ESRF	**Experiment title:** Electron phonon coupling in the record Seebeck effect compound FeSb2	**Experiment number**: HS 4388
Beamline: ID28	**Date of experiment**: from: 06.06.2011 to: 12.06.2011	**Date of report**: 20.03.2012
Shifts: 18	**Local contact(s)**: Michael Krisch (email: krisch@esrf.fr)	*Received at ESRF:*

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Report:

Within the beam time allocated for proposal HS 4388 the phonon dispersion curves in FeSb2 were investigated by means of inelastic X-ray scattering (IXS) at different temperatures using the experimental facilities provided at beamline ID18. This investigation was targeted on an understanding of the electron phonon coupling in this compound, which is assumed to be eventually responsible for the record Seebeck coefficient observed around 10 K in this system.

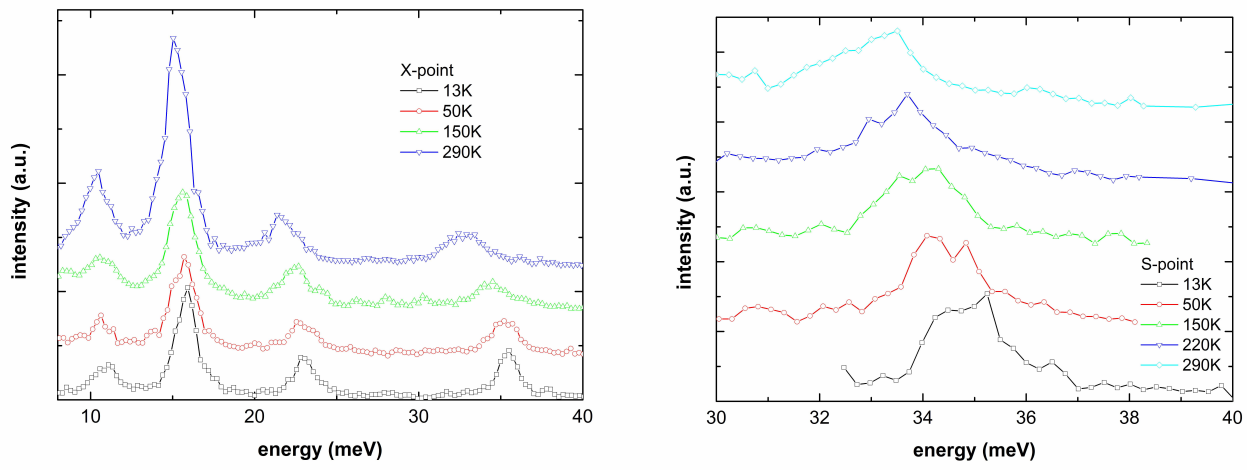
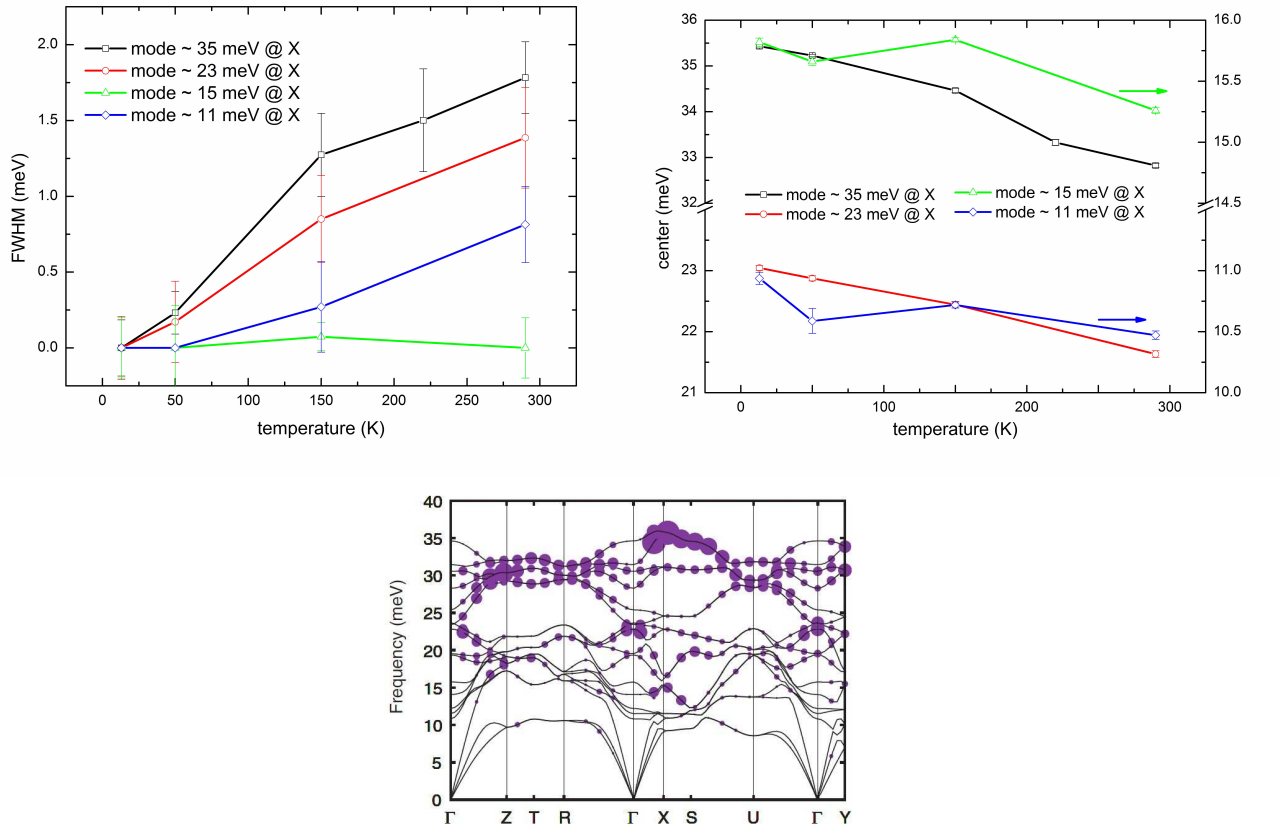


Fig. 1: Representative inelastic X-ray scattering spectra obtained by summation of several energy scans taken at different temperatures.

Representative inelastic X-ray spectra measured at X- and S-point in reciprocal space are shown in Fig. 1. Beside X and S, the phonon dispersion could be investigated at nine additional points each including at least four different temperatures. Phonon broadening as well as mode shifting was analyzed assuming a Lorentzian line shape and a pseudo-Voigt like resolution function (energy resolution of about 1.8 meV FWHM).

In general, the effect of electron-phonon coupling on the phonon line width in FeSb2 can be readily accessed using IXS. The FWHM changes of the modes at X with temperature as well as the corresponding center shifts are displayed in Fig. 2, upper part. While for the high energy modes at both X and S, ab-initio calculations (see Fig. 2, lower part) agree very well with the observed line widths, there is some discrepancy concerning the lower energies requiring further analysis.



Fi. 2: Representative analysis of IXS spectra yielding temperature dependent mode broadening (top left) and mode shifts (top right) for phonons at X. (bottom) Phonon dispersion obtained by ab-initio calculations [1]. Electron-phonon coupling strength at specific points is visualized by the dimension of the purple circles.

References

[1] M.S. Diakhate et al., Phys. Rev. B 84 (2011) 125210.