An Investigation of the Vibrational Properties of BGaN Alloys

Mark Turiansky

University of California, Santa Barbara
Department of Physics

December 5, 2017
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 quantities (entropy, heat capacity), phonon-phonon (thermal resistivity), electron-phonon (electronic resistivity).
For a 1D diatomic chain,

\[ \omega_{\pm} = \sqrt{\frac{\kappa_1 + \kappa_2}{m}} \pm \frac{1}{m} \sqrt{(\kappa_1 + \kappa_2)^2 - 4\kappa_1\kappa_2} \sin^2 \left(\frac{ka}{2}\right). \]

From the Debye model,

\[ U = \int d\omega D(\omega) \langle n(\omega) \rangle \hbar \omega \quad \rightarrow \quad C_V = \left(\frac{\partial}{\partial T}\right)_V. \]
Computational Methodology

- DFT calculations using the LDA functional 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.
Results

Dispersion Curves


M. Turiansky (UCSB Physics)
GaBN Dispersion Curves

![Graph of GaBN Dispersion Curves](image)
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.
Raman Activity of Zone-Center Phonons

Wavenumber [cm$^{-1}$]

B Concentration [1]

Low

Medium

High

Raman Activity [a.u.]