Modeling of Non-Equilibrium Phonons in Hot Carrier Solar Cells

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As fabrication techniques have improved and solar cell efficiencies are getting closer to the Shockley-Queisser limit, new designs which reconsider the fundamental assumptions of loss mechanisms are being explored. One such design is through hot-carrier solar cells in which the design of the cells is such that the photogenerated carriers are quickly extracted before the carriers have time to lose their excess energy to the lattice.

Reduced dimension systems have demonstrated in photo-luminescence (PL) measurements carrier temperatures in excess of the lattice temperature [1]. For 2D-MQW, it is theorized that the inhibited thermalization of carriers is due to the formation of a hot phonon bottleneck; as the phonon number N_{LO} increases, the rate of absorption and emission become approximately equal. This leads to an inhibition of the thermalization rate due to optical phonons. The dynamics of the system are not well understood, providing motivation for simulating these systems. Prior work has focused solely on the build up of polar LO phonons[2], however, the present work seeks to show that LA phonons could also play a role in the inhibition of carrier thermalization .

To simulate the system used in PL measurements, a modified Monte-Carlo (MC) method is used to solve the Boltzmann Transport Equation (BTE) with modifications to account for the build up of non-equilibrium phonons. The effects of confinement are included via the solution of a coupled non-parabolic Schrödinger-Poisson system. For recombination processes, an ABC model given as,

$$R(n) = An + Bn^2 + Cn^3 \tag{1}$$

is used, wherein the ABC coefficients are extracted from a fit to experimental measurements.

The non-equilibrium phonons are accounted for by introducing a discretized mesh of the phonon number $N_{LO}(\mathbf{q})$. When an emission or absorption event is selected in the MC, a value ΔN_{LO} is subtracted or added, respectively, for the corresponding $N_{LO}(\mathbf{q})$ value.

$$\Delta N_{LO} = \frac{2\pi}{\mathbf{q}^2 \Delta \mathbf{q} S} \tag{2}$$

This work also includes a discretization of the LA phonon branch. At the end of every synchronization time step, the decay and generation of LO phonons via Klemen's mechanism is modeled as:

$$\begin{aligned} \frac{\partial N}{\partial t} &= \Gamma_0 \left(G - \Gamma\right) \\ &= \Gamma_0 \left(N' N'' (N_{LO} + 1) - (N' + 1)(N'' + 1) N_{LO}\right) \end{aligned} \tag{3}$$

where N' and N'' are the LA phonon modes which are coupled to the LO phonon mode to conserve both energy and momentum. As such, the dynamics of both the LA and LO phonons can be studied.

The simulations predict a possible phonon bottleneck resulting from a build up of both optical and acoustic phonons. This can be advantageous for designing an effective hot carrier solar cell.

References

[1] H. Esmaielpour, B. K. Durant, K. R. Dorman, V. R. Whiteside, J. Garg, T. D. Mishima, M. B. Santos, I. R. Sellers, J.-F. Guillemoles, and D. Suchet. Hot carrier relaxation and inhibited thermalization in superlattice heterostructures: The potential for phonon management. *Applied Physics Letters*, 118(21):213902, May 2021. [doi:10.1063/5.0052600].

[2] Y. Zou, H. Esmaielpour, D. Suchet, J.-F. Guillemoles, and S. M. Goodnick. The role of nonequilibrium LO phonons, Pauli exclusion, and intervalley pathways on the relaxation of hot carriers in InGaAs/InGaAsP multi-quantum-wells. *Scientific Reports*, 13(1):5601, Apr. 2023. [doi:10.1038/s41598-023-32125-2].

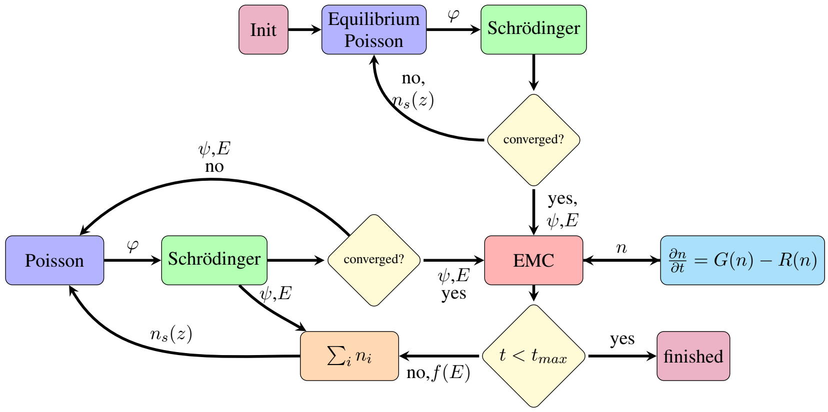

Fig. 1. Flowchart of the MC code

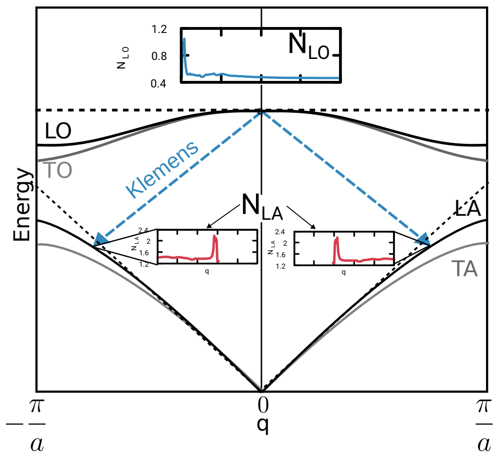

Fig. 2. Schematic diagram showing the considered LO phonon decay mechanism. The insets show the calculated phonon number vs wavenumber for the respective branch. Dotted lines show analytic dispersion used for LO and LA branches

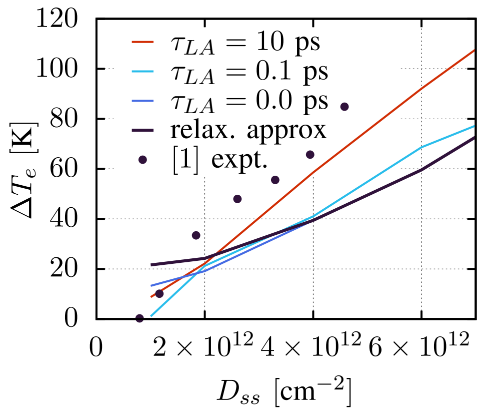

Fig. 3. Carrier temperature against steady-state sheet density for different acoustic phonon decay times compared to experimental results.

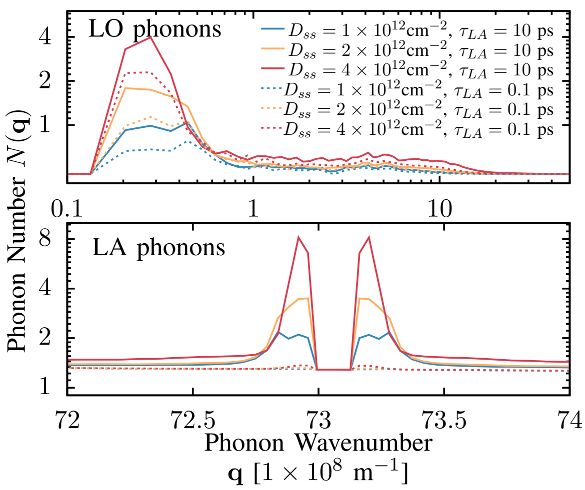

Fig. 4. Steady-state phonon number for both the acoustic and optical branches

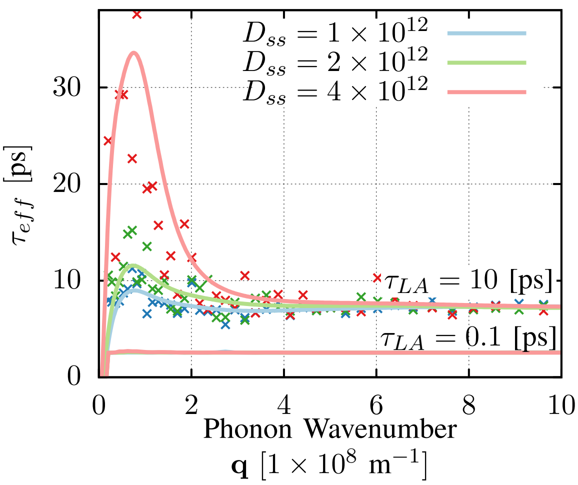

Fig. 5. Effective lifetimes for two different acoustic phonon decay times as a function of phonon wavenumber