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Experimental and theoretical studies of the lattice dynamics in superconducting BaNi2(As1-xPx)2.

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We present a combination of Thermal Diffuse Scattering (TDS) and Inelastic X-ray Scattering (IXS) measurements, and Density Functional Perturbation Theory (DFPT) calculations of the lattice dynamics in superconducting BaNi2(As1-xPx)2. At Ts=130 K, BaNi2As2 undergoes a structural phase transition from a tetragonal to a triclinic crystal structure. In addition, superconductivity emerges at Tc=0.7 K. Substitution of the arsenic with phosphorus leads to a suppression of Ts. Finally, at a substitution level of 7%, the structural phase transition is completely suppressed and the Tc jumps from 0.7 to 3.3 K. It is believed that the nature of the superconductivity displayed by this material is of the conventional BCS type. Furthermore, specific heat measurements suggest that a "Giant"phonon softening is responsible for the jump in Tc. In order determine if such a large phonon softening does occur in BaNi2(As1-xPx)2, we have undertaken a combined experimental and theoretical study of the lattice dynamics of this material. TDS measurements on BaNi2As2 have identified locations of significant diffuse scattering. Upon cooling, the scattering from these diffuse regions becomes stronger, collapsing into true Bragg structural reflections below Ts. The IXS measurements and DFPT calculations identify this to be the location of a significant softening of at least one phonon mode. Out results demonstrate that these phonons are strongly coupled to the structural phase transition, and therefore it is a strong candidate for being responsible for the jump in Tc. In order to ascertain if this is correct, we have extended our TDS and IXS measurements to phosphorus doped BaNi2As2. Results from these latest set of measurements will be presented. In addition, our results will be compared to the lattice dynamics to the iron pnictide unconventional superconductors.

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