DOS Inversions with Coherent Scattering

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This morning you saw how inversions of incoherent inelastic scattering from ^{57}Fe overcame the neutron-weighting problem.

More information is available through the Q- or $\vec{Q}$-dependence of coherent scattering.

Polycrystalline Average of Dynamical Structure Factor

- Polycrystalline Ni_3Al at HFIR with 4 values of Q.
  (We were looking at order-disorder phenomena...)
- Lattice dynamics on single crystal ordered Ni_3Al were done by C-K. Loong, et al.
  - Typo in a table of force constants.
  - O. G. Randl gave us some help getting 1nn, 2nn radial force constants of fair quality.
- Calculated incoherent scattering with Born–von Kármán code.
- Calculated coherent scattering from all orientations of crystallites w.r.t. $\vec{Q}$.
  (Coherent scattering was considered a nuisance to be overcome.)

The Q-dependence gives us more information about dynamics.

- Interpretable with powders and typical statistics.
- $\vec{Q}$-dependence is even better, but requires single crystals.

Possible Experiments

- Force constant softening in B2 NiTi, using polycrystalline samples.

- Temperature-dependence of lattice dynamics in bcc transition metals.
  - Ti phonons harden with increasing temperature(!)
  - Fe ?
  - Mo ?