A computationally efficient, non-equilibrium, carrier temperature dependent semiconductor gain model for FDTD simulation of optoelectronic devices

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Abstract—*We report a Finite Difference Time Domain (FDTD) model incorporating carrier heating/cooling for the first time. The proposed model thermalizes non equilibrium carrier distributions through carrier temperature dependent intraband transition terms. This multi-level, multi-electron model is formulated to be computationally efficient despite its physical complexity and hence presents potential for the development of powerful general optoelectronic device simulators for devices of arbitrary geometry.Results of carrier distribution thermalization and comparisons to non linear gain experiments are provided to validate the model.*

Keywords- Semiconductor Device Modelling, Finite Difference Methods, Semiconductor Opical Amplifiers.

I. INTRODUCTION

While the Finite Difference Time Domain (FDTD) method [1] is ubiquitous in the simulation of passive optical devices, it is yet to be extensively used for the simulation of devices with active gain media because of the computational challenges involved. In order to alleviate computational cost, a Multi-Level, Multi- Electron (MLME) model was proposed by the authors [2] for semiconductor gain media. However, this work did not consider the non linear gain effects caused by carrier heating/cooling which are essential to many applications. For instance, in all optical devices [3]-[5], modulation characteristics of lasers [6] and in Nanoscale lasers [7]. An FDTD simulator which can resolve the active medium dynamics for complex or arbitrary device geometries in a computationally efficient way is thus of great interest, especially in novel or complicated structures such as those of plasmonic devices or photonic crystal based devices. Here, we report the first such FDTD model for non linear gain in optoelectronic devices. Computational efficiency is achieved by a combination of broadened transition states, temperature dependent intraband transition terms and circumventing iterative procedures to calculate chemical potentials at each space-time grid.

II.THEORY

In the MLME method, the band structure of the semiconductor is spanned by a few broadened states as shown in Fig.1 which allows for tracking the dynamics of the complete carrier distribution while retaining computational efficiency. All notations and symbols presented henceforth are consistent with that of [2] and [8]. In order to introduce carrier temperature dependency, we introduce an upward intraband transition time as shown in Eq.(1). The detailed derivation is presented in [8]. These terms tend to drive an arbitrary distribution towards a Fermi-Dirac Distributions at the carrier temperature while circumventing the need to calculate chemical potentials at each time step.

$$\tau_{(i,i+1)_C}(r,t) = \frac{N^0_{C_i}}{N^0_{C_{i+1}}}\tau_{(i+1,i)_C}.e^{\frac{E_{C_{i+1}}-E_{C_i}}{k_B T_e(r,t)}} \quad (1)$$

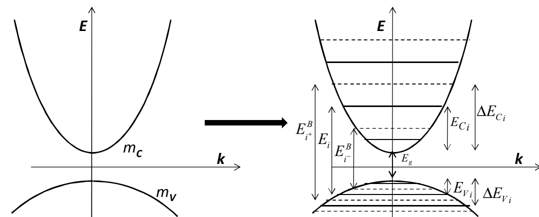

Fig.1.The parabolic semiconductor band structure as represented in the MLME model by broadened states centered at E_i. m_c,m_v correspond to the electron and hole effective masses and E_g corresponds to the bandgap energy.

A rate equation for the carrier temperature was derived based on energy conservation in [8] and is presented for electrons in Eq. (2). In (2), ΔN_i represents carrier changes in the ith level due to all interband processes and E. Here, C_{Ve}, and C_e are the partial derivatives of the carrier energy density w.r.t. carrier temperature and carrier number density respectively and are given by Eqs. (3) and (4). These expressions, derived in [8] are valid for carrier densties upto 40 $\times 10^{18}$cm-3 at 300K(larger for higher temperatures) avoid cumbersome series expansions or iterative processes at each spatial and temporal grid. The combination of these measures makes the formulation

computationally efficient. The last two terms in Eq.(2) are responsible for carrier cooling .

$$\frac{dT_e}{dt} = \left(C_{V_e}\right)^{-1}\left[-\sum_i E_{C_i}\Delta N_i(r,t) + C_e\sum_i \Delta N_i(r,t)\right] - \frac{T_e - T_L}{\tau_{e-p}} - \frac{T_e - T_h}{\tau_{e-h}} \quad (2)$$

$$C_{V_e} = \frac{\sqrt{2}m_c^{3/2}}{\pi^2\hbar^3}k_B^{5/2}T^{3/2}\left(\frac{s_e+0.02886}{0.7989+0.06283(s_e+0.02886)-1.124\times10^{-4}(s_e+0.02886)^2}\right) \quad (3)$$

$$C_e = k_B T\left(1.544 + 0.4879 s_e - 0.004382 s_e^{\,2} + 2.304\times10^{-5} s_e^{\,3}\right) \quad (4)$$

In Eqs.(3) and (4), $s_e = \left(k_B T_e^{\,3/2}\right)^{-1}\left(\frac{\sqrt{2}m_c^{3/2}}{\pi^2\hbar^3}\right)^{-1}\sum_i N_{C_i}$, where N_{Ci} is the electron density for each level i and is tracked by Eq.(5).

$$N_{C_i} = \Delta N_i - \Delta N_{C(i,i-1)} + \Delta N_{C(i+1,i)} \quad (5)$$

In (5), the second and third terms are intraband transition terms given by (6).

$$\Delta N_{C(i+1,i)} = \frac{N_{C_{i+1}}}{\tau_{(i+1,i)C}}\left(1-\frac{N_{C_i}}{N_{C_i}^{\,0}}\right) - \frac{N_{C_i}}{\tau_{(i,i+1)_C}(r,t)}\left(1-\frac{N_{C_{i+1}}}{N_{C_{i+1}}^{\,0}}\right) \quad (6)$$

A similar set of equations exist for hole densities. The electron and hole densities are coupled to the polarization as in [2] which are in turn coupled to the Maxwell curl equations.

II. SIMULATION RESULTS

We present simulation results of an active medium with bandgap of 834.8nm, spanned by 20 pairs of levels. In Fig.2, we examine the process of thermalization.Two situations of quasi-equilibrium exist. The first one occurs at an elevated carrier temperature in <100fs and the next occurs close to the lattice temperature on a picosecond time scale. This represents the heating and eventual cooling of the distributions. In Fig.3, we present comparisons to the non linear pump-probe experiments from [9] which show good quantitative agreement.

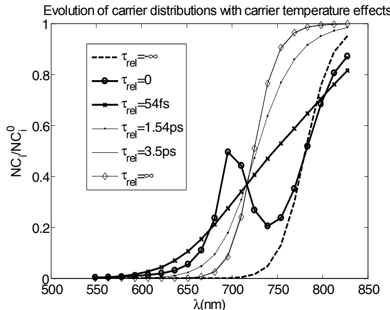

Fig.2. (a) Evolution of distributions when a 90fs 700nm pulse with peak intensity of 10GWcm-2 is incident on a medium biased at transparency at ≈822nm. Carrier heating causes smearing of the distribution. Carrier cooling to the lattice temperature leads to a compressed distribution. $\tau_{e-p} = 0.75ps, \tau_{h-p} = 0.25ps, \tau_{e-h} = 2ps$

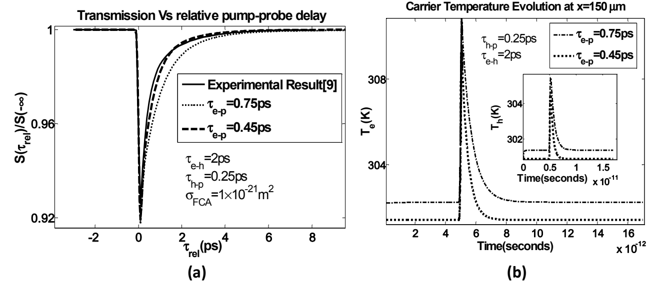

Fig.3. (a) Transmission curves for $\tau_{e-p} = 0.75ps, 0.45ps$ biased at transparency at 822nm(other parameters same as that of Fig.2) shows two component relaxation corresponding to carrier heating and cooling and agree with experiments (b) The evolution of the carrier temperatures at the center of the waveguide also shows carrier heating and cooling to lattice temperature.

III. CONCLUSION

A new scheme for incorporating dynamic carrier temperatures in the semiconductor gain medium using FDTD was presented. The model showed good quantitative agreement with experiments in [9]. The novel formulation resulted in a computationally efficient model with only a 5 fold increase over the passive simulation time. The current work has high potential for the development of a general optoelectronic device simulator. Further improvements to the model such as the inclusion of carrier diffusion would make it highly efficacious in visualizing device physics and useful to device realization.

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