# Nonequilibrium Electron and Phonon Dynamics in Advanced Concept Solar Cells

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The realization of advanced concept solar cells that circumvent the assumptions inherent in the Shockley-Queisser limit depends strongly on the competition between carrier energy relaxation processes to the lattice and high energy processes that do useful work. Nanostructured systems offer advantages in terms of reduced channels for energy relaxation in reduced dimensional systems, and the possibility of bandgap engineered structures for improved collection and charge separation. Here we use ensemble Monte Carlo simulation of electrons and holes to investigate the role of ultrafast carrier processes in the realization of two advanced concept devices, hot carrier capture and multi-exciton generation. The particle based simulation approach includes the electron-phonon scattering in quantum wells and quantum wires, intercarrier scattering, and nonequilibrium phonon effects.

In the case of hot carrier solar cell architectures, we have simulated carrier relaxation dynamics including the dynamical nonequilibrium population of optical phonons that are generated in III-V quantum well structures through primarily polar optical phonon emission, assuming a phenomenological anharmonic phonon decay time from an optical mode to two acoustic modes. Acoustic modes are assumed to propagate the excess energy away as classical heat conduction, whereas the energy of the optical modes is retained within the optical excitation volume due to the low group velocity of such modes. With increasing phonon lifetime, simulation results show an evolution of energy loss dominated by the polar emission rate, to one dominated by the anharmonic decay time, depending on the injected carrier density. While typical III-V bulk materials have short anharmonic decay times, less that 10 ps, recent experimental work has indicated slow decay in 'phononic bandgap' materials like InN, where the separation of the optical and acoustic modes is large enough to suppress the dominant two phonon decay process.[1]

Impact ionization plays a critical role for high energy electrons and holes during photoexcitation. Here we investigate the role of impact ionization in nanowires using an atomistic tight binding representation of the nanowires, and calculating the full multi-subband impact ionization rate from perturbation theory. The short time carrier dynamics in nanowires under varying photoexcitation conditions are investigated using a full band Cellular Monte Carlo (CMC) simulation based on an atomistic representation.[2] The CMC also includes the scattering rates due to optical and acoustic phonons that tend to the bulk material scattering rates for larger nanowire widths. The effect of impact ionization is shown to be prominent smaller width nanowires due to the increase in the band gaps as the nanowire width decreases. The percentage of electrons undergoing an impact ionizing event, thereby creating multiple electron hole pairs, is also shown to drastically above the threshold given by twice the bandgap of the nanowire, showing a strong potential for multiexciton generation in such systems.

1. Y. Zhang et al., Applied Physics Letters 108, 131904 (2016)
2. R. Hathwar, M. Saraniti, and S. M. Goodnick, J. Appl. Phys. 120, 044307 (2016)