ESRF	**Experiment title:** Inelastic X-ray scattering studies of the giant phonon softening in BaNi2(As1-xPx)2	**Experiment number:** HC-1697
Beamline: ID28	**Date of experiment:** from: 10/09/14 to: 15/09/14	**Date of report:** 05/09/15
Shifts: 18	**Local contact(s):** Thomas Forrest	*Received at ESRF:*
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Report:

Background

At room temperature $BaNi_2As_2$ exists in a tetragonal $ThCr_2Si_2$-type structure (space group *I4/mmm*). Upon cooling the system undergoes a first-order structural phase transition into a triclinic phase (space group *P1*), and superconductivity emerges at 0.7 K. It is believed that the nature of this superconductivity is of the conventional BCS type [1]. Isovalent doping at the Arsenic site with Phosphorus initially leads to a suppression of the structural phase transition, and a slight increase in the superconducting transition temperature (T_c). At a doping level of x=0.067, the structural phase transition is completely suppressed, and an abrupt increase in T_c from 0.7 to 3.3 K is observed [2]. It has been suggested that there is a soft of a phonon mode in the tetragonal phase, which is suppressed by the structural phase transition. In fact, this softening could be as much as 50% (ref.2 describes it as "giant"). Therefore this phonon softening leads to an enhancement of the electron-phonon coupling in the tetragonal phase, and hence the jump in T_C as the doping suppress the structural phase transition [2].

Prior to our experiment, we conducted a series of X-ray diffuse scattering measurements on the parent compound ($BaNi_2A_2$), at several temperatures above and below T_S. These measurements showed significant diffuse scattering around the periodic position: *(H=even, K=odd±1/4, L=odd)*. Furthermore, with cooling the diffuse scattering became stronger, and finally upon crossing the structural phase transition at T_S~135 K, this diffuse scattering collapses into a focused superstructure reflection (see figure 1). Therefore this diffuse scattering is likely to be the location on the giant phonon softening that has been predicted [1].

Experiment

We have performed a series of Inelastic X-ray Scattering (IXS) measurements to study the lattice dynamics in BaNi2(As1-xPx)2, as a function of temperature. These measurements were taken on a high quality single crystal of $BaNi_2As_2$, with ID28 in the Si(11 11 11) backscattering configuration (E= 21.747 keV), this gave an energy resolution of ~1.5 meV. IXS scans were taken between ±20 meV, at several Q-points that cross the (4 0.75 1) position (a location of significant diffuse scattering). The IXS measurements at room temperature indeed confirmed that the (4 0.75 1) is the location of the phonon mode softening. Furthermore this softening is excellently reproduced by our D.F.P.T. calculations.

Interestingly upon cooling the sample, the scattering close to zero energy transfer increases dramatically (see fig 2.). This scattering is broader in energy than the instrument resolution, and is therefore quasi-elastic in nature. As the temperature is reduced through T_S the scattering becomes limited by the instrument resolution, becoming truly elastic (see insert of fig 2).

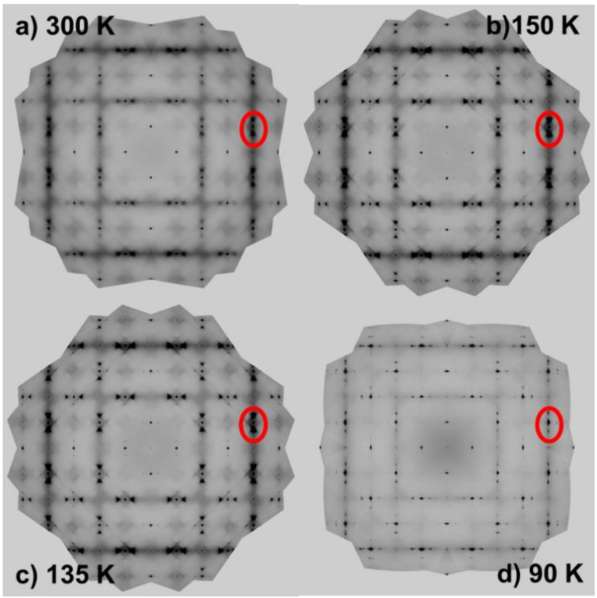

Figure 1: TDS scattering from the (HK1) plane at 4 temperatures: a) room temperature, b) 150 K, c) 135 K & d) 90K. The red ellipse show examples of the diffuse scattering above T_S (fig1a-c) and the superstructure reflections below T_s (fig 1d).

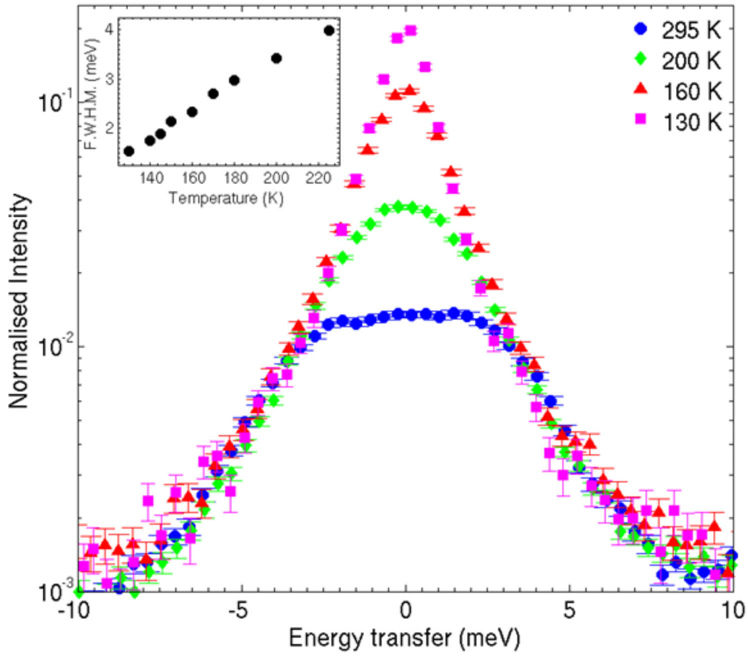

Figure 2: A log plot of IXS spectra at (4 0.75 1), between 295 K & 130 K. The insert shows the FWHM from a Gaussian fit of the central peak between 225 K & 130 K.

Our result shows that there is indeed a significant and unusual phonon softening in the tetragonal phase of $BaNi_2As_2$. Unfortunately due to the experiment being run in 16 bunch mode, we did not have a high enough X-ray flux to be able to measure the doped compound during 18 shifts. Therefore we plan to submit a new proposal to complete this project.

References

1. Subedi et al., Phys. Rev. B **78**, 132511 (2008).
2. Kudo et al., Phys. Rev. Let. **109**, 097002 (2012).