Direct Measurement of the Orientation of Atomic Vibrations Using Inelastic Neutron Scattering

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(Mentee of Daniel Parshall)
What is a phonon?

- Vibrational wave
- Occurs in crystals and other condensed matter
- Can be detected with neutron scattering

Animation of phonons courtesy of Dan Parshall's program SNAXS
How are phonons detected?

→ Bounce a beam of neutrons off of a sample
→ Measure energy and momentum transferred
→ New machines collect massive amounts of data, but the tools to analyze the data do not exist

The Wide Angular-Range Chopper Spectrometer (ARCS) at Oak Ridge National Laboratory
Data Fitting

- New program can find a fit at any point in the crystal
- Phonons repeat in reciprocal space, but their intensities can vary based on direction
- Center and width fit globally, height and background fit individually
Simultaneous Fitting

- Individual data sets are noisy and incomplete
- Utilizes many datasets at the same time to clean up the fit
Eigenvalues are the energy of each phonon.

Eigenvectors are the direction of atomic displacement.

Crystals can be approximated as a lattice of masses on springs.
→ Distribution of electrons determines force constants
→ Normally only compare energy
→ Force constants can be wrong but still give correct phonon energy values
→ We plan to compare force constants directly

And we care because...?

Theory (ex. DFT)

Force Constants

Eigenvectors

Phonon Intensities and Energy Values

Data side

Force Constants

Eigenvectors

(Data is Fit)

Theory side

Data
Finding Eigenvectors

→ Use intensities found previously to fit the eigenvectors
→ Compare fitted intensities to values calculated from eigenvectors

Leasqr is a Levenberg-Marquardt nonlinear regression function from the Octave package Optim
Results...

Phonopy model of eigenvector

Eigenvector fitted from data directly
Visualizing Results

- Phonopy model of eigenvector
- Eigenvector fitted from data directly

111 Direction
Thanks be unto:

★ Daniel Parshall
★ Julie Borchers
★ Yamali Hernandez
★ Dan Neumann
★ Yang Zhao
★ The SHIP administration
BKBO is a superconductor with a maximum $T_c$ of $\sim 30K$

Phonons are most likely involved in the superconductivity

Electron-phonon interactions as yet unobserved

Ba$_{1-x}$K$_x$BiO$_3$ unit cell structure