ESRF	**Experiment title: Strong electron-phonon coupling and the superconducting energy gap in SrPt3P**	**Experiment number**: HC-859
Beamline: ID28	**Date of experiment**: from: 03 Apr 2013 to: 09 Apr 2013	**Date of report**: 18 Feb 2014
Shifts: 18	**Local contact(s)**: Thomas Forrest	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Sven Krannich*, Karlsruhe Institute of Technology, Germany

Frank Weber*, Karlsruhe Institute of Technology, Germany

Diego Zocco*, Karlsruhe Institute of Technology, Germany

Report:

Specific-heat measurements of the recently discovered superconductor $SrPt_3P$ (T_c = 8.4 K) reveal evidence for very strong coupling *s*-wave superconductivity ($2\Delta/k_BT_c \sim 5$) [1], consistent with our *ab initio* calculations which yield a large electron-phonon coupling constant $\lambda \sim 2$. In order to test the lattice dynamical properties of $SrPt_3P$ and the possible strong electron-phonon coupling effects on the superconducting state, we have investigated this material via high-resolution inelastic x-ray scattering experiments. The measurements were performed on a polycrystalline sample in 18 shifts of beam time at the inelastic x-ray scattering beamline ID28. The incident beam energy was set to 21747 eV, with an instrumental energy resolution of approximately 1.5 meV. Low temperatures were obtained using a continuous flow cryostat. A total of 153 energy (E) scans were performed at four temperatures: 300 K, 100 K, 10 K and 2.5 K. Typical counting times varied from 60 to 120 seconds using 0.5 meV energy steps.

Samples were grown at our intitute in Karlsruhe. X-ray diffraction revealed powders containing more than 90% of the desired $SrPt_3P$ superconducting phase. Diffraction scans (2θ) were performed before measurements to determine the position of elastic peaks. Preferable angles (Q-vectors) with low number of elastic counts were selected to match the initial position of one of the analyzers (analyzer #2 in our case). Elastic peaks were fitted with a pseudo-Voight function and substracted from the raw data to result in the inelastic contribution [Fig. 1(a)].

At 300 K, data were collected with an array of 8 analyzers spanning ~ 5.3°, so a total of 7 scans were sufficient for covering the whole 2θ range ($8° \leq 2\theta \leq 45°$ or equivalently 1.5 $Å^{-1} \leq Q \leq 8.5$ $Å^{-1}$). An E vs. Q intensity map was created with these data and compared with our calculations of the phonon density of states (PDOS). An initial analysis of the data yielded a rather different result, although this could be due to the different efficiencies of the 8 analyzers. Further analyis will be carried out to account for this effect.

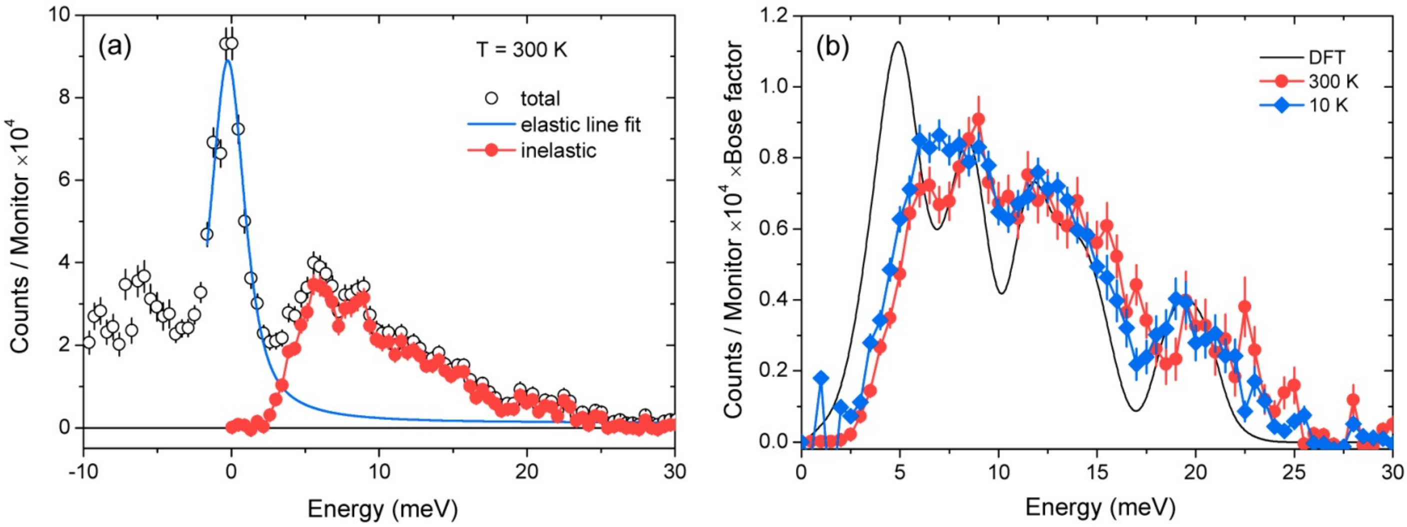

Fig. 1 - (a) A representative energy scan between −10 meV and 30 meV measured at 300 K and Q = 5.7 $Å^{-1}$ (black circles). The inelastic component (red circles) is obtained after substracting the fit to the incoherent-elastic peak contribution (blue line). (b) Inelastic data from energy scans at Q = 5.7 $Å^{-1}$ obtained at 300 K (red circles) and 10 K (blue diamonds). The black line corresponds to the DFPT calculation.

In order to avoid the problem arising from comparing data obtained with different analyzers, in the following we focused in the scans of analizer #2 alone. Data-sets measured at different temperatures were corrected with the corresponding Bose-factor. Fig. 1(b) shows the combined data taken at 300 K for analyzer #2 at Q = 5.7 $Å^{-1}$. Our density functional perturbation theory (DFPT) calculations describe the experimental data fairly well above 10 meV. A discrepancy of the data with the calculations exists at low energies. While theory predicts a phonon mode at 4.9 meV, the experiments at 300 K show a peak centered around 6.5 meV. If the calculations were adjusted to increase the energy of this phonon, then it would result automatically in a decrease in the strength of the estimated electron-phonon coupling. We conclude that our calculations underestimate the energy of the lowest band of phonon modes indicating that the coupling of these modes to the electronic subsystem is overestimated.

As a function of temperature, we observe an overall softening of the low temperature spectra with respect to the room temperature measurements. In particular, a pronounced transfer of spectral weight towards lower energies occurs below 10 meV when cooling from 300 K to 10 K [Fig. 1(b)].

As temperature is reduced from 10 K to 2.5 K, the inelastic data show no variation within the statistical error. For this reason, we conclude that no clear effects are observed upon entering the superconducting state.

[1] T. Takayama *et al.*, Phys. Rev. Lett. **108**, 237001 (2012).