Towards a semi-classical simulator for the energy distribution functions in optically excited hot carrier semiconductor devices

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Abstract

Progress is reported on the semi-classical component of a proposed hybrid quantum /classical simulator [1] for the efficient design and analysis of macroscopic photovoltaic semiconductor devices [2,3] with nanoscale insertions and hot photoexcited carriers.

INTRODUCTION AND MODEL

The determination of the energy distributions of carriers, photons and phonons is crucial for photo-voltaic device modelling, ideally on time/space scales from very small to very large (fig.1-3),
The physical processes involve externally incident photons at high temperature which are absorbed by electron and hole photo-excitation. The excited carriers re-distribute energy and momentum by inter-carrier interactions. Ultimately, the photon and carrier distributions thermalise to the lattice via interaction with optical and acoustic phonons with carrier recombination leading to photon emission processes that produce a steady state photon distribution.. Our long term aim is to couple a simplified version of the NEGF methodology with the semi-classical kinetic equation methodology to obtain a phenomenological parameterised computational model that determines the mobilty, diffusion coefficients, and the temperatures and chemical potentials of both carriers *and* photons on multiple time scales for which quasi-steady state processes occur. The aim is to explore nanostructured inserts that provoke *persistent* hot carrier states that improve device efficiency.

We consider coupled transport equations (fig3) for the energy distributions of photons, electrons and holes in the energy-space domain on different quasi-stationary time scales. Here, we will present results for computation of the electron and hole distributions in a homogeneous slice of an absorber region subject to a quasi-stationary photon distribution intermediate to the incident Bose-Einstein photon flux and the lattice thermalized photon flux at a fixed photon chemical potential. The method involves iterative solving of coupled non-linear integral equations for the carrier energy (E) distribution functions $F[K=(E/k_BT)^{1/2}]$ of Fig.4-5. Fig.6 illustrates a simple sub-case: the energy distribution function of electrons photo-excited by high temperature photons incident on neutral donors in a compensated model semiconductor. Using precise forms for the electron-photon and electron-trap recombination we find that the distributions are non-equilibrium mixtures of the incident excitation function and the scaled thermal electron distribution. Fig. 6 illustrates the typical form of the distributions for weak, intermediate and strong inelastic acoustic phonon scattering. Of course realistic models require optical phonon scattering and phonon and trap-assisted band to band recombination.

References

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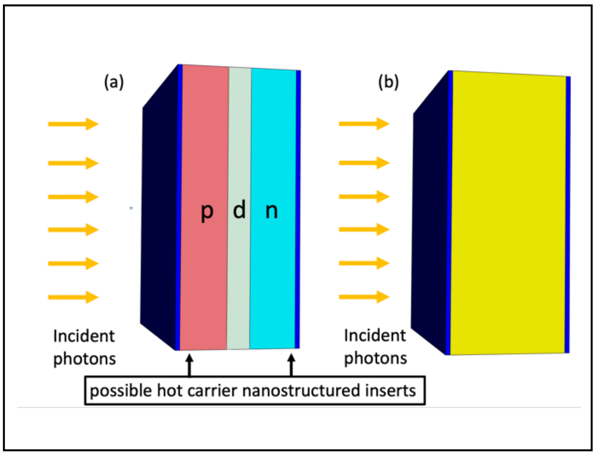

Fig. **1.** (a) Schematic of a solar cell; (b) photo-excited compensated semiconductor: trap recombination

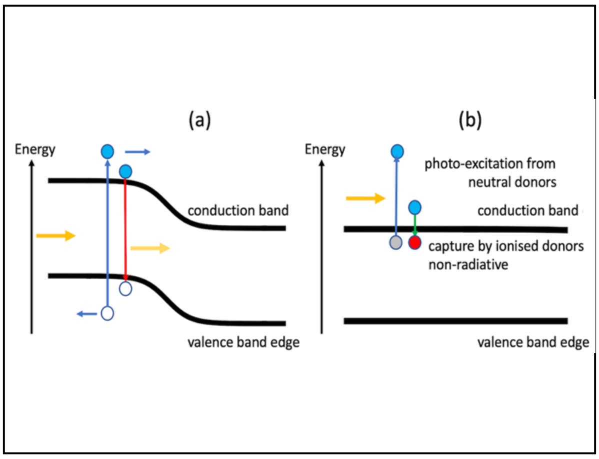

Fig. 2. Band edge profile of (a)solar cell;
(b) photo-excited compensated semiconductor

General Coupled Continuity equations for:

n_γ photon density, n_e *and* n_h electron and hole densities, n_{ph} phonon densities

$$\frac{\partial n_\gamma}{\partial t} + \nabla \cdot \mathbf{j}_\gamma = G_\gamma - R_\gamma$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{j}_e = G_e - R_e \qquad \frac{\partial n_h}{\partial t} + \nabla \cdot \mathbf{j}_h = G_h - R_h$$

$$\frac{\partial n_{ph}}{\partial t} + \nabla \cdot \mathbf{j}_{ph} = G_{ph} - R_{ph}$$

Similarly, the coupled equations for the photon, electron, hole and phonon phase space distribution functions exist with scattering integrals involving

$e-e, e-h, h-h, e-\gamma, h-\gamma, \gamma-traps/dopants$

$e-ph, e\,h-ph, ph-\gamma, ph-ph, ph-traps/dopants$ and higher order processes

STUDY STEADY STATE and SEEK REDUCTION OF THE 6-DIMENSIONAL PHASE SPACE TO LOWER DIMENSIONS

Fig. 3. Coupled system equations

Integral equation for the dimensionless electron energy distribution $F[K]$

$$F[\varepsilon_{\mathbf{k}}] \equiv F(K = (\frac{\varepsilon_{\mathbf{k}}}{k_B T_{lattice}})^{\frac{1}{2}})$$

$$F(K) = \frac{G(K) + C_{in}[F(K)]}{R(K) + C_{out}(K)}$$

G: Electron photo-excitation rate parameterised by effective photon distribution

R: Electron recombination rate

$F(K)C_{out}(K)$: Electron inelastic phonon scattering - out rate

$C_{in}[F(K)]$: Electron inelastic phonon scattering - in rate

G=R=0 yields the thermalised distribution.

Fig. 4. Energy distribution in a homogeneous region satisfying non-linear Volterra integral equation of second kind

$$C_{in} = C_0\{\int_{K_1'}^{K_2'} - \int_{K_1''}^{K_2''}\}\frac{dK'K'(K^2 - K'^2)}{1-\exp[K^2 - K'^2]}F(K')$$

$$F(K)C_{out} = C_0\{\int_{K_1'}^{K_2'} - \int_{K_1''}^{K_2''}\}\frac{dK'K'(K^2 - K'^2)}{1-\exp[K^2 - K'^2]}$$

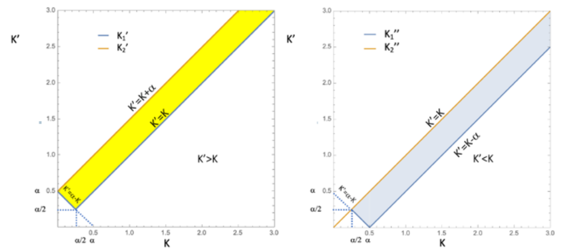

Fig. 5. Acoustic phonon ccattering and boundary conditions.

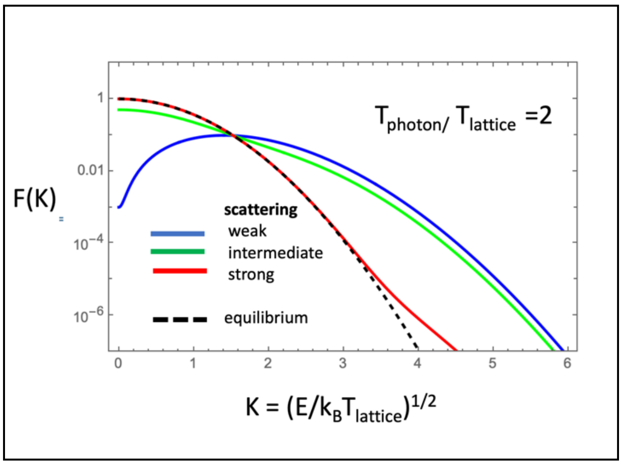

Fig. 6. Energy distributions as a function of recombination and weak to strong energy relaxation parameters.