Measuring Vibrational Energy

**AlN Phonon Dispersion**

![Graph showing AlN phonon dispersion](image)

A phonon describes the transport of vibrational energy in a material. A phonon dispersion depicts available frequencies in a system.

![Diagram showing Raman spectroscopy](image)

**Raman spectroscopy** is a light-based, experimental method that can probe certain vibrational modes.

![Diagram showing vibrational energy states](image)

Symmetry determines which frequencies are Raman active, due to changes in polarizability.

![Diagram showing DFT electronic approximation](image)

**Density Functional Theory (DFT)** can calculate phonon dispersions and Raman activity.

Raman Spectra of AlN & GaN

**AlN Raman Spectrum (ONCVPS v0.4, Unit Cell)**

![Graph showing AlN Raman spectrum](image)

Simulation results for AlN place A1, E2, and E1 Raman peaks in the correct order, and locate these peaks with reasonable accuracy. Relative intensities, however, are not accurate.

![Graph showing GaN Raman spectrum](image)

**GaN Raman Spectrum (ONCVPS v0.4, Unit Cell)**

Calculation results for GaN correctly place the E2 Raman peak, but fail to capture the A1 peak at approximately 735 cm⁻¹.

AlN-GaN Superlattice

**AlN-GaN Raman Spectrum (ONCVPS v0.4, ASR)**

![Graph showing AlN-GaN Raman spectrum](image)

- DFT can accurately calculate phonon frequencies and Raman-active modes.
- Unique modes arise in the superlattice, representing potential interface or hybrid modes.

![Table showing calculated vibrational modes](image)

Increasing the size of this system and improving convergence may yield improved intensity data and the calculation of additional active peaks, which would improve the trustworthiness of calculations.

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