Proposed Use of Step Quantum Wells for Terahertz Quantum Cascade Lasers

Will Freeman
Naval Air Warfare Center
Physics and Computational Sciences Division
China Lake, CA 93555, USA

Gamani Karunasiri
Naval Postgraduate School
Physics Department
Monterey, CA 93943, USA

Terahertz (THz) quantum cascade lasers (QCLs) have been designed by a number of approaches and variations using square quantum wells. Here, a step quantum well structure is analyzed for use in LO-phonon assisted QCLs where the radiative transition and LO-phonon transition are within the same well. The electron-phonon and electron-electron scattering rates are calculated for this step well and a QCL structure for operating in the THz frequencies is proposed.

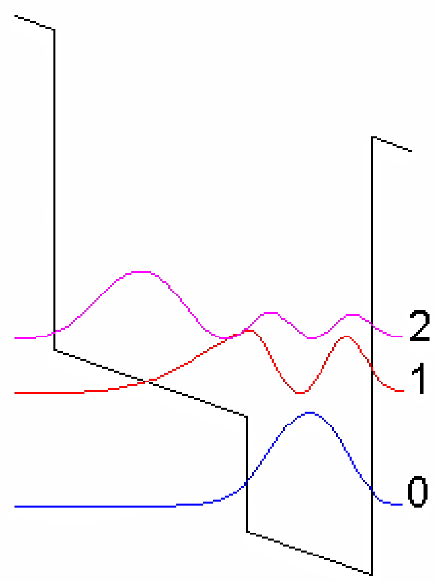
Introduction

The first terahertz QCL that used electron-phonon scattering for depopulation similar to that of Faist's *et al.* mid-infrared QCL, was by Williams *et al*. Variations of the terahertz LO-phonon based designs have essentially been within the same framework. All of these design approaches used square quantum wells, i.e., quantum wells that are symmetric when not under bias.

It is not possible to have an upper radiative terahertz energy spacing and LO-phonon energy spacing within a single square quantum well. A step quantum well, in which two different material compositions are used, breaks this restriction. In this approach, the radiative transition and LO-phonon transition are within the same step well. While intrawell radiative transitions can have large overlap of the electron wavefunctions which can yield large oscillator strengths, there can be a trade off between the oscillator strength and upper state lifetime as the parasitic scattering from the upper radiative state to the ground state can be increased.

Terahertz Step Quantum Well

Consider the following step well with the radiative energy spacing E_{21} = 17.9 meV (4.2 THz). The 1 to 0 transition has E_{10} = 36.5 meV which is near the LO-phonon energy. An external electric field of 10.1 kV/cm was applied. This approach can be used to engineer radiative frequencies lower and higher than the 4.2 THz value as well.



Conduction band profile of a step quantum well comprised of $Al_xGa_{1-x}As$ layers with compositions of 0.143/0.035/0/0.143 and well thicknesses in nm of 20.9/13.5. The radiative transition is from 2 to 1 and the 1 to 0 transition is near the LO-phonon energy.

Rate Analysis

The scattering rates (W_{21} and W_{10}) must be calculated for the step quantum well structure to estimate if a population inversion is likely between states 2 and 1. The simplest rate equation analysis allows us to write the population of the middle state 1 (n_1) as

$$\frac{dn_1}{dt} = n_2 W_{21} - n_1 W_{10}$$

where n_2 is the population of state 2. The necessary condition at steady state for a population inversion to exist ($n_2 > n_1$) is $W_{10} > W_{21}$ (in terms of corresponding lifetimes $\tau_{10} < \tau_{21}$). In general, the scattering rates are a combination of all possible scattering mechanisms, i.e., electron-phonon, electron-electron, impurity, and interface roughness scattering. The scattering rates were estimated by taking into account the electron-phonon and electron-electron scattering rates. For the calculations that follow, the lattice temperature will be taken to be 25 K and the electron temperature 100 K.

Electron-phonon Scattering

The Fröhlich interaction for the electron-phonon scattering was computed using the bulk LO-phonon potential.

$$V_{e^- - phonon} = \sum_q \frac{i}{q} \sqrt{\frac{e^2 E_{LO}}{2V} \left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_{st}} \right)} \left(\mathrm{a}_{\mathbf{q}} - \mathrm{a}_{-\mathbf{q}}{}^\dagger \right) \mathrm{e}^{i\mathbf{q}\cdot\mathbf{x}}$$

$$W_{e^- - phonon,\ mean} = \frac{\int dE_{k_i}\ W_{e^- - phonon, i}\ f_{FD,i}(k_i)\left[1 - f_{FD,f}(k_f)\right]}{\int dE_{k_i}\ f_{FD,i}(k_i)}$$

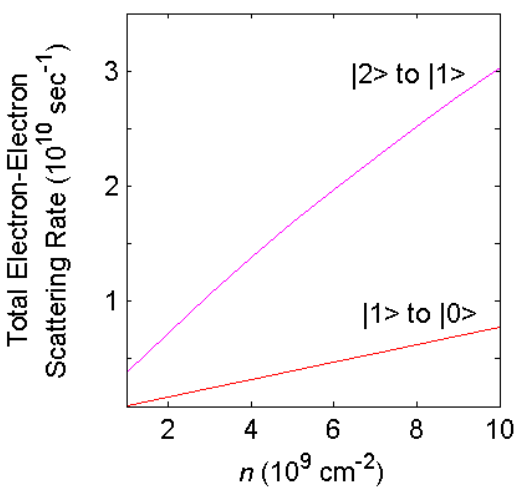
The mean scattering rates are on the order of ~ 10^{12} sec^{-1}. The corresponding lifetimes are listed below (reciprocals of the essentially constant scattering rates, from $n = 1\times10^9$ cm^{-2} to 1×10^{10} cm^{-2}).

τ_{10} = 0.37 psec
τ_{21} = 5.6 psec ($\tau_{21\ max}$ = 0.63 psec)
τ_{20} = 1.8 psec

Electron-Electron Scattering

The electron-electron scattering rates due to antiparallel spin electrons is considered (noting that parallel spin collisions with the exchange term produce a lower scattering rate). The following matrix element is computed for the electron-electron scattering and the mean rates are found for n = 1×10^{9} cm^{-2} to 1×10^{10} cm^{-2}).

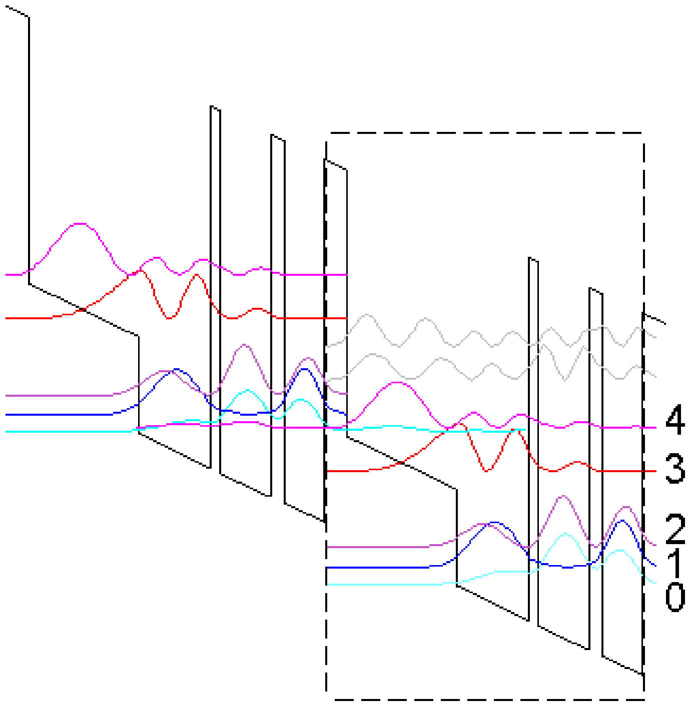
$$\langle f, g | V | i, j \rangle = \langle f, g | \frac{e^2}{4\pi\varepsilon|\mathbf{x}-\mathbf{x}'|} | i, j \rangle \qquad W_{e^- - e^-, mean} = \frac{\int dE_{k_i} \, W_{e^- - e^-, i} \, f_{FD,i}(k_i)}{\int dE_{k_i} \, f_{FD,i}(k_i)}$$



The total electron-electron scattering rates for the 2 to 1 and the 1 to 0 transitions, based on the processes for the simplified rate equation analysis.

The analysis indicates that the electron-phonon scattering rates are about an order of magnitude larger than the electron-electron scattering rates. This indicates that this type of structure is likely capable of keeping a population inversion for the temperatures and range of carrier concentrations considered.

Proposed Structure



The radiative transition: E_{43} = 17.3 meV (4.2 THz or λ ~ 72 μm).

The primary LO-phonon assisted transition: E_{31} = 37.3 meV which is near $\hbar w_{LO}$.

Conduction band profile of a proposed step well quantum cascade laser found using a self-consistent solution to the Schrödinger and Poisson equations. The step well and resonant tunneling double barriers of one module are outlined. Beginning with the left injector, the $Al_xGa_{1-x}As$ layers compositions are 0.143/0.035/0/0.143/0/0.143/0 and thicknesses in nm are 4.3/20.9/13.5/1.7/9.6/2.5/7.6. The radiative transition is from 4 to 3 and the 3 to 1 transition is near the LO-phonon energy. The applied field is 10.1 kV/cm and the 9.6 nm well is doped 2.9×10^{16} cm^{-3} which corresponds to a sheet density of 2.8×10^{10} cm^{-2}.

Analysis

The electron-phonon scattering gives $\tau_{3 \text{ to } (2,\ 1,\ 0)}$ ~ 0.4 psec
Oscillator strength = 1.52
The parasitic scattering rate gives $\tau_{4 \text{ to } (2,\ 1,\ 0)}$ ~ 1.4 psec

The estimated 2D population inversion at threshold approximating the lower state as empty is 2.7×10^{9} cm^{-2} (within the carrier densities used in our analysis, assuming a total loss of ~ 41 cm^{-1}, *FWHM* ~ 4 meV)

$$gain = \frac{2e^2\hbar^2 \Delta n_{3D}}{m^2\ \varepsilon\ n_{index}\ c\ \omega\ FWHM}\left|\left\langle f \left| \frac{d}{dx} \right| i \right\rangle\right|^2$$

The total upper radiative state 4 lifetime is estimated to be ~ 0.56 psec. This implies that tunneling rather than the relatively fast parasitic scattering rate from state 4 to (2, 1, 0) is what dominates the total upper state lifetime.

The current density is estimated to be J ~ 810 A/cm^{-2}

$$\Delta n_{2D} \sim (J/e)\ \tau_4\ (1 - \tau_3/\ \tau_{4,3})$$

Summary

Our analysis indicates that step quantum wells may be capable of maintaining a population inversion for low carrier concentrations expected in QCLs. A full structure that uses a step well and a double barrier section for injection to the next module has been proposed. The vertical nature of the radiative transition yields a relatively high oscillator strength, and also an increased parasitic scattering rate from the upper state to the ground states. Though, similar upper state lifetimes were found from previously reported QCL structures. Further analysis is needed to see if such structures are practical for QCL devices and to accurately determine the electron temperatures and subband populations of the full structure.