Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Simulations of Non-Equilibrium Phonon Dynamics in III-V Materials SRIDHAR SADASIVAM, YI XIA, MARIA CHAN, PIERRE DARANCET, Argonne Natl Lab — Understanding non-equilibrium energy transfer between hot electrons and phonons is important to improving the efficiency of solar-energy conversion and nanoelectronic devices. As photo- or electrically-excited electrons excite non-thermal phonons, they generate transient and/or steady-state non-equilibrium phonon distributions known as "phonon bottlenecks", impacting thermal transport and structural properties. In this work, we develop a first-principles method that captures these effects, by computing the transient dynamics of non-equilibrium phonon distribution using the Bloch-Boltzmann-Peierls equations along with first-principles calculations of electron-phonon and phonon-phonon interactions. We apply our method to the description of phonon thermalization in III-V semiconductors. We examine the effects of polarity and phonon-phonon scattering phase space on the thermalization time, and discuss the deviation from simple two-temperature models that are commonly used to interpret ultrafast-laser experiments.

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Date submitted: 11 Nov 2016 Electronic form version 1.4