An Investigation of the Vibrational Properties of BGaN Alloys

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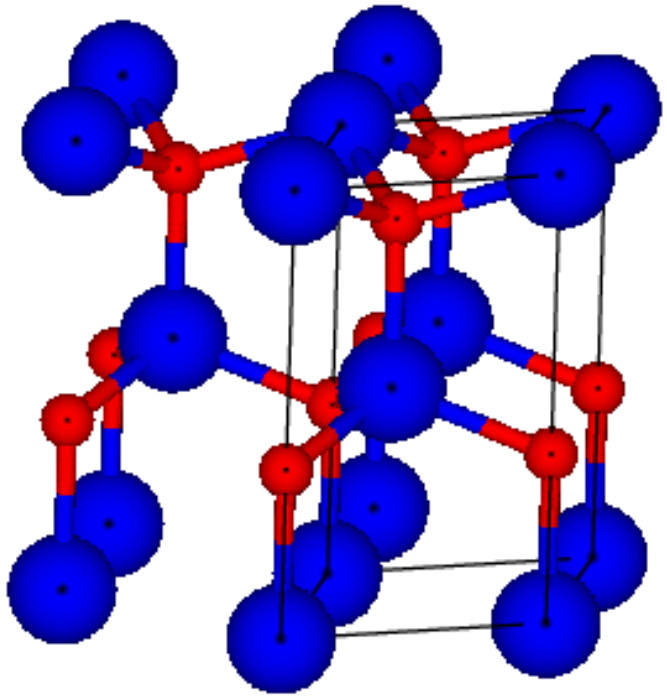
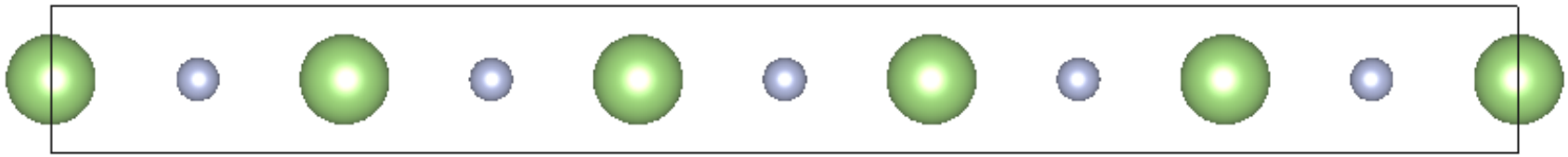
Motivation

- Alloys of III-nitrides such as AlN, GaN, and InN are important for electronics and optoelectronics.
- BN is a natural next choice as we push into the UV spectrum.
- Vibrational properties are of prime importance for understanding thermal and electronic properties.
  - integrated quantitites (entropy, heat capacity)
  - phonon-phonon (thermal resistivity)
  - electron-phonon (electronic resistivity)



Gaining Intuition

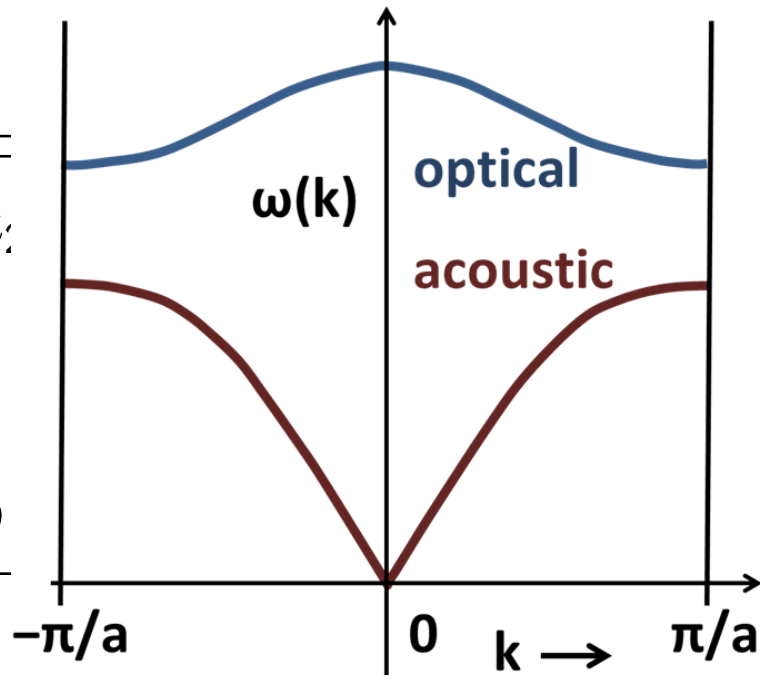


For a 1D diatomic chain,

$$\omega_{\pm} = \sqrt{\frac{\kappa_1 + \kappa_2}{m} \pm \frac{1}{m}\sqrt{(\kappa_1 + \kappa_2)^2 - 4\kappa_1\kappa_2}}$$

From the Debye model,

$$U = \int d\omega D(\omega) \langle n(\omega) \rangle \hbar\omega \quad \rightarrow \quad C_V = \left(\frac{\partial}{\partial}\right.$$



[1] By Brews ohare — Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=19037365

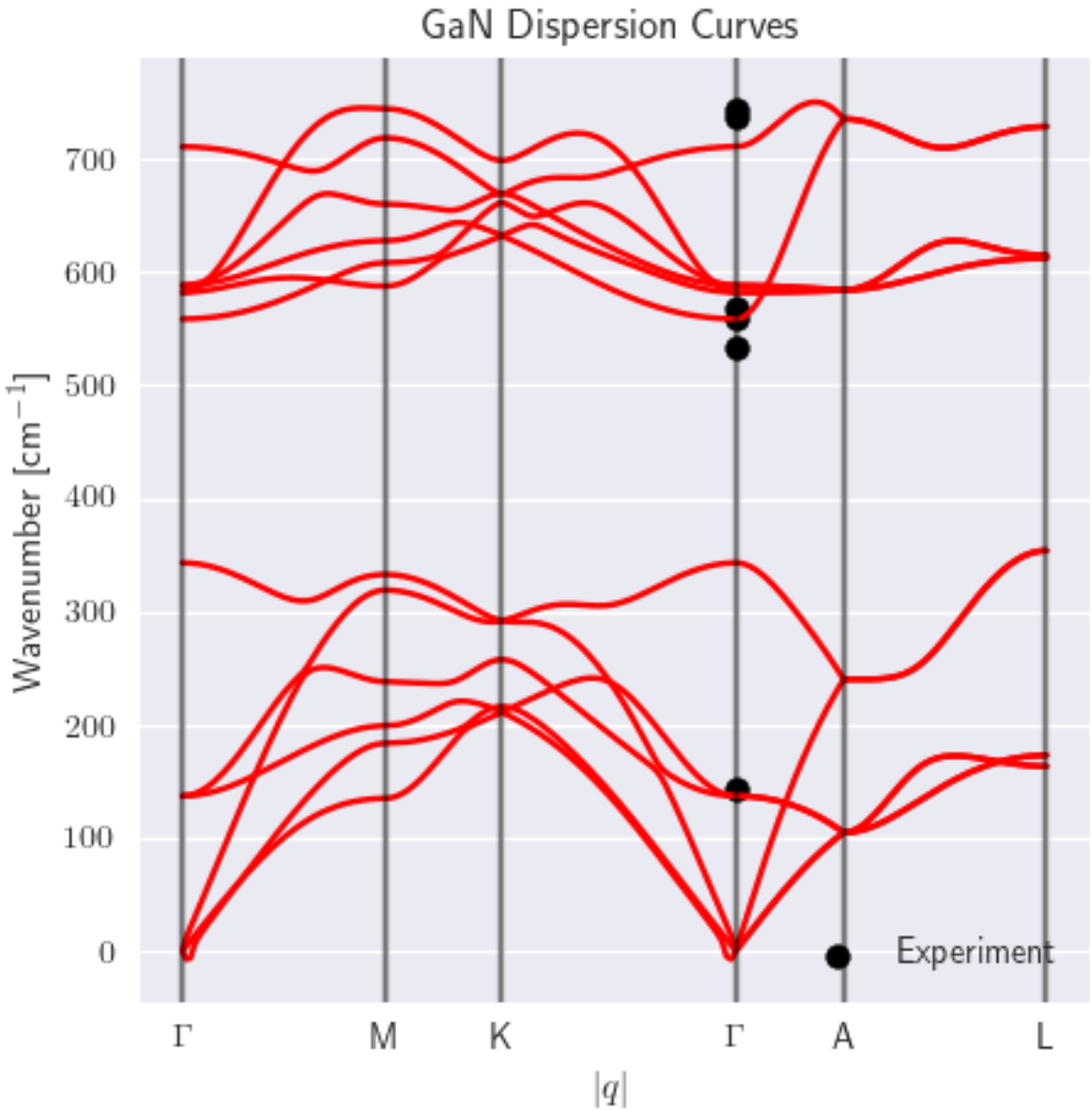
Computational Methodology

- DFT calculations using the LDA fuctional as implemented in VASP.
- Use PAW pseudopotentials and an ENCUT of 520 eV.
- "DFPT" (IBRION = 8) to calculate zone-center frequencies and Hessian matrix.
  - "frozen phonons"
  - $\Delta E < 10^{-7}$ eV
  - forces < 5 meV/Å
- Phonopy to calculate dispersion curves.

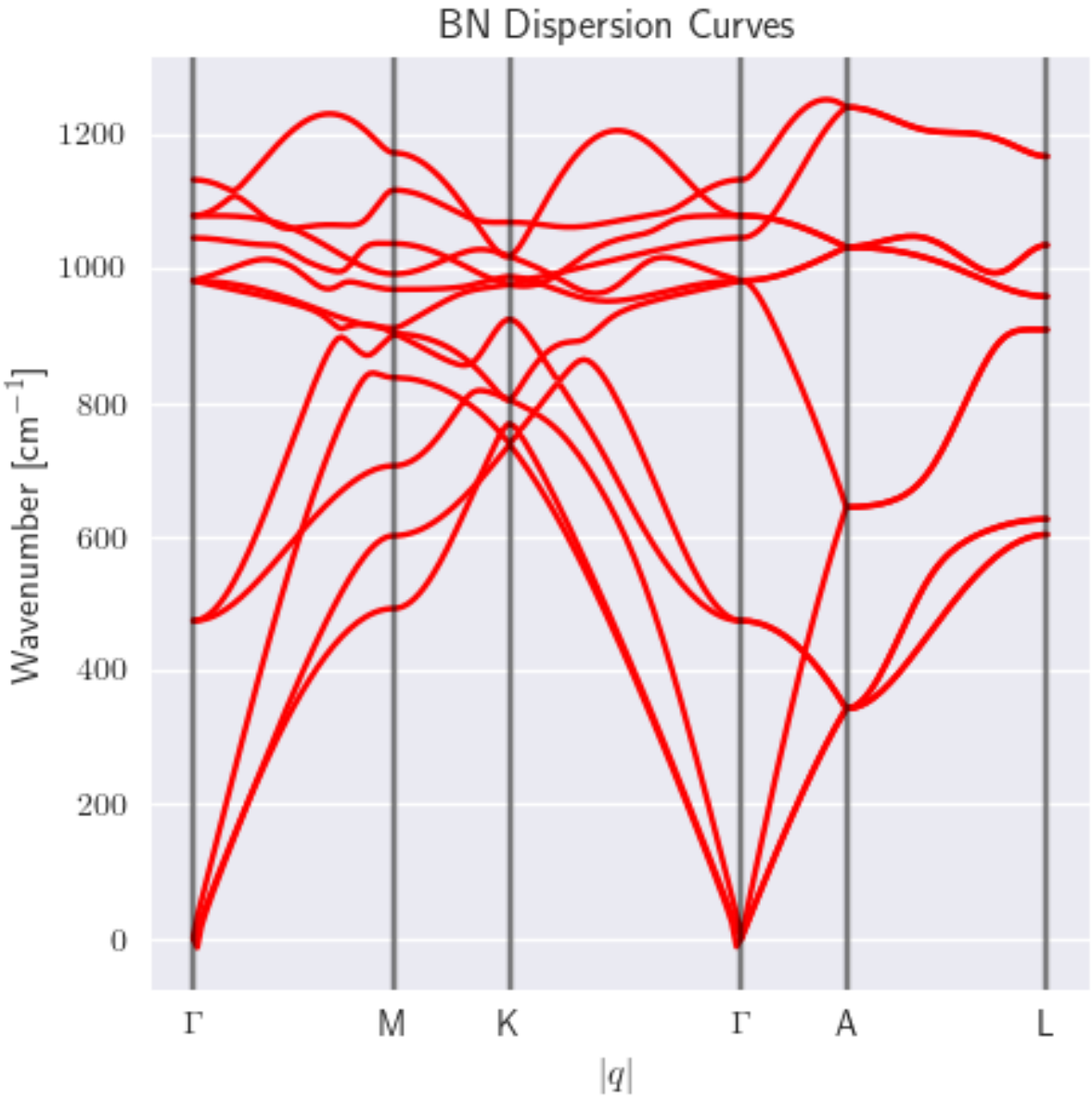
How do we simulate an alloy?

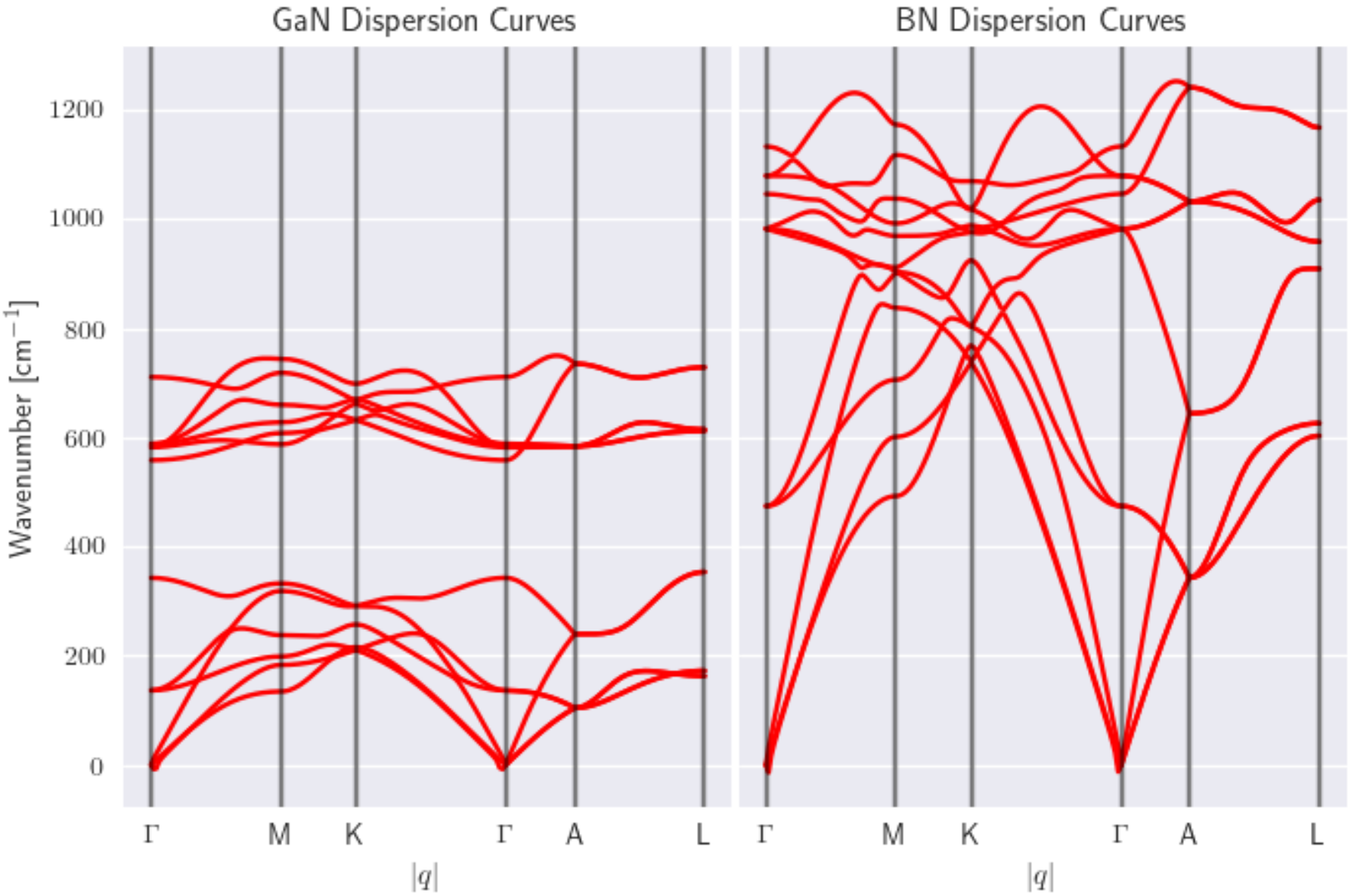
- special quasi-random structures (SQS)
- random structure averaging

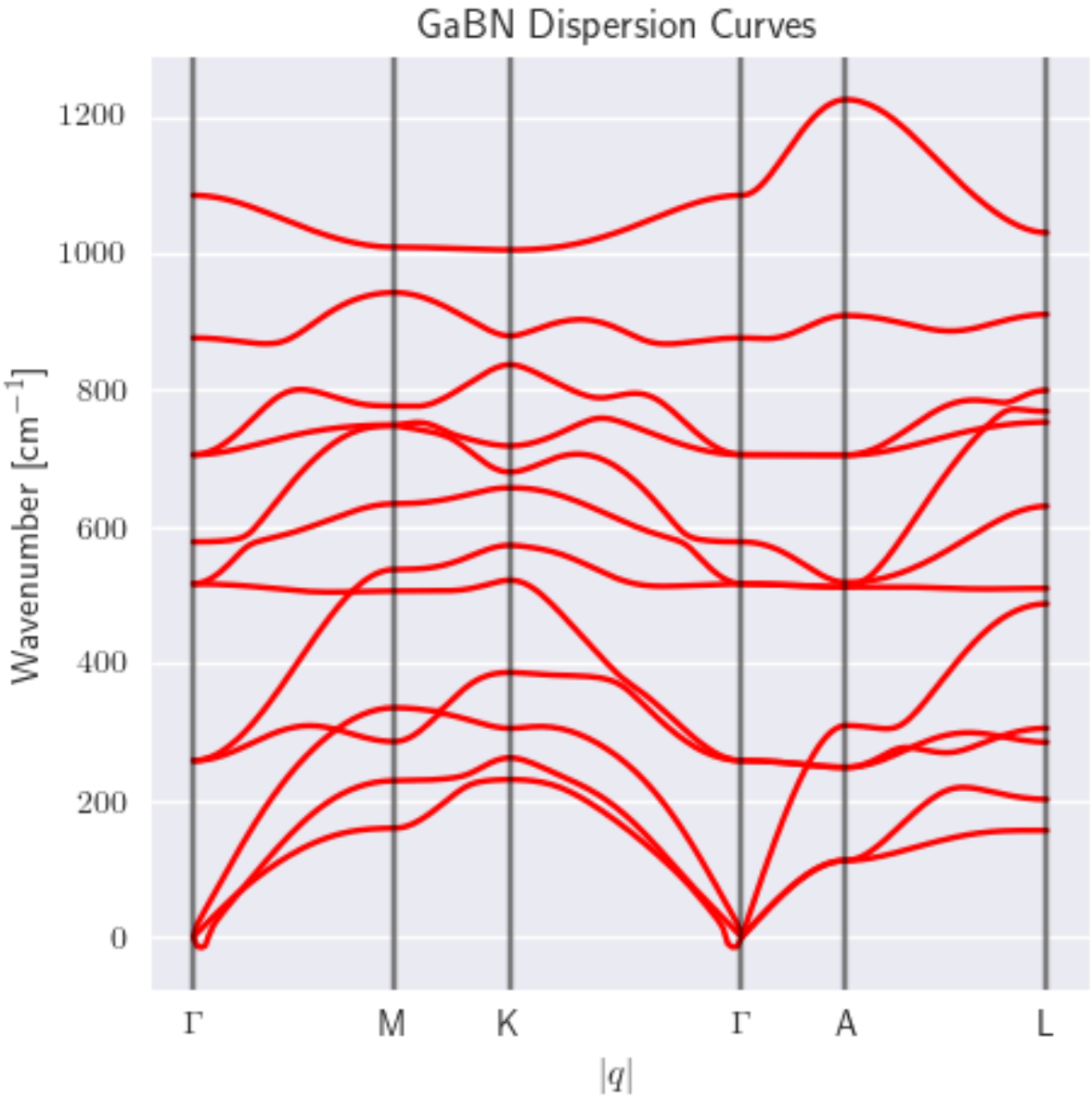
However, we will use the ordered compound, $GaBN_2$, to approximate a 50% B concentration alloy.

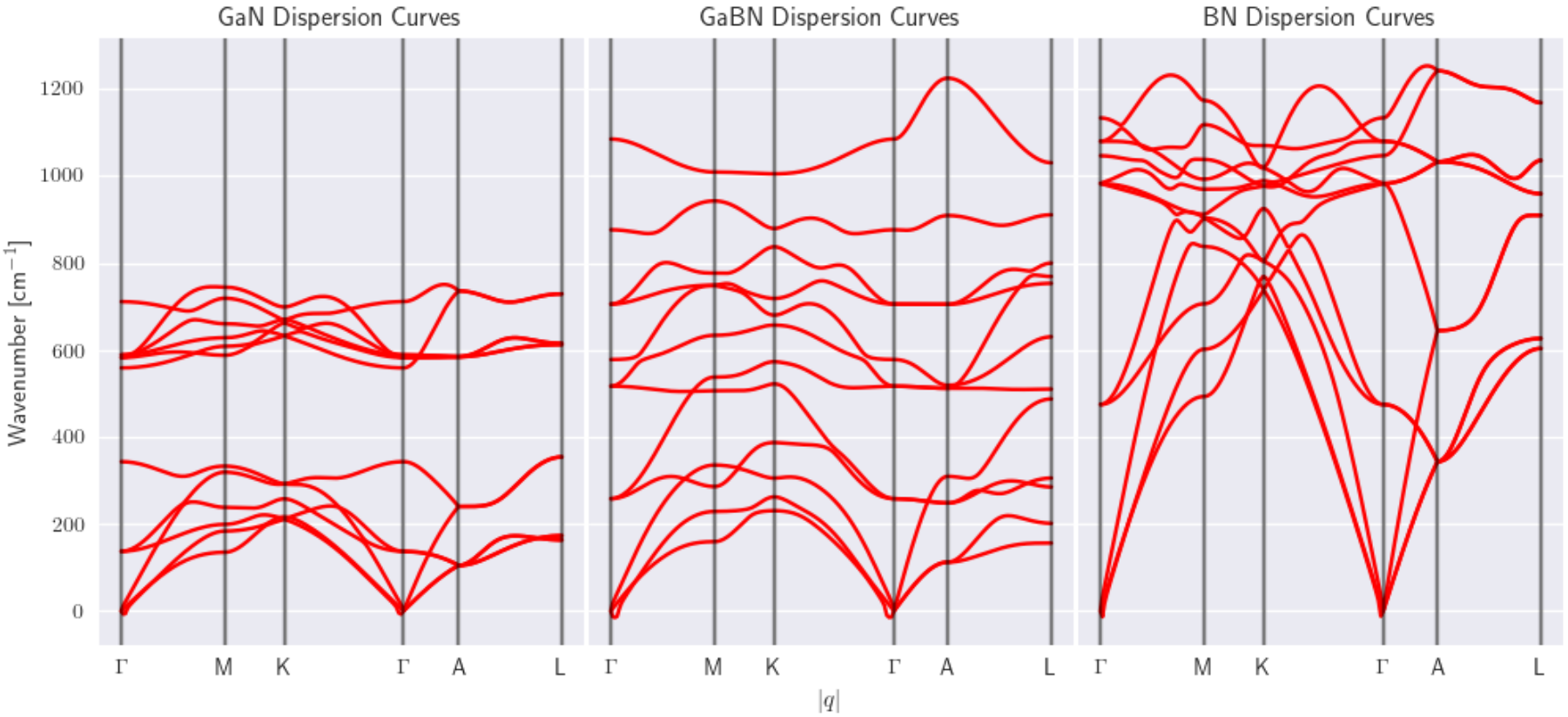


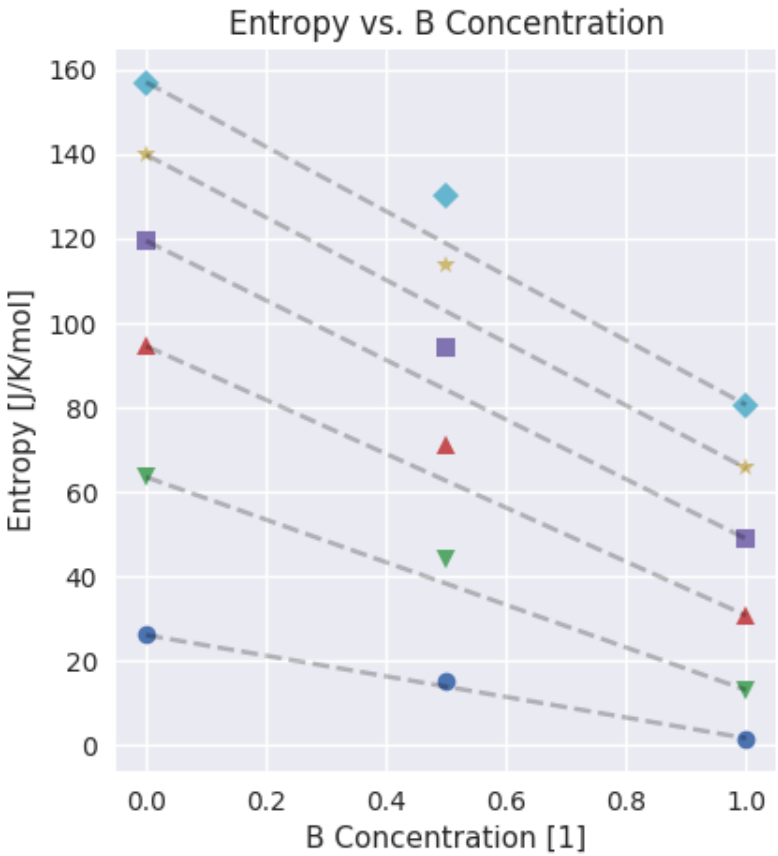
[1] Kuball, 2001.

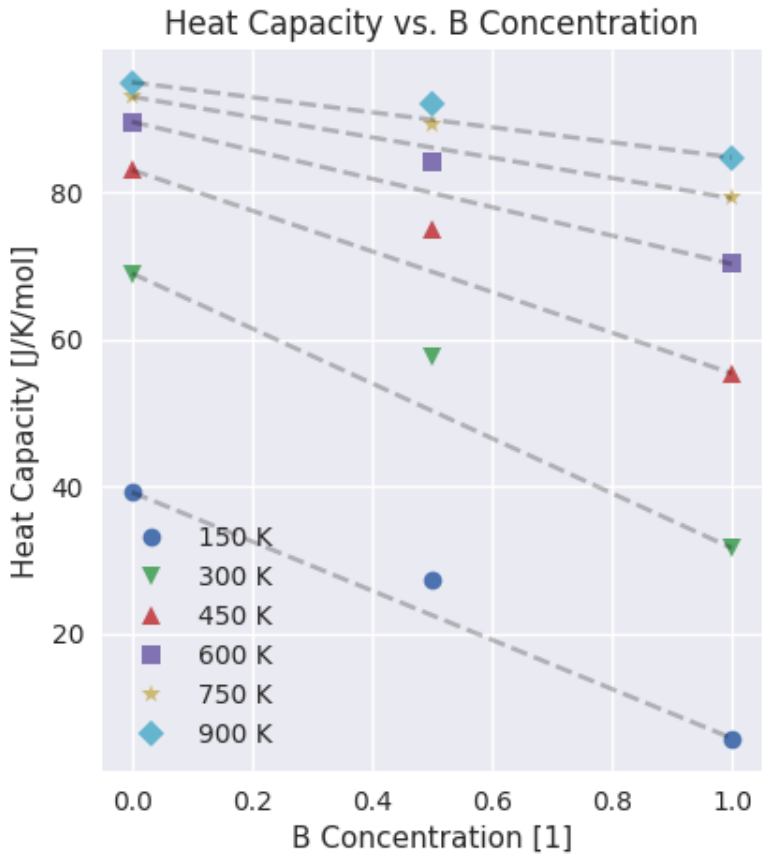

BN Dispersion Curves
Wavenumber [cm^{-1}]
1200
1000
800
600
400
200
0
Γ
M
K
Γ
A
L
|q|


GaN Dispersion Curves
BN Dispersion Curves
Wavenumber [cm^{-1}]
1200
1000
800
600
400
200
0
Γ
M
K
Γ
A
L
|q|


GaBN Dispersion Curves
Wavenumber [cm^{-1}]
1200
1000
800
600
400
200
0
Γ
M
K
Γ
A
L
|q|


GaN Dispersion Curves
GaBN Dispersion Curves
BN Dispersion Curves
Wavenumber [cm^{-1}]
1200
1000
800
600
400
200
0
Γ M K Γ A L
|q|


Entropy vs. B Concentration
Entropy [J/K/mol]
160
140
120
100
80
60
40
20
0
0.0
0.2
0.4
0.6
0.8
1.0
B Concentration [1]


Heat Capacity vs. B Concentration
Heat Capacity [J/K/mol]
80
60
40
20
150 K
300 K
450 K
600 K
750 K
900 K
0.0
0.2
0.4
0.6
0.8
1.0
B Concentration [1]

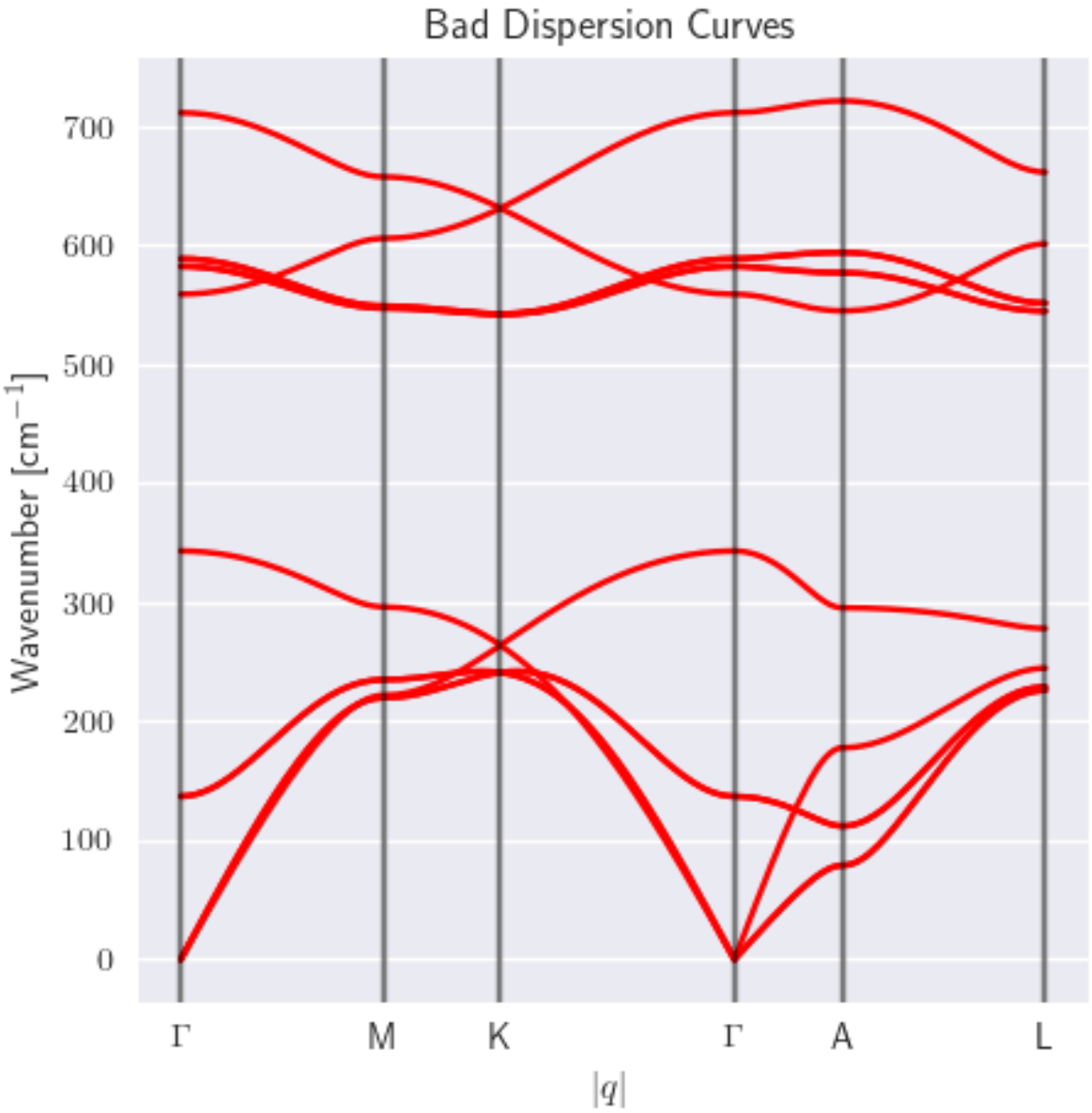
Summary

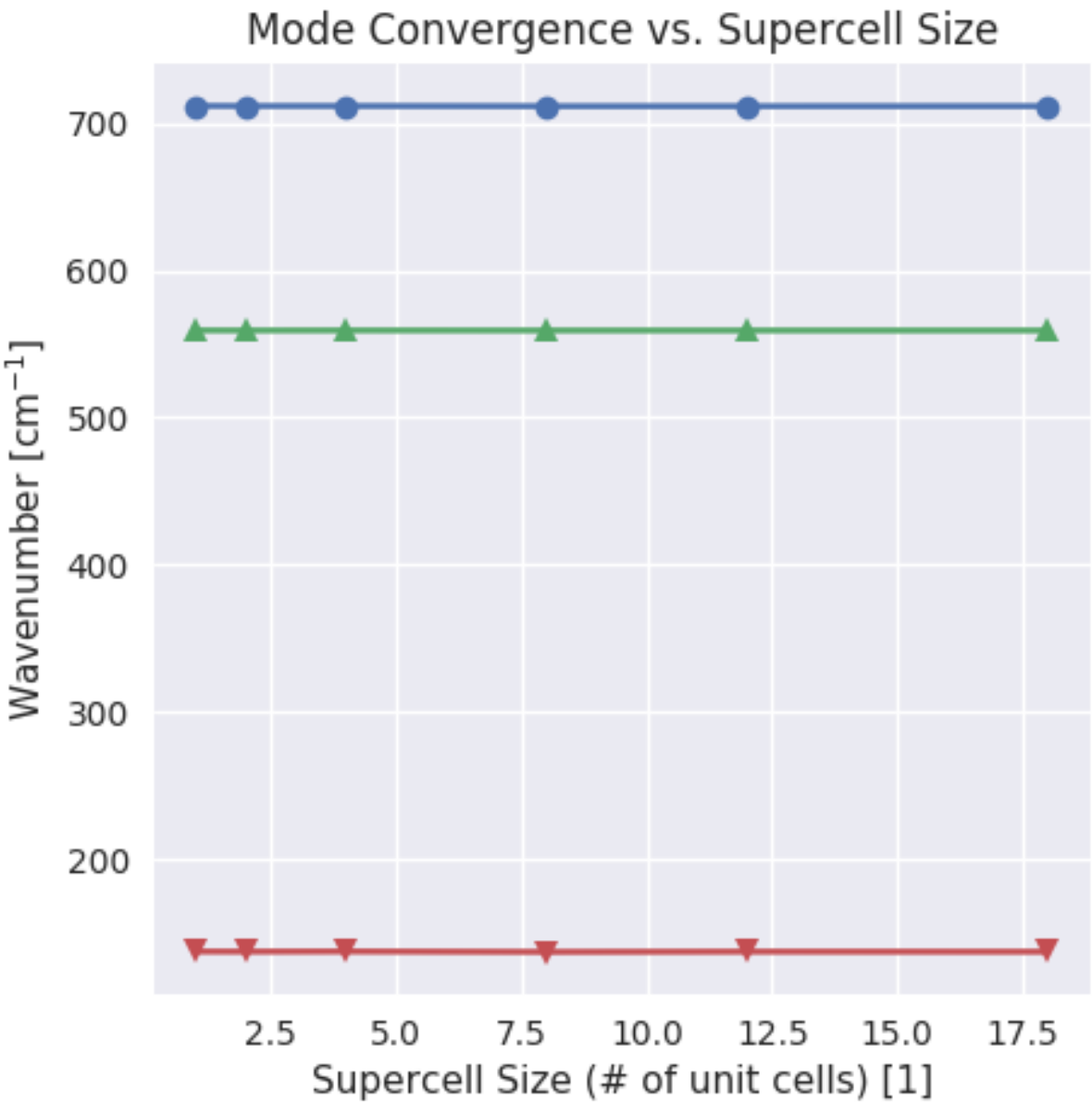
In conclusion, we have shown:

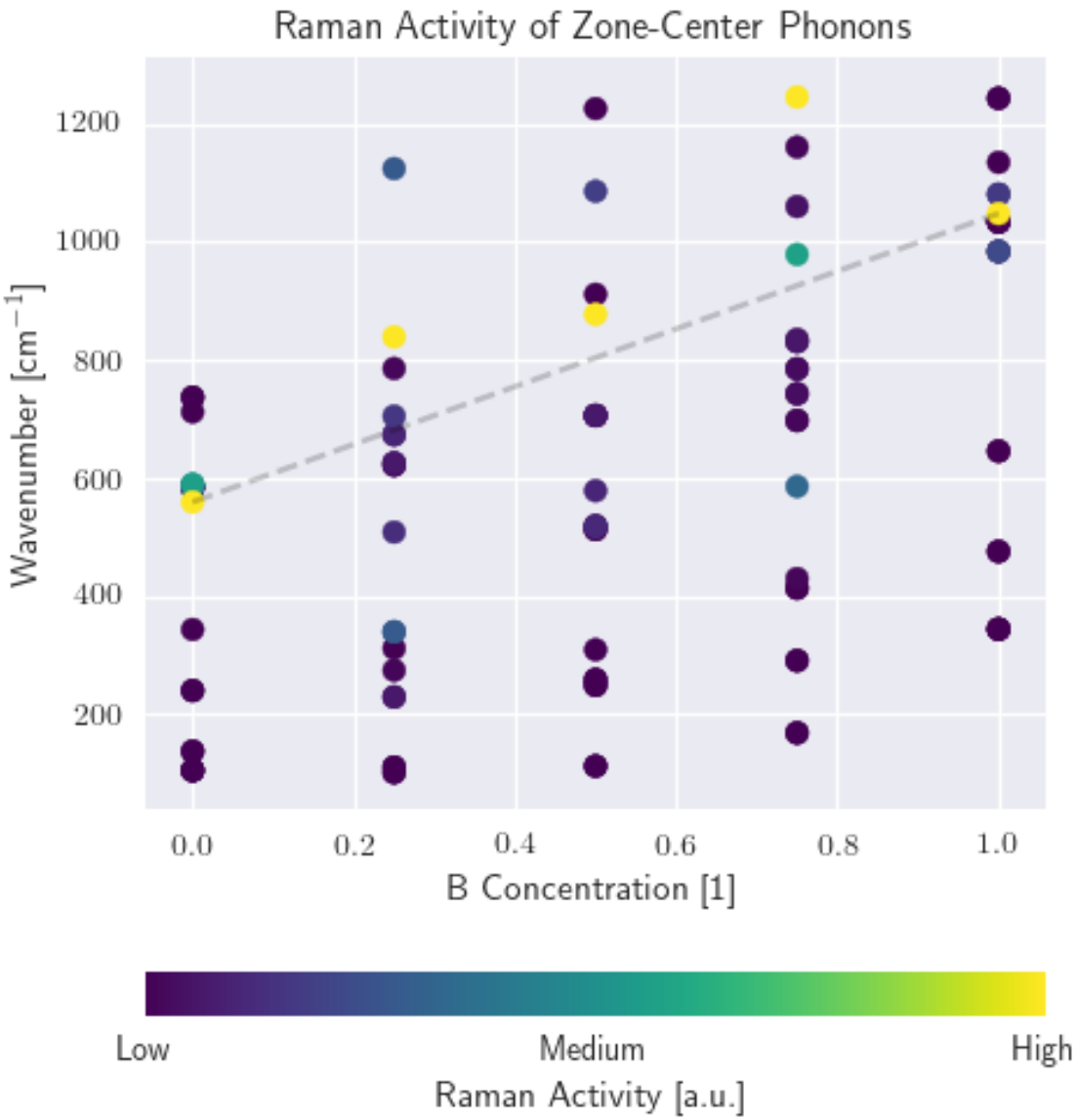
- Using VASP and the frozen phonon method, the phonon dispersion curves can be generated that agree well with experiment.
  - Quantum Espresso may be a better option for phonon calculations.
- There appears to be a deviation from a linear interpolation of B concentration for integrated quantities.

Future work includes:

- Using larger alloy supercells to track the progression of various modes as a function of B content.
- Tracking the progression of raman activity as a function of B content.


Bad Dispersion Curves
Wavenumber [cm^{-1}]
700
600
500
400
300
200
100
0
Γ
M
K
Γ
A
L
|q|


Mode Convergence vs. Supercell Size
Wavenumber [cm^{-1}]
700
600
500
400
300
200
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Supercell Size (# of unit cells) [1]


Raman Activity of Zone-Center Phonons
Wavenumber [cm^{-1}]
1200
1000
800
600
400
200
0.0
0.2
0.4
0.6
0.8
1.0
B Concentration [1]
Low
Medium
High
Raman Activity [a.u.]