Phonon Spectra and Thermal Properties of InGaAs <100> NW

M. Salmani-Jelodar, A. Paul, T. Boykin, G. Klimeck

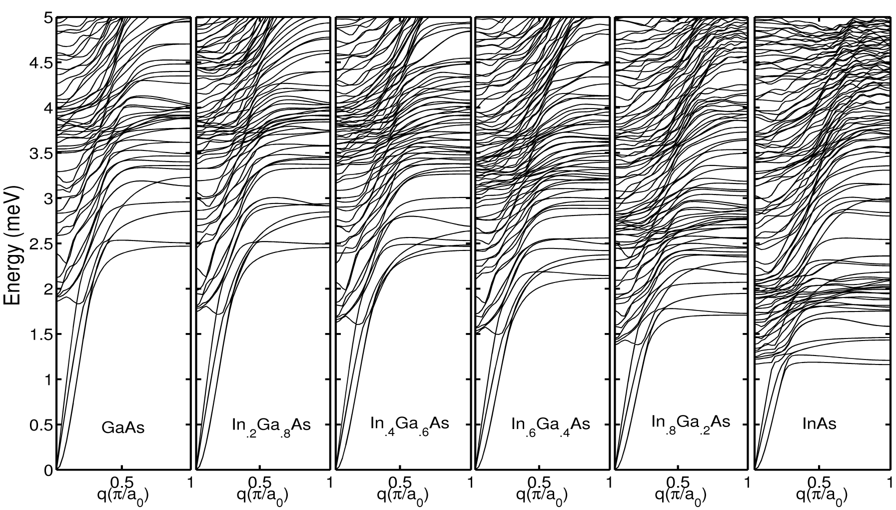
Objective:

- Calculation of phonon dispersion and thermal properties including sound velocities, specific heat (Cv) and ballistic thermal conductance (κ_l)

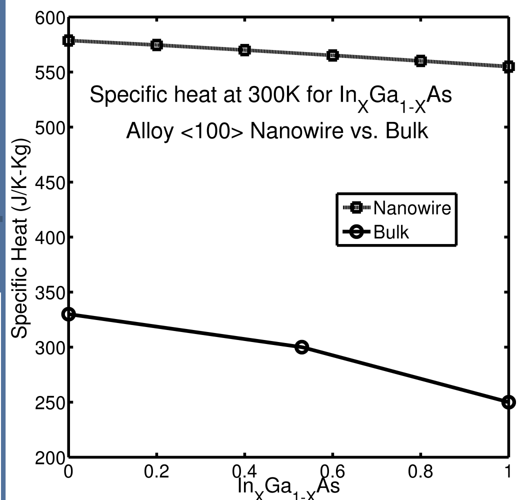
Approach:

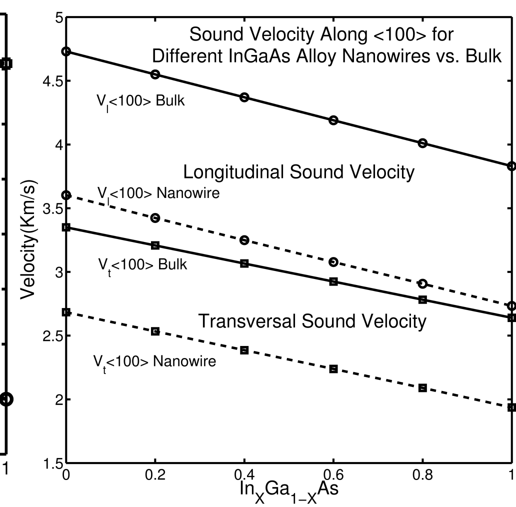
- Enhance Valance Force Field (EVFF) with virtual crystal approximation to calculate phonon dispersion
- Sound velocity: slope of acoustical branches near q→0

Impact/Results:



- Flattening in NWs phonon dispersion
  - ➢ Phonon confinement
- Sound velocities more than 20% in <100> NWs less than bulk
  - ➢ Flattening in acoustical modes
- Specific heat of NWs is about twice as bulk
  - ➢ Higher surface to volume ratio
  - ➢ Phonon confinement





1. M. Salmani-Jelodar, A. Paul, T. Boykin, G. Klimeck, "Calculation of Phonon Spectrum and Thermal Properties in Suspended <100> $In_XGa_{1-X}As$ Nanowires" accepted for publication *Journal of Computational Electronics* (2012)
2. M. Salmani-Jelodar, A. Paul, T. Boykin, G. Klimeck "Phonon Spectrum and Thermal Properties of free standing <100> and <111> InGaAs alloy nanowires" APS March Meeting 2012

Mehdi Salmani