ESRF	**Experiment title: ^{57}Fe NIS studies of phonon DOS in superconducting FeSe systems as function of pressure and composition**	**Experiment number**: HS-4098
Beamline: ID18	**Date of experiment**: from: 2. March 2010 to: 8. March 2010	**Date of report:** 18. Aug. 2010
Shifts: 18	**Local contact:** Dr. Aleksandr Chumakov	*Received at ESRF:*

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Report:

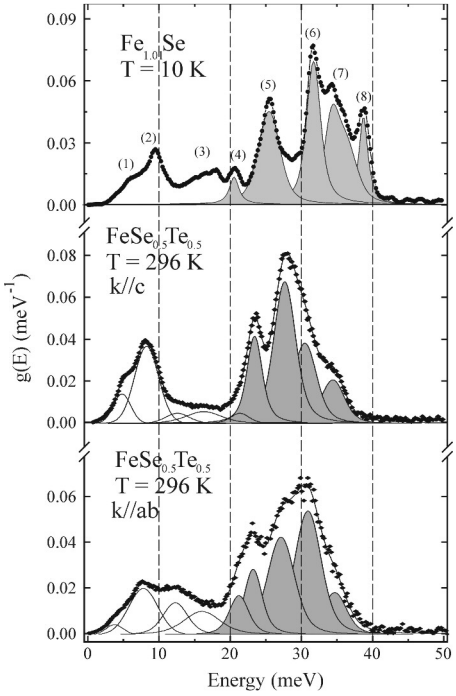

Fig.1: Fe partial phonon-DOS for $Fe_{1.01}Se$ at 10 K ([7]) and of $FeSe_{0.5}Te_{0.5}$ X-tals at RT measured with different orientation of the SR k-vector.

FeSe and $FeSe_{0.5}Te_{0.5}$ are model systems for the new high-T_C superconductors with FeX (X = As and Se) layers. In the previous beamtime HS-3978, we studied in detail the temperature and pressure dependence of the local Fe phonon-DOS in a superconducting (s.c.) $Fe_{1.01}Se$ sample, well characterized and intensively investigated by the applicants in cooperation with Princeton University and Max-Planck Institute of Chemistry, Mainz [1-5]. FeSe could be, because its much simpler structure but still with the same FeX layers a clue compound [6] for the understanding of the principal mechanisms of superconductivity in these FeX-based systems. In particular, the dramatic increase of T_C from 8 K at ambient pressure to 37 K at 9.0 GPa [2] points to a pressure modulated mechanism for superconductivity in FeSe systems. Similar to the s.c. FeAs systems $Ba_{1-x}K_xFe_2As_2$ and $SmFeAsO_{1-x}F_x$, a large isotope effect on T_C has been detected for the FeSe system [6]. Therefore a detailed study of the local phonon density-of-states (DOS) at the Fe sites, which are here the active "players", is of actual scientific interest [6]. We have just published the results of the ^{57}Fe-NIS study on the temperature and pressure dependence of the partial phonon-DOS in $Fe_{1.01}Se$ [7].

In the present beamtime we studied in detail the phonon-DOS in $FeSe_{0.5}Te_{0.5}$ as function of temperature and, by the use of single crystals, the polarisation dependence of the phonon modes. We applied again ^{57}Fe nuclear inelastic scattering (NIS) spectroscopy, with the high energy resolution of 0.7 meV for the 14.413 keV radiation, provided at beamline ID18. The present sample, 100% enriched in ^{57}Fe, was prepared by Vladimir Tsurkan from the group of Prof. Alois Loidl (Univ. Augsburg), specialised in this system [8]. The investigated sample had a s.c. temperature of T_C = 14 K at ambient pressure. Application of pressure leads to an increase of T_C up to 25 K at 3 GPa, as determined in Mainz, similar to the reports of other groups [9]. In Fig. 1 we present the phonon-DOS of the $FeSe_{0.5}Te_{0.5}$ X-tal, measured at 296 K with the k-vector of the monochromatized synchrotron radiation parallel and perpendicular to the c-axis of the tetragonal structure. For comparison, we show on top of Fig.1 the phonon-DOS of $Fe_{1.01}Se$, measured at 10 K in the previous beamtime [7]. We refer to our recent publication for details of the analysis of the pronounced structures of the DOS, labelled 1-3 for acoustic and 4-8 for optical phonon modes [7]. The same principal features are present in the phonon-DOS of the $FeSe_{0.5}Te_{0.5}$ X-tal sample, exhibiting now a pronounced polarization dependence, which allows us to prove (or disprove) our assignment of certain optical modes in our publication, based in part on comparison with theoretical

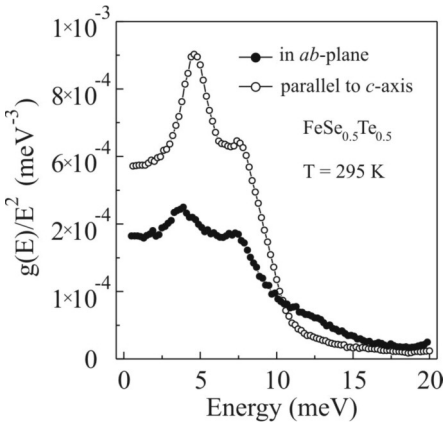

Fig.2: Reduced form of Fe phonon-DOS for $FeSe_{0.5}Te_{0.5}$ X-tals with different orientations.

calculations of the phonon-dispersions and phonon-DOS of FeSe (see refs. in [7]). In addition a pronounced shift to lower energy is observed, different for different modes in the phonon-DOS of $FeSe_{0.5}Te_{0.5}$, by ~4% for mode 5, assigned to the B_{1g} Raman mode, and up to 13% for the lowest acoustic mode 1, in comparison to $Fe_{1.01}Se$ [7]. These shifts result from the combined effects of a lattice expansion by ~10% and an increase of the effective mass m* by ~8%, both caused by the substitution of Se by Te. Of course, the highly anisotropic elastic properties of the layered PbO-structure with a ~3-fold stronger compression (expansion) of the c-axis than the a,b-plane result in different pressure/volume induced variations of the phonon-mode energies (see below). In addition, the random substitution of the Se sites by Te caused obviously a broadening of certain structures resulting from a combined motion of the Fe and Se,Te atoms, most pronounced in the optical modes 6–8, which also exhibit a lowering of their energies by ~8%. In contrast, the mode 5, assigned by us to the B_{1g} mode [7], which originates mainly from Fe atoms vibrating in opposite direction parallel to the c-axis, exhibit only a small shift of ~4% from 24.4 meV (FeSe) to 23.4 meV ($FeSe_{0.5}Te_{0.5}$) with no resolvable spectral broadening. This is easily explained by the fact that mainly the Fe atoms are involved in this mode. The assignment to B_{1g} is further supported by the observation of this mode at 23.0 meV in the Raman spectrum of isostructural $FeSe_{0.3}Te_{0.7}$ [10]. In Fig. 2 we present a plot of the phonon-DOS g(E) in the reduced form, $g(E)/E^2$, exemplifying the strong anisotropy of the acoustic modes, with a "soft" acoustic mode at 4.7(2) meV clearly connected with the soft c-axis (for details, see [7]). These anisotropic properties are reflected in the derived parameters like the Debye temperatures, the sound velocities and the Lamb-Mössbauer f-factors, similar to the case of $Fe_{1.01}Se$ [7].

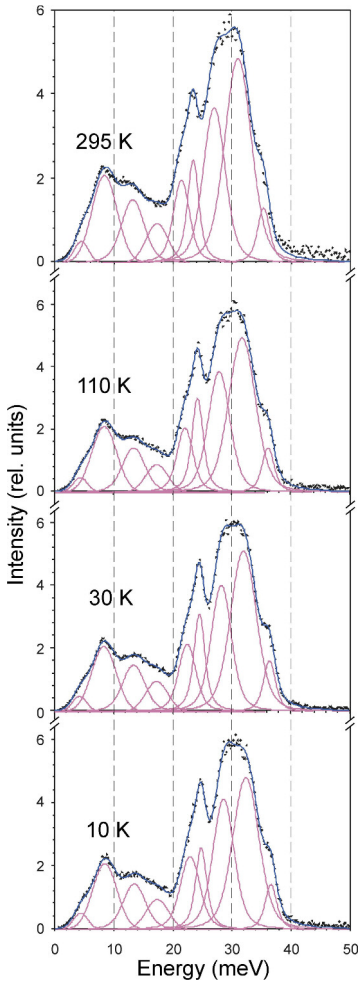

Fig.3: Phonon-DOS of polycryst. $FeSe_{0.5}Te_{0.5}$ at different temperatures.

In Fig. 3 we present the phonon-DOS of a polycrystalline, but textured (resembling the k//ab phonon-DOS) $FeSe_{0.5}Te_{0.5}$ sample at different temperature, e.g. 10 K and 30 K, below and above the s.c. transition, also at 110 K, above the tetragonal-orthorhombic transition and at 295 K for comparison with the oriented X-tal samples shown in Fig. 1. Again we see with decreasing temperature a sharpening of the spectral features, not as pronounced as for $Fe_{1.01}Se$, and shift of the phonon-modes by ~4% to higher energies, very similar to $Fe_{1.01}Se$ [7]. Here the data analysis is, as for the data of $FeSe_{0.5}Te_{0.5}$ in Fig. 1, in a preliminary stage. We want to use the information obtainable from difference spectra, evaluated similar as in a ^{119}Sn-NIS study of SnO with the same PbO structure [11], to search for subtle details in the phonon-DOS above/below T_C and the tetragonal/orthorhombic transition, respectively. As a preliminary resume, we obtained new and highly informative data from the polarisation-dependent phonon-DOS of X-tal samples of $FeSe_{0.5}Te_{0.5}$ as well as from their temp.-dependent behaviour important for their (possible) connections to the s.c. properties. These new data on $FeSe_{0.5}Te_{0.5}$ will be published together with the Augsburg group, where the well-defined ^{57}Fe-enriched samples were prepared [12].

References

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