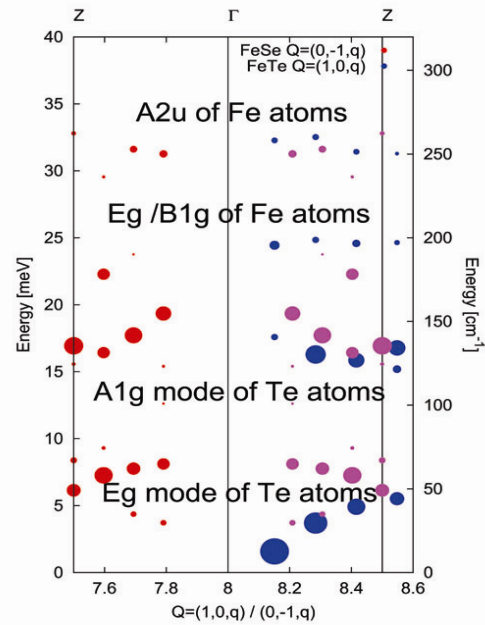


Fig. 1: The phonons dispersions from gamma point to Z direction (0, 0, 1/2). The red points and mirror one, purple points, shows the FeSe crystal phonons branch and blue points for FeTe compounds.

References

- [1] F. C. Hsu, J. Y. Luo, M. K. Wu *et. al.*, PNAS **105**, 14262 (2008).
- [2] P. Terzieff and K. L. Komarek, Monatshefte für Chemie **109**, 651 (1978).
- [3] W. Schuster, H. Mimer, and K. L. Komarek, Monatshefte für Chemie **110**, 1153 (1979).
- [4] Y. Kamihara, T. Watanabe, M. Hirano, and H. J. Hosono, Am. Chem. Soc. **130**, 3296 (2008).
- [5] Alaska Subedi *et. al.*, Physical Review B **78**, 134514 (2008).