Temperature Dependence of the Lattice Dynamics of Nickel

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Abstract:

• The majority of the entropy of a solid comes from the vibrations of atoms about their equilibria (phonons).

• As the temperature increases, the inter-atomic forces change, causing shifts in the phonon spectrum.

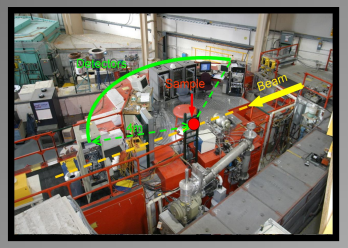
• In this study we investigate the changes in the nickel phonon Density of States (DOS) at temperatures from 300K – 1275 K.

• We also consider data from two generations of time-of-flight, direct geometry, inelastic chopper spectrometers.

Neutron Scattering Measurements:

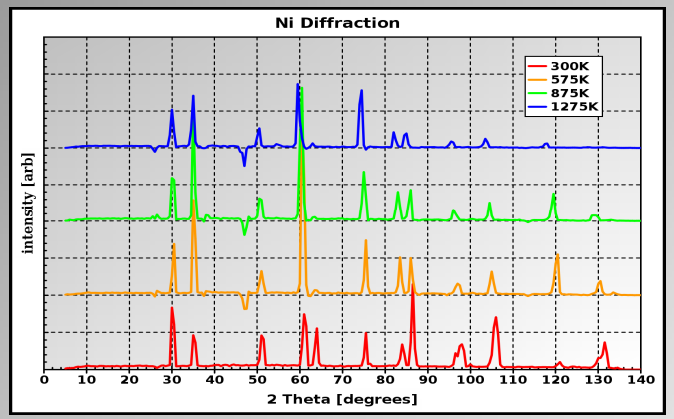
• Measurements made on two spectrometers.
  • Pharos Ei = 70 meV (Los Alamos Neutron Science Center)
  • LRMECS Ei = 60 meV (Intense Pulsed Neutron Source, Argonne)

• Samples were flat plate,10% scatterers, displex mounted.



Neutron Diffraction:

Neutron diffraction patterns were taken in-situ at Pharos.



Phonon DOS and Modeling:

• The phonon DOS were obtained from S(E) after performing multiphonon, Debye-Waller and thermal corrections.

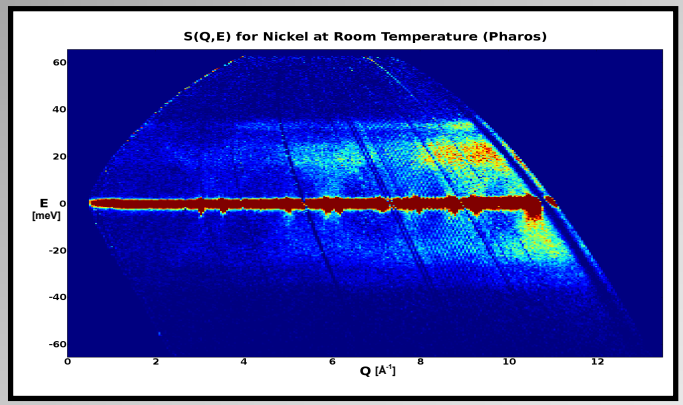
• The DOS were fit with Born-von Kármán (BvK) models of the lattice dynamics.

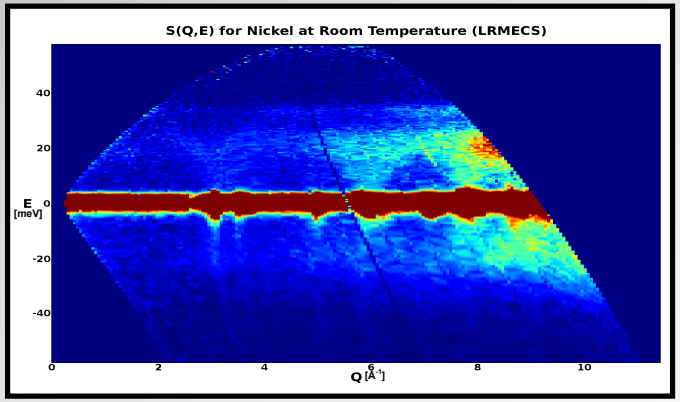
Coherent Inelastic Scattering:

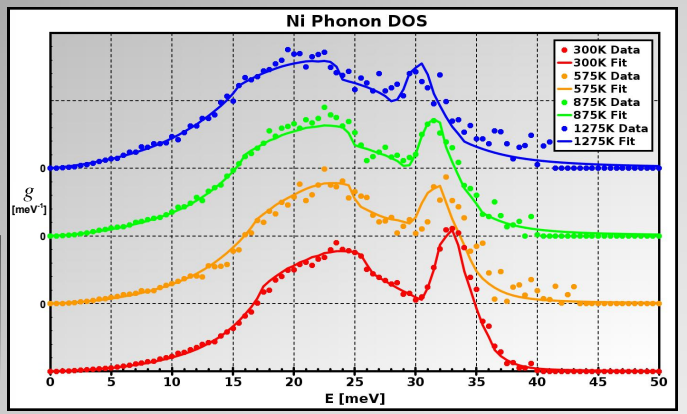
• Maps of S(Q,E) were produced from data collected at two different spectrometers.

• Two data processing techniques were employed:
  • Pharos → `rebinning` methods
  • LRMECS → transformation and linear extrapolation

• Coherent scattering in S(Q,E) gives information about the polycrystalline average of phonon dispersions.







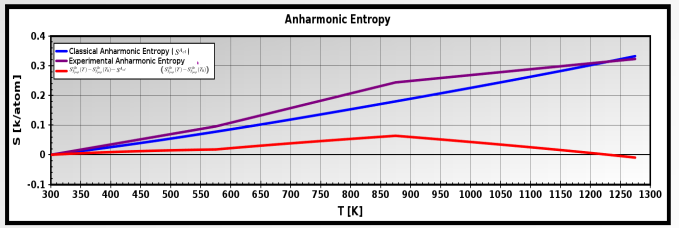
Vibrational Entropy

•The vibrational entropy is given by

$$S^{vib}_{T_{pop}} = 3k_B \int g\left[(n_{T_{pop}}+1)ln(n_{T_{pop}}+1) - n_{T_{pop}} ln(n_{T_{pop}})\right] dE$$

•By considering the DOS at two temperatures, populated at the same temperature, we make comparisons to the classical formula for the anharmoic entropy of a solid.

$$S^{An_{cl}} = \int_{T_0}^{T} \frac{C_P - C_V}{T'} dT' = \int_{T_0}^{T} \frac{9B\alpha^2}{\rho_N} dT' \; ? = ? \; S^{vib}_{T_{pop}} - S^{vib}_{T_{pop}}$$



Summary and Future Work:

• The Ni phonon DOS was measured at temperatures from 300K – 1275K.

• The DOS were fit with BvK models of the lattice dynamics.

• The softening of the DOS was consistent with the expansion of the Ni lattice.

• Work is currently under way to fir S(Q,E) directly with a BvK model.