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Phonon Spectrum and Thermal Properties of free standing <100> and <111> InGaAs alloy nanowires MEHDI SALMANI JELODAR, ABHIJEET PAUL, Purdue University, TIMOTHY BOYKIN, University of Alabama in Huntsville, GERHARD KLIMECK, Purdue University — The phonon spectra in zinc blende InAs, GaAs and their ternary alloy nanowires (NWs) are computed using an enhanced valence force field (EVFF) model. The physical and thermal properties of these nanowires such as sound velocity, elastic constant, specific heat (Cv), phonon density of states, phonon modes, and the ballistic thermal conductance are explored. The calculated transverse and longitudinal sound velocities along <100> direction in these NWs are ∼25% and 20% smaller compared to the bulk velocities, respectively. These velocities along <111> direction are about twice smaller than bulk values. The Cv for NWs are about twice as large as the bulk values due to higher surface to volume ratio (SVR) and strong phonon confinement in the nanostructures. The temperature dependent Cv for InAs and GaAs nanowires show a cross-over at 180K and 155K along <100> and <111> directions respectively. It happens due to higher phonon density in InAs nanowires at lower temperatures. With the phonon spectra and Landauer's model the ballistic thermal conductance is reported for these III-V NWs. The results in this work demonstrate the potential to engineer the thermal behavior of III-V NWs.

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