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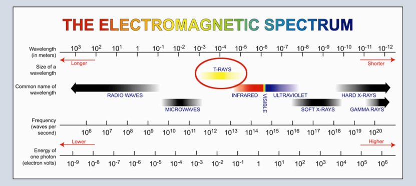
Simulation of electron and phonon dynamics in terahertz semiconductor devices within the framework of a microscopic density matrix approach

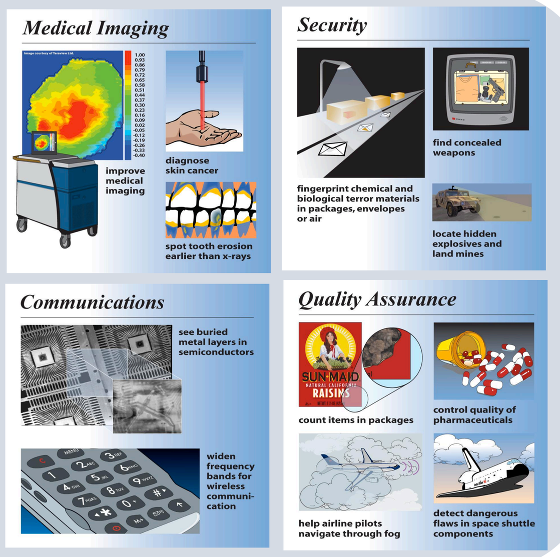
Inès (Waldmueller) Montaño, Michael C. Wanke, and Weng W. Chow

Sandia National Laboratories

Email: iwaldmu@sandia.gov

Why THz?

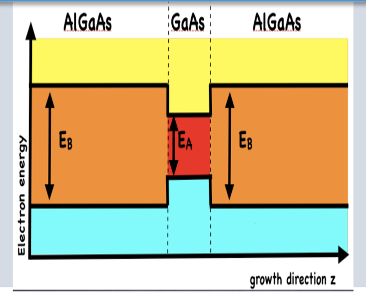


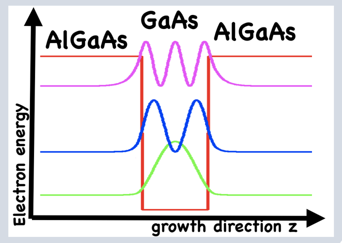


- Many materials are transparent to THz
- THz radiation is non-invasive, does not damage biological tissue
- Explosives have unique chemical signatures (THz fingerprints)

Why semiconductor nanostructures?

- Eigenstates can be changed over layer thickness and bias
- Wide range of frequencies can be targeted in same material system



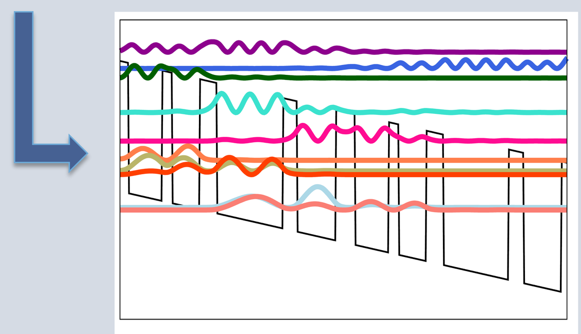


Theory

1. Band structure

solve Schrodinger Equation (k.pmethod, 8x8 Hamiltonian) in fourier space

$$\hat{\underline{\mathbf{H}}}(\mathbf{k})\ \underline{\psi}(\mathbf{k}) = \mathbf{E}\ \underline{\psi}(\mathbf{k})$$



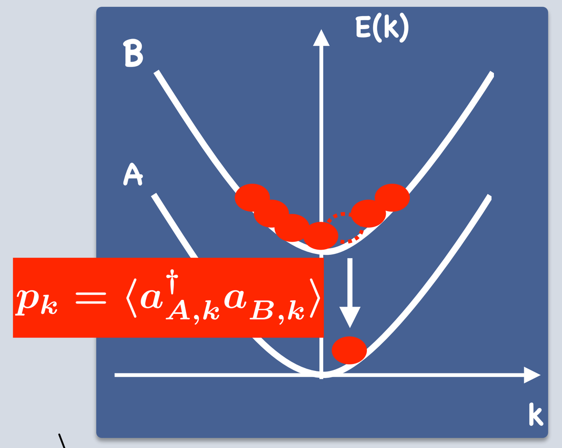
2. Material Dynamics

solve Heisenberg equations (in Markov and 2nd order Born approximation) to determine k-resolved

- intersubband coherences $p^{AB}_{\mathbf{k}} = \langle a^\dagger_{A,\mathbf{k}} a_{B,\mathbf{k}} \rangle$
- subband populations $n^A_{\mathbf{k}} = \langle a^\dagger_{A,\mathbf{k}} a_{A,\mathbf{k}} \rangle$
- Phonons $n_{\mathbf{q}}(q_\perp, q'_\perp) = \langle b^\dagger_{\mathbf{q},q_\perp} b_{\mathbf{q},q'_\perp} \rangle$

$$-i\hbar \frac{\mathrm{d}}{\mathrm{dt}} \langle a^\dagger_{\mathbf{k}} a_{\mathbf{l}} \rangle = \langle [\mathbf{H_0} + \mathbf{H_{cf}} + \mathbf{H_{cp}} + \mathbf{H_{cc}} + \mathbf{H_{ci}}, a^\dagger_{\mathbf{k}} a_{\mathbf{l}}] \rangle$$

$$-i\hbar \frac{\mathrm{d}}{\mathrm{dt}} \langle b^\dagger_{\mathbf{q},q_\perp} b_{\mathbf{q},q'_\perp} \rangle = \langle [\mathbf{H_0} + \mathbf{H_{cp}} + \mathbf{H_{pp}}, b^\dagger_{\mathbf{q},q_\perp} b_{\mathbf{q},q'_\perp}] \rangle$$



$$H_0 = \sum_{a,\mathbf{k}} \epsilon^a_{\mathbf{k}} a^\dagger_{a\mathbf{k}} a_{a\mathbf{k}} + \sum_{\mathbf{Q}} \hbar\omega_{LO} b^\dagger_{\mathbf{Q}} b_{\mathbf{Q}}$$

$$H_{cl} = \sum_{a,b,\mathbf{k}} \int \mathrm{d}z\, \mathbf{d}_{ab}(z) \cdot \mathbf{E}(z,t)\, a^\dagger_{a\mathbf{k}} a_{b\mathbf{k}}$$

$$H_{cc} = \frac{1}{2} \sum_{abcd} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V^{abcd}_{\mathbf{q}} a^\dagger_{a\mathbf{k}+\mathbf{q}} a^\dagger_{b\mathbf{k}'-\mathbf{q}} a_{d\mathbf{k}'} a_{c\mathbf{k}}$$

$$H_{cp} = \sum_{a,b,\mathbf{k}} \sum_{\mathbf{Q}} [g^{ab}_{\mathbf{Q}} a^\dagger_{a\mathbf{k}} b_{\mathbf{Q}} a_{b\mathbf{k}-\mathbf{Q}_{||}} + h.a.]$$

$$H_{ci} = \sum_{c,d} \sum_{l} \sum_{\mathbf{q},\mathbf{k}} V^l_{cd}(\mathbf{q}) a^\dagger_{c,\mathbf{k}+\mathbf{q}} a_{d,\mathbf{k}}$$

For the contribution from H_{pp} we use the relaxation time approximation.

3. Field Dynamics

solve Maxwell's wave equation

$$(\nabla^2 + \frac{n^2}{c^2}\frac{\partial^2}{\partial t^2}) E_i(r,t) = -\mu_0 \frac{\partial^2}{\partial t^2} P_i(r,t)$$

where the resonant part of the material response is been treated dynamically in terms of the macroscopic optical polarization

$$P(r,t) = \sum_{\mathbf{q}_{||}} \tilde{P}(\mathbf{q}_{||}, z, t) \exp^{i\mathbf{q}_{||}\cdot\mathbf{r}_{||}}$$

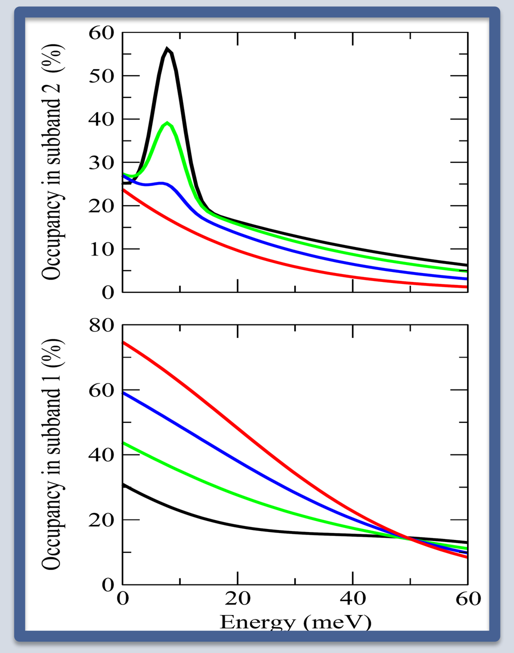
with

$$\tilde{P}(\mathbf{q}_{||}, z, t) = \frac{1}{A} \sum_{\mathbf{k}_{||}} p^{AB}_{\mathbf{k}_{||}-\mathbf{q}_{||},\mathbf{k}_{||}}(t) d_{AB}(z) + c.c.$$

Depending on the problem at hand, the three parts (1. band structure, 2. material dynamics, and 3. field dynamics) have to be solved simultaneously or iteratively.

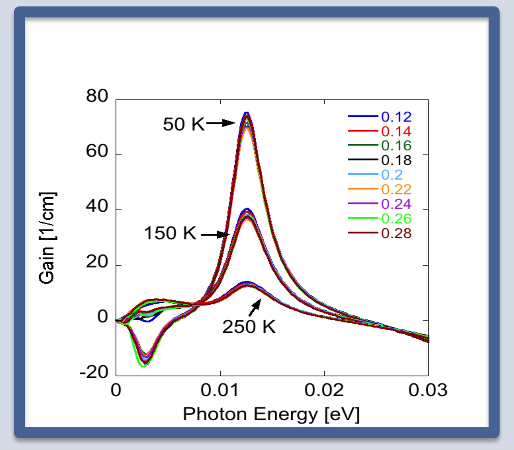
Selected Applications

1. Quantum wells & Quantum Cascade Lasers



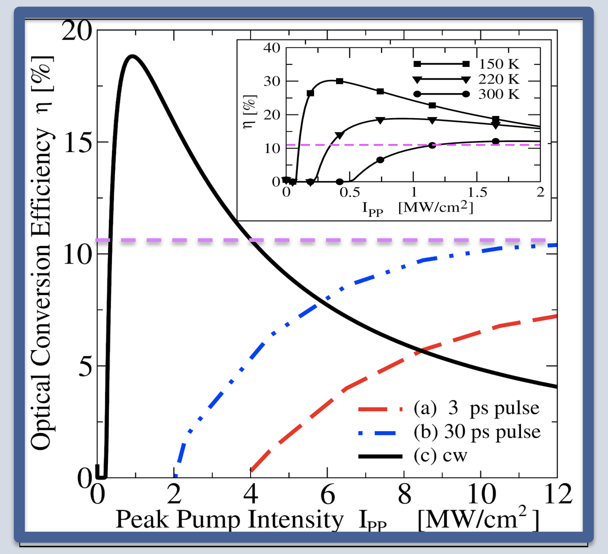
Time- and k-resolved electron occupations and intersubband coherences are calculated including both diagonal, and non-diagonal correlation contributions

Gain spectra, showing the different gain contributions, are calculated microscopically without any fit-parameters

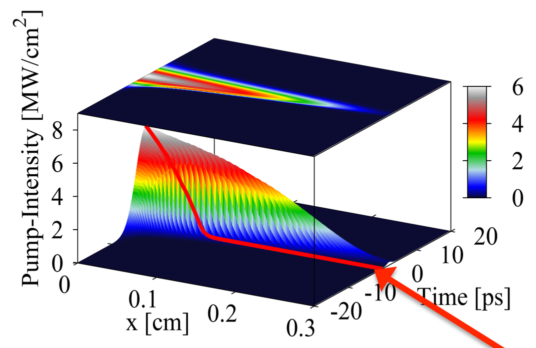


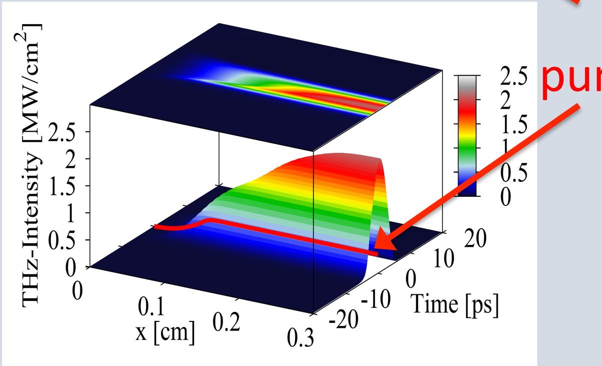
2. Optically-pumped, electrically driven THz QCL[1]

- circumvents the Manley-Rowe limit by coherently recovering the pump phonons
- THz generation via stimulated emission but also from automatically phase-matched quantum coherence contributions

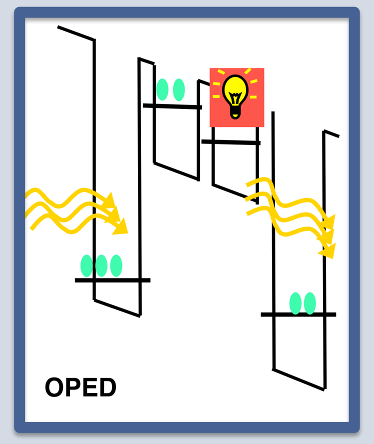


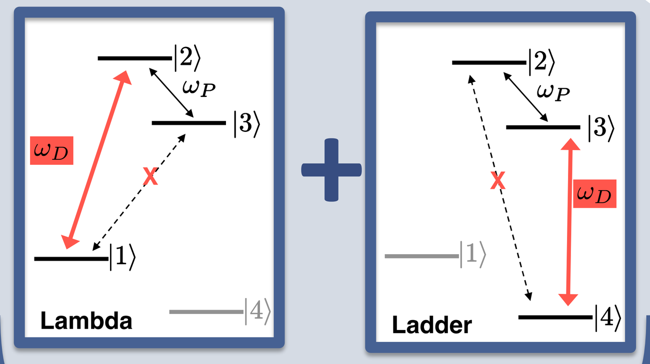
exceeds Manley-Rowe limit !

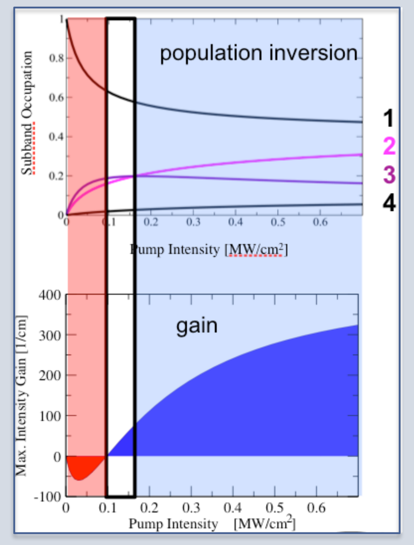


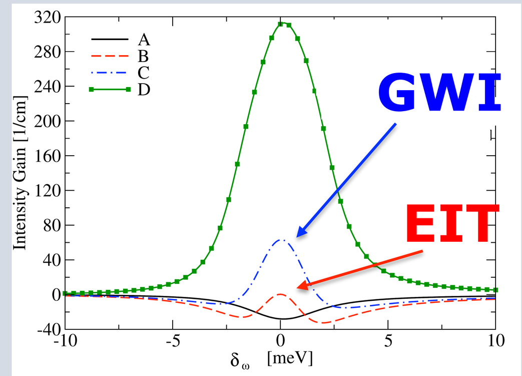


without pump recyling









Model systems for quantum coherence effects (GWI, EIT)

Linear stimulated emission | auto-correlation | cross-correlation | automatically phase-matched q.c. effects

$$\frac{\mathrm{d}}{\mathrm{dt}} E_{THz} \propto d^2_{THz} E_{THz} \frac{(N_2 - N_3) 4\hbar^2\gamma^2 + (N_2 - N_3) d^2_{THz} |E_{THz}|^2 + (N_1 + N_2 - N_3 - N_4) d^2_D |E_D|^2}{2\hbar\gamma(4 d^2_D |E_D|^2 + d^2_{THz}|E_{THz}|^2 + 4\hbar^2\gamma^2)}$$

Conclusions

Our microscopic simulator has been applied successfully to the description of ultrafast phenomena (including high excitation and fast modulation conditions) as well as to the steady-state characteristics (electron distributions, non-equilibrium phonon populations, absorption/gain spectra, current densities) of complex 2d-heterostructures. Furthermore, it has been used to showcase that automatically phase-matched quantum coherence contributions can give rise to THz radiation.

References

[1] Waldmueller et al., 'Circumventing the Manley-Rowe Quantum Efficiency Limit in an Optically Pumped Terahertz Quantum-Cascade Amplifier', Phys Rev. Lett. 99 (2007)

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