Tutorial - THz GaAs/AlGaAs (Fathololoumi)

Summary

This tutorial is based on the following publication.

[Fathololoumi2012]
Terahertz quantum cascade lasers operating up to ~200 K with optimized oscillator strength and improved injection tunneling
S. Fathololoumi, E. Dupont, C.W.I. Chan, Z.R. Wasilewski, S.R. Laframboise, D. Ban, A. Mátyás, C. Jirauschek, Q. Hu, H. C. Liu
Optics Express 20, 3866 (2012)

This article describes an AlGaAs/GaAs THz quantum cascade laser (QCL) operating at around 2.6 to 3.22 THz. This layout of this laser is a resonant phonon based three-well design. The corresonding input file is called
`THz_QCL_GaAs_AlGaAs_Fathololoumi_OptExpress2012_10K-MEDIUM.xml`.

Note that we also provide an input file called
`THz_QCL_GaAs_AlGaAs_Fathololoumi_OptExpress2012_10K-FAST.xml` which is faster but does not produce accurate result. This `*-FAST.xml` file is only intended to show the user how to run a “quick” simulation. The results shown here correspond to the `*-MEDIUM.xml` file.
`[Fathololoumi2012]` designed the laser to operate at an electric field of -12.2 kV/cm.

Simulation details

We simulate the structure at a temperature of 10 K.

```
 <Temperature unit="K"> 10 </Temperature>
```

Device definition

First, the materials used in the structure (GaAs and AlGaAs) have to be defined. Each material is referred by an alias, which is here 'well' for GaAs and 'barrier' and AlGaAs.

```
  <Materials>

    <Material>
      <Name>GaAs</Name>
      <Alias>well</Alias>
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
    </Material>

    <Material>
      <Name>Al(x)Ga(1-x)As</Name>
```

```
      <Alloy_Composition>0.15</Alloy_Composition>
      <Alias>barrier</Alias>
<Effective_mass_from_kp_parameters>yes</Effective_mass_from_kp_parameters>
    </Material>
    <!-- Model nonparabolicity -->
    <NonParabolicity>yes</NonParabolicity>

    <UseConductionBandOffset>yes</UseConductionBandOffset>

  </Materials>
```

In addition, it is specified that the effective mass is calculated from the k.p parameters. Also, non

Then, alternating layers consisting of barrier and well have to be specified, i.e. **4.1** / 16.0 / **4.3** / 8.9 / **2.46** / 8.15, where AlGaAs is in bold fonts and the doping region is underlined, i.e. the wide GaAs quantum well is doped. The total length of one period is thus 43.91 nm. This layout is consistent to [Fathololoumi2012].

```
  <Layer>   <!-- #1 -->
   <Barrier_Thickness unit="nm"> 4.1 </Barrier_Thickness>
   <   Well_Thickness unit="nm"> 16.0 </   Well_Thickness>
  </Layer>

  <Layer>   <!-- #2 -->
   <Barrier_Thickness unit="nm"> 4.3 </Barrier_Thickness>
   <   Well_Thickness unit="nm"> 8.9 </   Well_Thickness>
  </Layer>

  <Layer>   <!-- #3 -->
   <Barrier_Thickness unit="nm"> 2.46 </Barrier_Thickness>
   <   Well_Thickness unit="nm"> 8.15 </   Well_Thickness>
  </Layer>
```

The resulting conduction band edge profile can be found in the file called BandEdge_conduction.dat. This file includes the (small) band bending due to the electrostatic potential. At a bias voltage of 54 mV per period, it looks as follows.

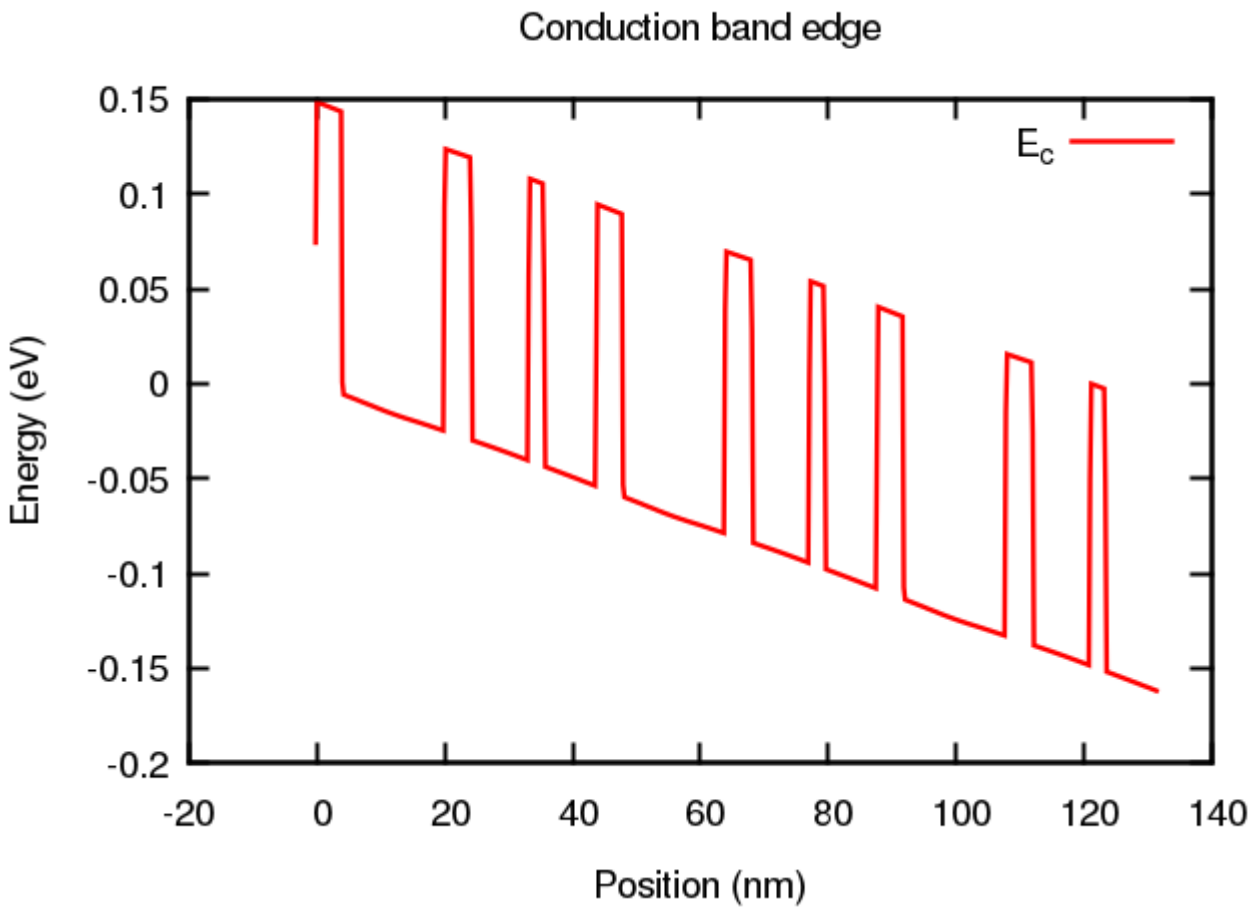

Figure 1: Conduction band edge at a bias of 54 mV/period which corresponds to an electric field of -12.3 kV/cm

Doping

Here, we use a doping sheet density of $3 \cdot 10^{10}{\rm~cm}^{-2}$. The 16 nm GaAs quantum well starts at 4.1 nm and ends at 20.1 nm and is thus centered at 12.05 nm. We distribute the doping sheet density homogeneously over a region of width 5 nm with respect to the center of the quantum well, i.e. from 9.6 nm to 14.6 nm. The sheet density and its distribution is consistent to [Fathololoumi2012].

```
     <Doping>
      <DopingStart unit="nm">  9.6 </DopingStart>
      <DopingEnd   unit="nm"> 14.6 </DopingEnd>
      <Doping_Specification> 0 </Doping_Specification>
      <Doping_Density> 3e10 </Doping_Density> <!-- doping sheet density
[cm^-2]-->
     </Doping>
```

Material parameters

We set the conduction band offset (CBO) between GaAs and $Al_{0.15}Ga_{0.85}As$ to 0.120 eV, i.e. we

overwrite the default material parameters that are contained in the material database.

```
<Material_Parameters>
 <Overwrite_ConductionBandOffset>true</Overwrite_ConductionBandOffset>
 <ConductionBandOffset unit="meV"> 120 </ConductionBandOffset>
</Material_Parameters>
```

(In fact, the figures shown in the tutorial were generated using a different CBO of 0.149 eV.)

Electric field

The total length of one period is L = 43.91 nm. A bias of V = 54 mV per period then corresponds to an electric field of F = V/L = -12.3 kV/cm.

Wannier-Stark states

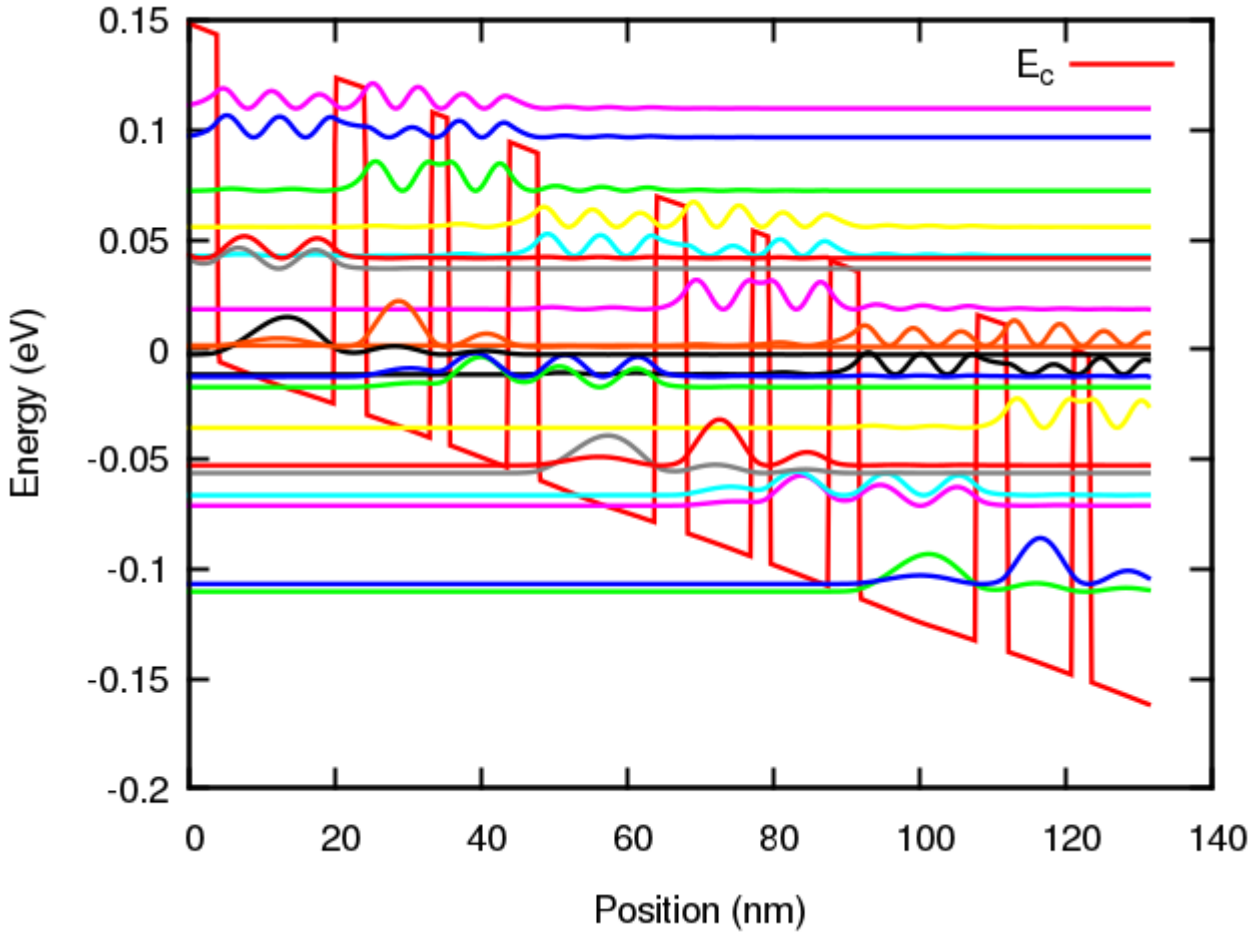

Figure 2: Conduction band edge at a bias of 54 mV/period which corresponds to an electric field of -12.3 kV/cm and corresponding probability densities ($\left|\psi_i(x)\right|^2$) of the Wannier-Stark states.

The following two figures show the Wannier-Stark states at an applied bias of 56 mV/period (-12.8

kV/cm). They compare Fig. 1 of the publication of T. Grange, PRB 92, 241306(R) (2015) with the results of this input file.

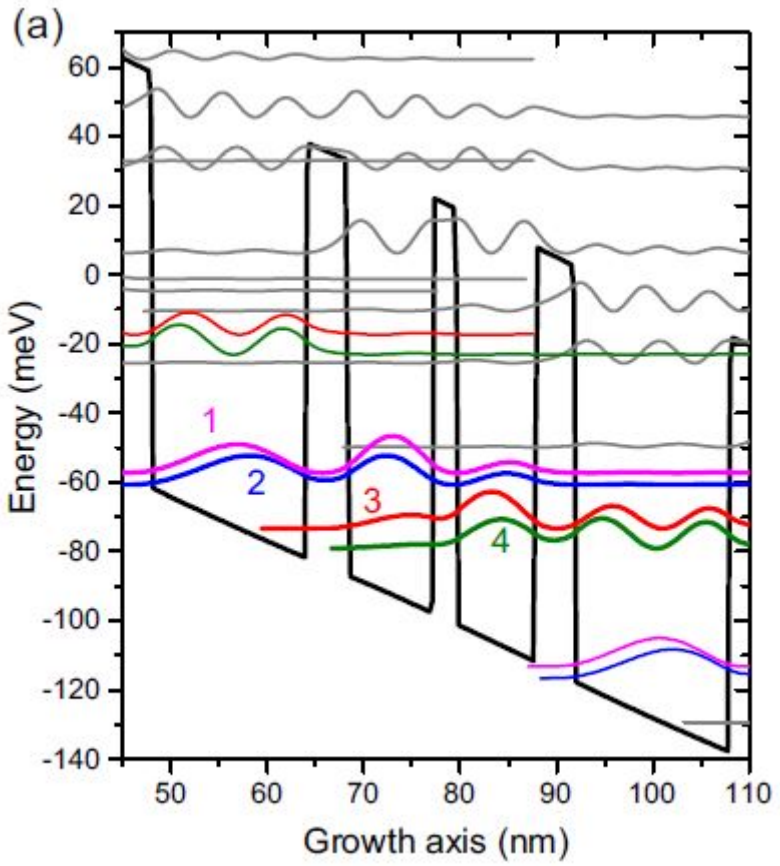

Figure 3: Wannier-Stark states at a bias of 56 mV/period (-12.8 kV/cm) (Fig. 1 of T. Grange, PRB 92, 241306(R) (2015)). The three-well design consists of one large well and two small wells. The optical photon transition is a diagonal transition (i.e. from the left thin well to the right thin well) and occurs between the states 2 (blue) and 3 (red). Each of the large wells contains an injector state 1 (purple) and an extractor state 4 (green). The injector state fills the upper laser level 2 (blue) with electrons while the extractor state empties the lower laser level 3 (red).

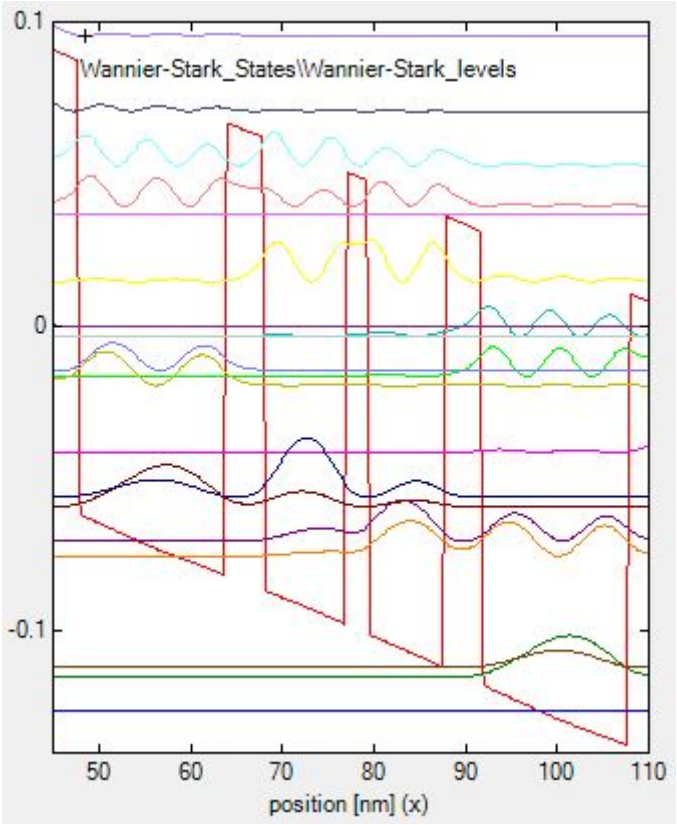

Figure 4: Wannier-Stark states at a bias of 56 mV/period (-12.8 kV/cm) (Results of this input file)

Local density of states

The following figure shows the local density of states (LDOS) at a bias of 54 mV / period corresponding to -12.3 kV/cm). The LDOS tells us where and at which energy electronic states are available that the charge carriers can occupy. The LDOS is shown for $k_\parallel=0$, i.e. there are also electronic states available for $k_\parallel \ne 0$. But they are not shown in this plot because then the picture could not show the minimum energy of each subband , which is at $k_\parallel=0$, so nicely.

Figure 5: Local density of states $\rho(x,E)$ and conduction band edge $E_{\rm c}$

Electron density

The following figure shows the energy resolved electron density $n(x,E)$ at a bias of 54 mV / period corresponding to -12.3 kV/cm). The electron density is obtained from occupying the LDOS (for both $k_\parallel=0$ and $k_\parallel \ne 0$) with charge carriers. The occupation is not described by a Fermi distribution (equilibrium). It is a nonequilibrium occupation which leads to population inversion in this case which is a necessary requirement for a laser to operate.

Figure 6: Energy resolved electron density $n(x,E)$ and conduction band edge $E_{\rm c}$ at a bias of 54 mV / period (-12.3 kV/cm)

If one integrates the energy resolved electron density $n(x,E)$ over energy E, then one obtains the electron density $n(x)$ which is shown in the following graph.

Figure 7: Electron density $n(x)$ at a bias of 54 mV/period which corresponds to an electric field of -12.3 kV/cm

The following two figures show the energy resolved electron density at an applied bias of 58 mV/period (-13.2 kV/cm). They compare Fig. 3 (a) of the publication of T. Grange, PRB 92, 241306(R) (2015) with the results of this input file.

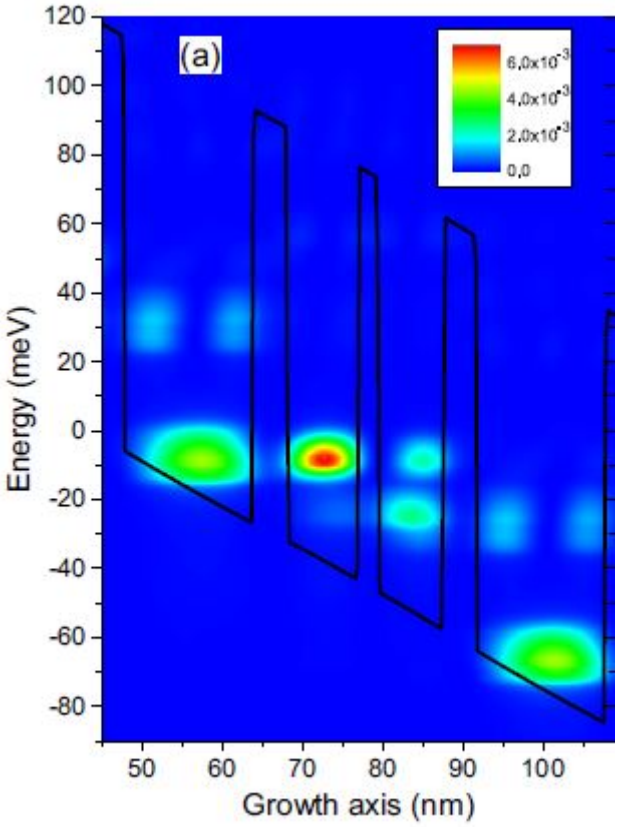

Figure 8: Energy resolved electron density $n(x,E)$ at a bias of 58 mV/period (-13.2 kV/cm) (Fig. 3(a) of T. Grange, PRB 92, 241306(R) (2015))

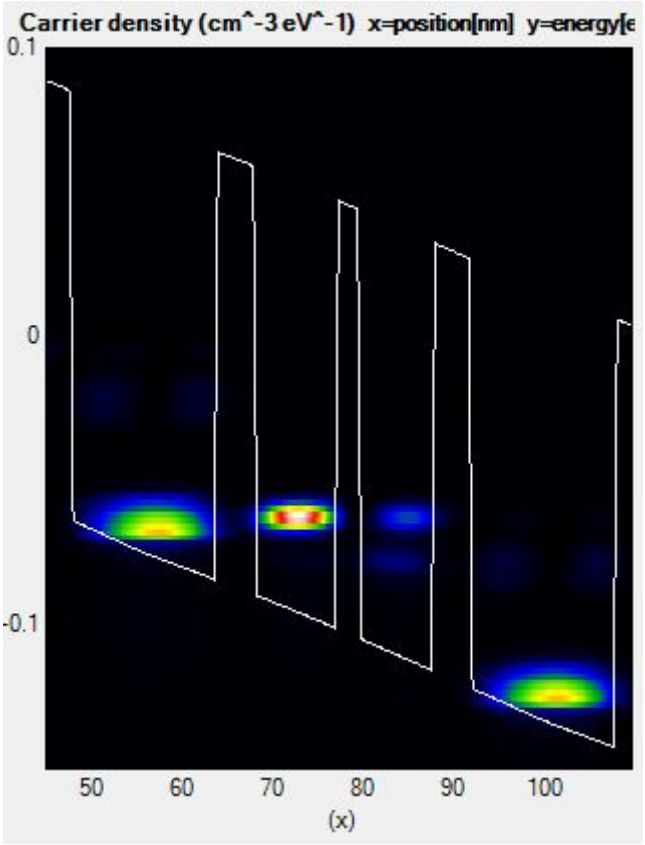

Figure 9: Energy resolved electron density $n(x,E)$ at a bias of 58 mV/period (-13.2 kV/cm) (Results of this input file)

Current density

The following figure shows the energy resolved current density $j(x,E)$ at a bias of 54 mV / period corresponding to -12.3 kV/cm).

Figure 10: Current density $j(x,E)$ and conduction band edge $E_{\rm c}$. One can clearly see that the current density inside the thick quantum well changes abruptly because the electrons lose energy of order 35 meV. The reason is that the electrons scattering resonantly with LO phonons ($E_{\rm LO}=35{\rm~meV}$).

Longitudinal polar-optical phonon scattering

The material parameter for the LO phonon energy is specified in the material database.

```
   <LOPhononEnergy Unit="eV"> 36.75e-3 </LOPhononEnergy>
```

Gain

The following figure shows the energy resolved gain $g(x,E_{\rm ph})$ at a bias of 54 mV / period corresponding to -12.3 kV/cm). Note that the energy axis corresponds to the photon energy $E_{\rm ph}$. The thin white lines indicate the barrier/well interfaces and are only a guide to the eye. Regions

with large positive gain are white (and read), regions with strong absorption are black (and blue).

Figure 11: Gain $g(x,E_{\rm ph})$ (self-consistent calculation). The white maxima in this plot show nicely that the photon transition is diagonal, i.e. it occurs from the left thin well to the right thin well.

The following shows the same as above but this time the gain was not calculated self-consistently. Nevertheless, the results are very similar.

Figure 12: Gain $g(x,E_{\rm ph})$ (nonself-consistent calculation)

For the difference between self-consistent and nonself-consistent gain calculation (`GainMethod`), please refer to the documentation of the input file syntax.

If one integrates the position resolved gain $g(x,E_{\rm ph})$ over position x, one obtains the gain as a function of photon energy $g(E_{\rm ph})$ as shown below.

Figure 13: Gain $g(E_{\rm ph})$. The red line is the self-consistently calculated gain, the gray one the nonself-consistent one. Values of $g(E_{\rm ph})>0$ correspond to gain, values of $g(E_{\rm ph})<0$ to absorption of photons.

Gain-Voltage characteristics

The following figure shows the maximum gain (red) in units of [1/cm] as a function of applied bias. The corresponding photon energy (blue) for each maximum gain is also shown. For voltages $54 \le V \le 62 $, the photon energy is 14 meV which corresponds to 3.39 THz.

Figure 14: Maximum Gain $g_{\rm max}(V)$ (red line) vs. applied bias per period V and corresponding photon energy $E_{\rm ph}$ (blue). $E_{\rm ph}=14 {\rm~meV}$ corresponds to a laser emission at a frequency of 3.39 THz.

We calculate the gain only for interesting voltages, i.e. only between the values of potential drop per period from 42 mV to 64 mV. Photon energies between 2 meV and 50 meV are considered. The energy spacing between two photon energies is set to 2 meV.

```
<Gain>
  ...
  <dE_Phot unit="meV"> 2 </dE_Phot>
  <Ephoton_Min unit="meV">  2 </Ephoton_Min>
  <Ephoton_Max unit="meV"> 50 </Ephoton_Max>
  <Vmin unit="mV"> 42 </Vmin>
  <Vmax unit="mV"> 64 </Vmax>
</Gain>
```

Details of the simulation

The file `Current-miscellaneous.txt` contains additional information. For instance, in this file we can find the **electric field** that corresponds to the applied bias per period or the current density.

```
Current density = 513.793479050054 A.cm^-2
Average electron velocity = 4.93162777325326  nm / ps
Time for electron to travel through one period = 8.90375389605566 ps

Electric Field = -12.2978820314279 kV/cm
Doping sheet density per period 30000000000 cm^-2
Average 3D doping density  6.83215668412662E+15 cm^-3

Effective electronic temperature 113.778348225956 K
```

Current-voltage characteristics

The IV curve for all voltages is shown next.

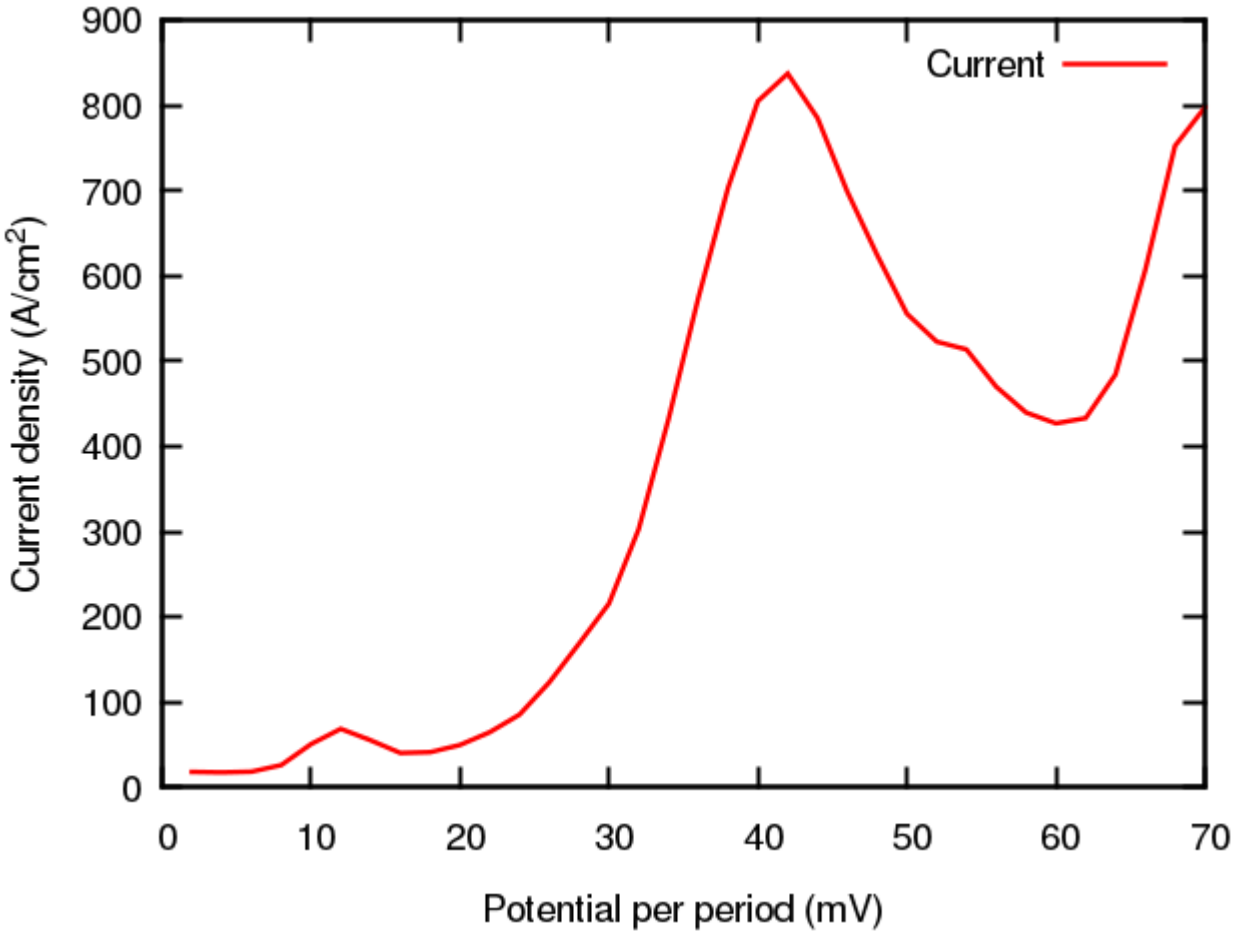

Figure 15: Current-voltage (IV) characteristics of the Fathololoumi quantum cascade laser. All the

figures discussed in this tutorial correspond to an applied bias of 54 mV/period which gives a current density of 514 A/cm^2.

The voltage is swept from 2 mV to 70 mV in steps of 2 mV. The voltage refers to mV/period.

```
<SweepParameters>
  <Min   unit="mV">  2 </Min>
  <Max   unit="mV"> 70 </Max>
  <Delta unit="mV">  2 </Delta>
</SweepParameters>
```

Interface roughness scattering

For interface roughness we assume typical values of an amplitude of 0.1 nm and an exponential correlation length of 8 nm.

```
<Roughness>
  <Interface_Roughness>
    <Amplitude_in_Z unit="nm"> 0.1 </Amplitude_in_Z>
    <InterfaceAutoCorrelationType> 0 </InterfaceAutoCorrelationType>
             <!-- Correlation type: 0=Exponential, 1=Gaussian -->
    <Correlation_Length_in_XY unit="nm"> 8 </Correlation_Length_in_XY>
    <Asymmetric_Interfaces> false </Asymmetric_Interfaces>
    <Amplitude_in_Z_Left>  0.1 </Amplitude_in_Z_Left>
    <Amplitude_in_Z_Right> 0.2 </Amplitude_in_Z_Right>
  </Interface_Roughness>
</Roughness>
```

Computational resources

The CPU time was about 5-6 hours and used about 9 GB RAM.

Feedback

If you have questions regarding this tutorial or if you have comments how we can improve it, please contact us at support@nextnano.com.