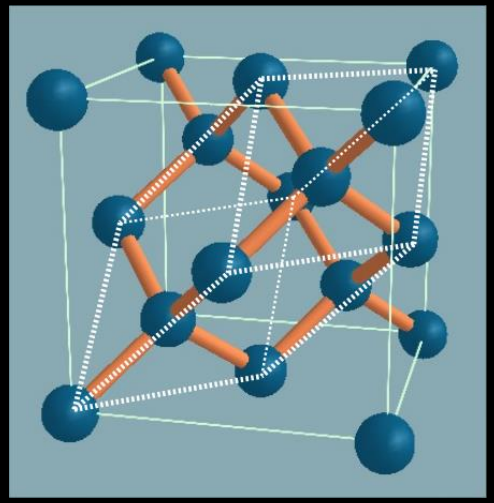

Direct Measurement of the Orientation of Atomic Vibrations Using Inelastic Neutron Scattering

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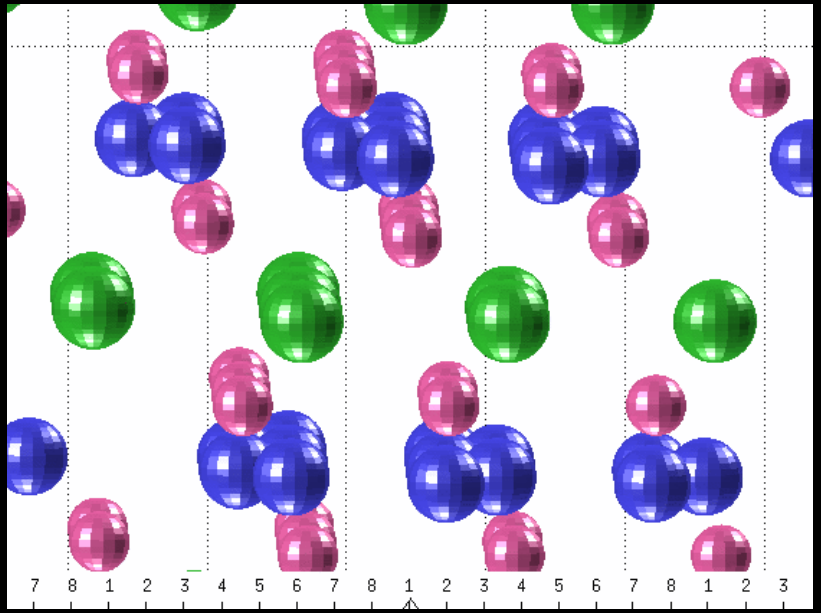
(Mentee of Daniel Parshall)

National Institute of Standards and Technology
U.S. Department of Commerce

What is a phonon?

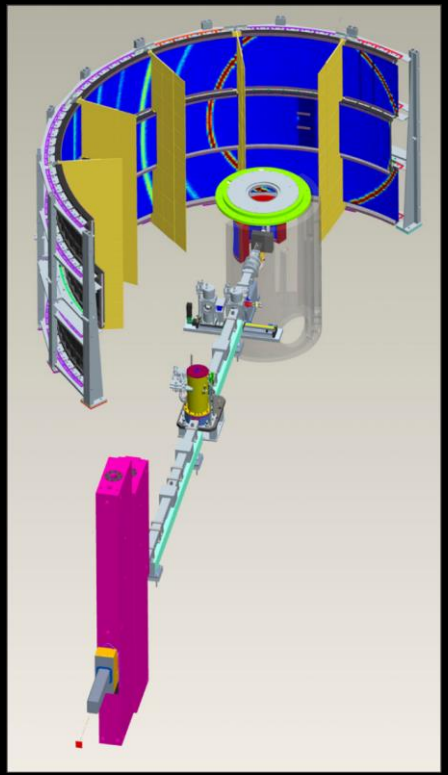
- ➔ Vibrational wave
- ➔ Occurs in crystals and other condensed matter
- ➔ Can be detected with neutron scattering



Animation of phonons courtesy of Dan Parshall's program SNAXS

How are phonons detected?

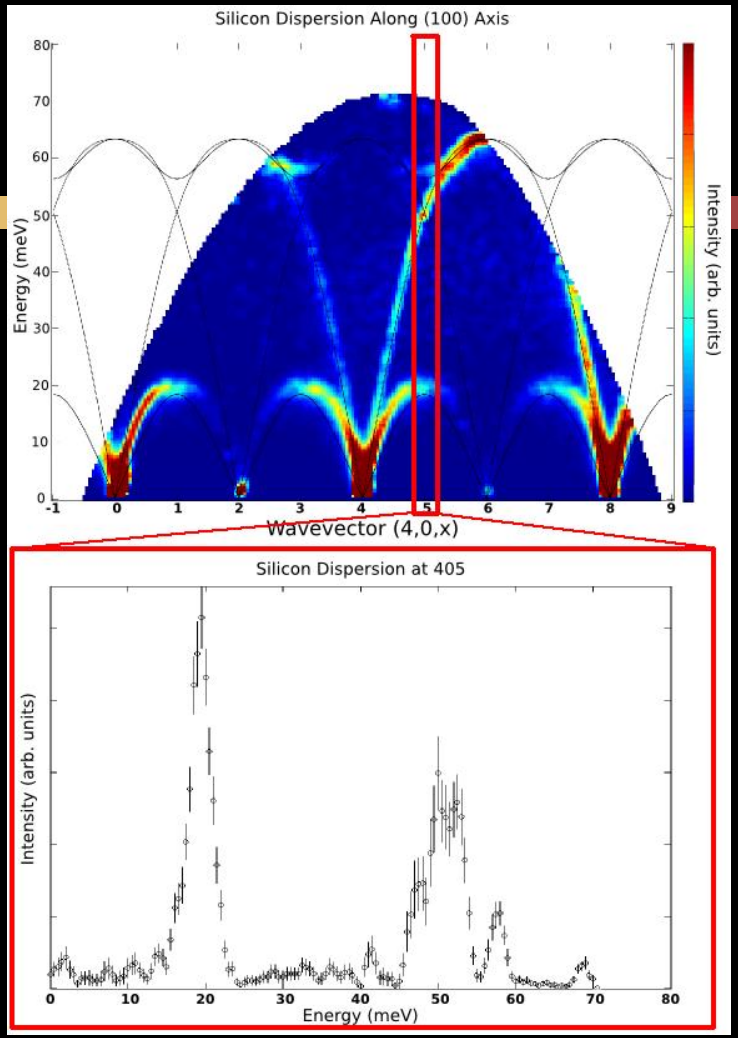
- ➔ Bounce a beam of neutrons off of a sample
- ➔ Measure energy and momentum transferred
- ➔ New machines collect massive amounts of data, but the tools to analyze the data do not exist



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

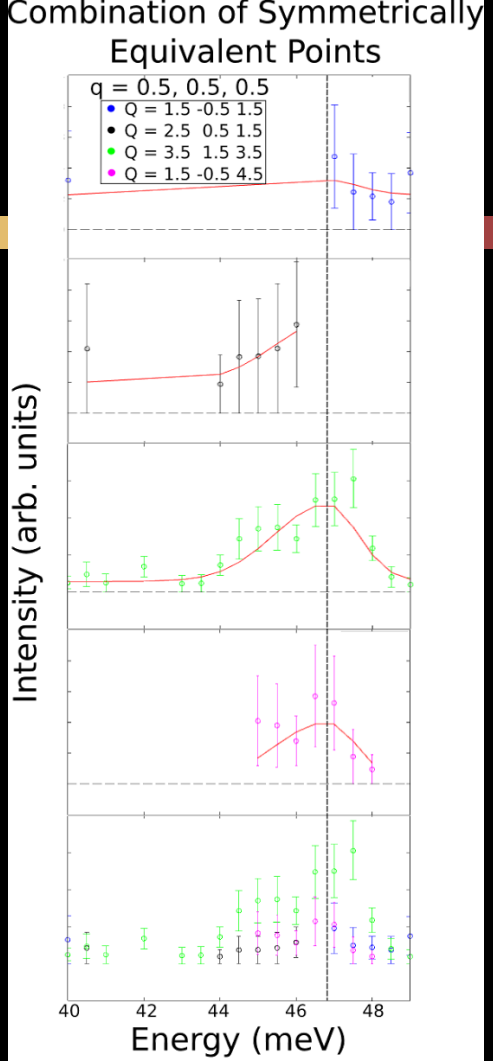
Data Fitting

- ➔ 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



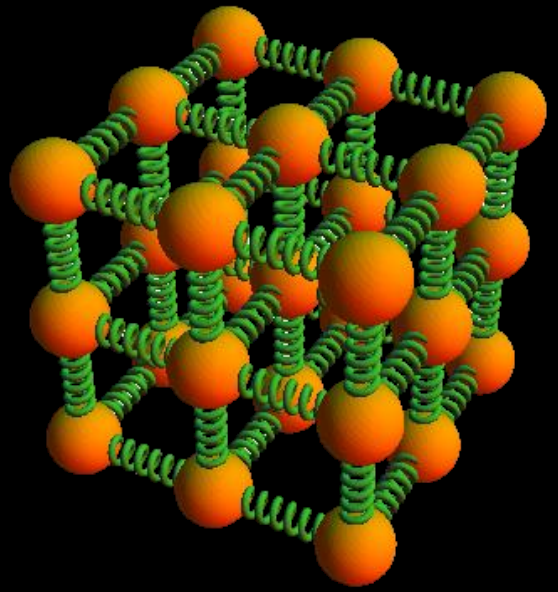
Simultaneous Fitting

- ➔ Individual data sets are noisy and incomplete
- ➔ Utilizes many datasets at the same time to clean up the fit



Eigenvectors and Phonons

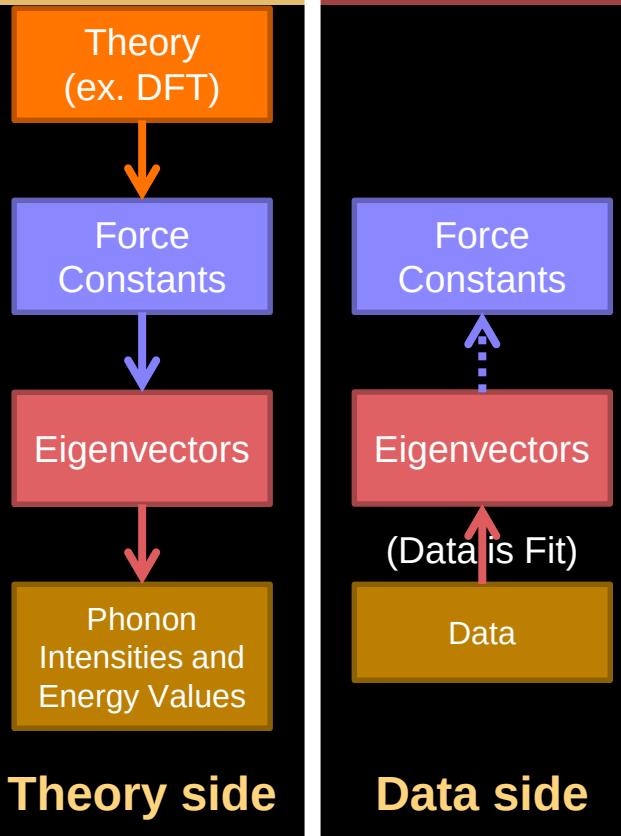
- ➔ Eigen**values** are the energy of each phonon
- ➔ Eigen**vectors** are the direction of atomic displacement



Crystals can be approximated as a lattice of masses on springs

And we care because…?

- ➔ 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



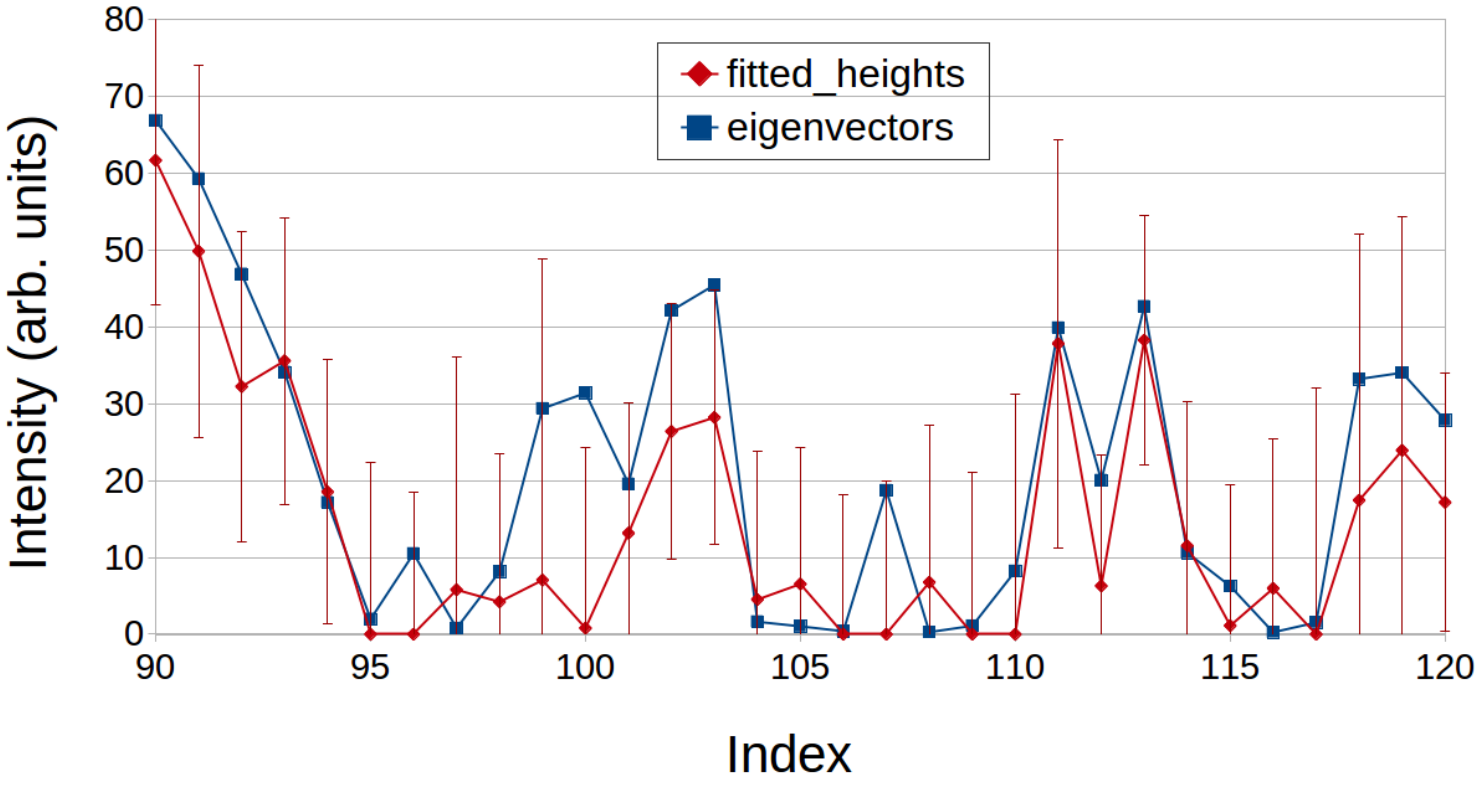
Finding Eigenvectors

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

```
hdatin = SQW{1}.VARS.allvars(phonon_mode,mask+1,1);% grabs the fit heights
hdatin = hdatin(:);
varsin = zeros(6*PARAMS.CRYSTAL.N_atom,1);
stol=1E-4;
niter=100;
wt = .1*ones(length(hdatin),1);%calc_uncertainty(SQW,phonon_mode);%
dp=0.001*ones(size(varsin));

PARAMS.hdatin = hdatin;
PARAMS.wdatin = wt;

%[funcout,varsout] = leasqr(PARAMS,hdatin,varsin,'eig_calc',stol,niter,wt,dp,dFdp);
[funcout,varsout] = leasqr(PARAMS,hdatin,varsin,'eig_calc',stol,niter,wt,dp);

eigenvectors = reshape(varsout,3*PARAMS.CRYSTAL.N_atom,2);
```

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

Intensity from Eigenvectors Overlayed with Fitted Heights



Results...

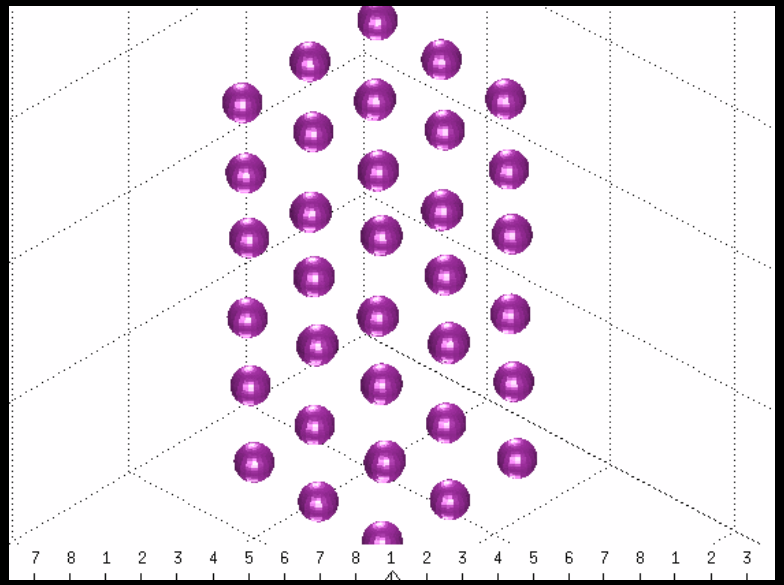
```
- # 3
  frequency:     5.1317473718
  eigenvector:
  - # atom 1
    - [ -0.40824829046386,  0.00000000000000 ]
    - [ -0.40824829046386, -0.00000000000000 ]
    - [ -0.40824829046386, -0.00000000000000 ]
  - # atom 2
    - [ -0.37489139457916,  0.16162644875501 ]
    - [ -0.37489139457917,  0.16162644875501 ]
    - [ -0.37489139457917,  0.16162644875501 ]
```

Phonopy model of eigenvector

```
eigens =

  -0.55290  - 0.00000i
  -0.36513  + 0.13357i
  -0.48845  - 0.04804i
  -0.24493  + 0.10230i
  -0.33578  - 0.14649i
  -0.32458  + 0.02698i
```

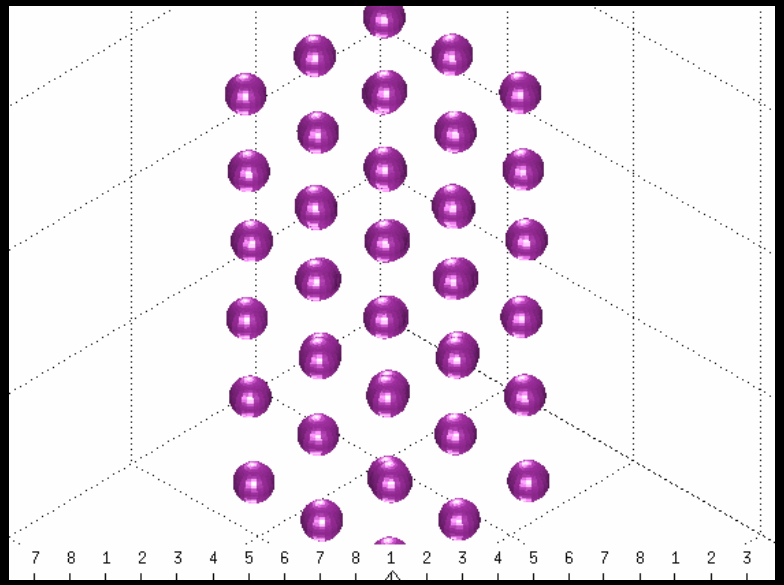
Eigenvector fitted from data directly

Visualizing Results



Phonopy model of eigenvector

111 Direction



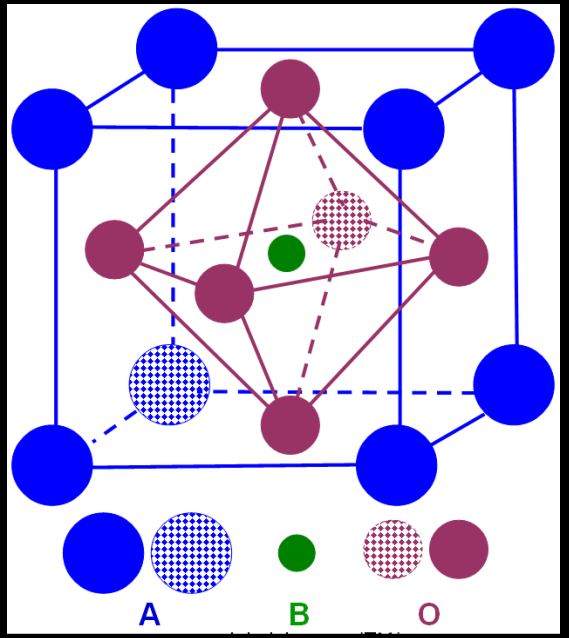
Eigenvector fitted from data directly

Thanks be unto:

- ★ Daniel Parshall
- ★ Julie Borchers
- ★ Yamali Hernandez
- ★ Dan Neumann
- ★ Yang Zhao
- ★ The SHIP administration

Where do we go from here?

- ➔ BKBO is a superconductor with a maximum T_c of ~30K
- ➔ Phonons are most likely involved in the superconductivity
- ➔ Electron-phonon interactions as yet unobserved



$Ba_{1-X}K_XBiO_3$ unit cell structure