An Investigation of the Vibrational Properties of BGaN Alloys

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MOTIVATION

- Alloys of III-nitrides such as AIN, 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

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For a 1D diatomic chain,

$$\omega_{\pm} = \sqrt{rac{\kappa_1 + \kappa_2}{m} \pm rac{1}{m} \sqrt{\left(\kappa_1 + \kappa_2
ight)^2 - 4\kappa_1\kappa_2\sin^2(ka/2)}}$$
 .

From the Debye model,

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



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

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VIBRATION OF BGAN ALLOYS

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"
 - $\Delta E < 10^{-7} \text{ eV}$
 - 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.



¹Kuball, 2001.

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DISPERSION CURVES









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.



Extra Slides



Extra Slides

