Three-step model

Absorption – Transmission – Emission

The goal of the COMSOL model is to cover step 2 based on a given step 1 (from Band Gap model) and an external step 3.

So how do I plan for it to work?

A given absorption coefficient and refractive index (material driven) is given to COMSOL to calculate energy (Fermi-level) w/ respect to depth

Additionally, a given doping profile is used to produce the correct band-bending expected in the material.

These two controls are uses to generate the study COMSOL performs which will be explain in step across the following slides.

Before I go any further...

It seems it may help to have a derivation of QE...

We define two quantities in addition to QE, namely

Charge Flow

$$I = \frac{N_e q}{t}$$

Photon Flux

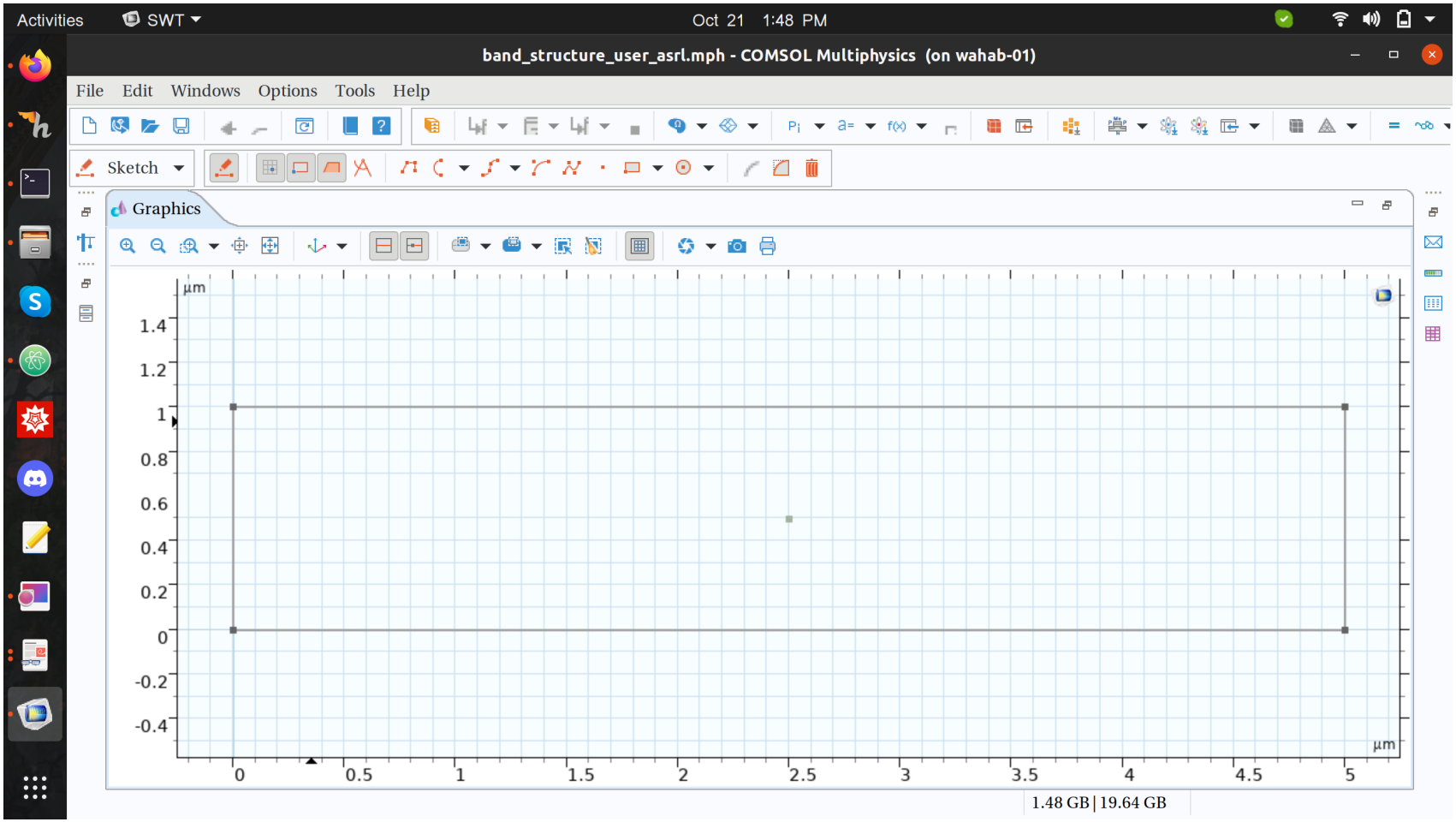
$$P = \frac{hc}{\lambda}\Phi = \frac{hc}{\lambda}\frac{N_\gamma}{t}$$

The photon flux Φ assumes the area includes all photons, hence no surface area in the denominator. We could instead include an area in the power definition but we assume all power is captured. Thus...

$$\eta = \frac{N_e}{N_\gamma} = \frac{It}{q}\frac{hc}{\lambda t P} = \frac{hc}{\lambda q}\frac{I}{P}$$

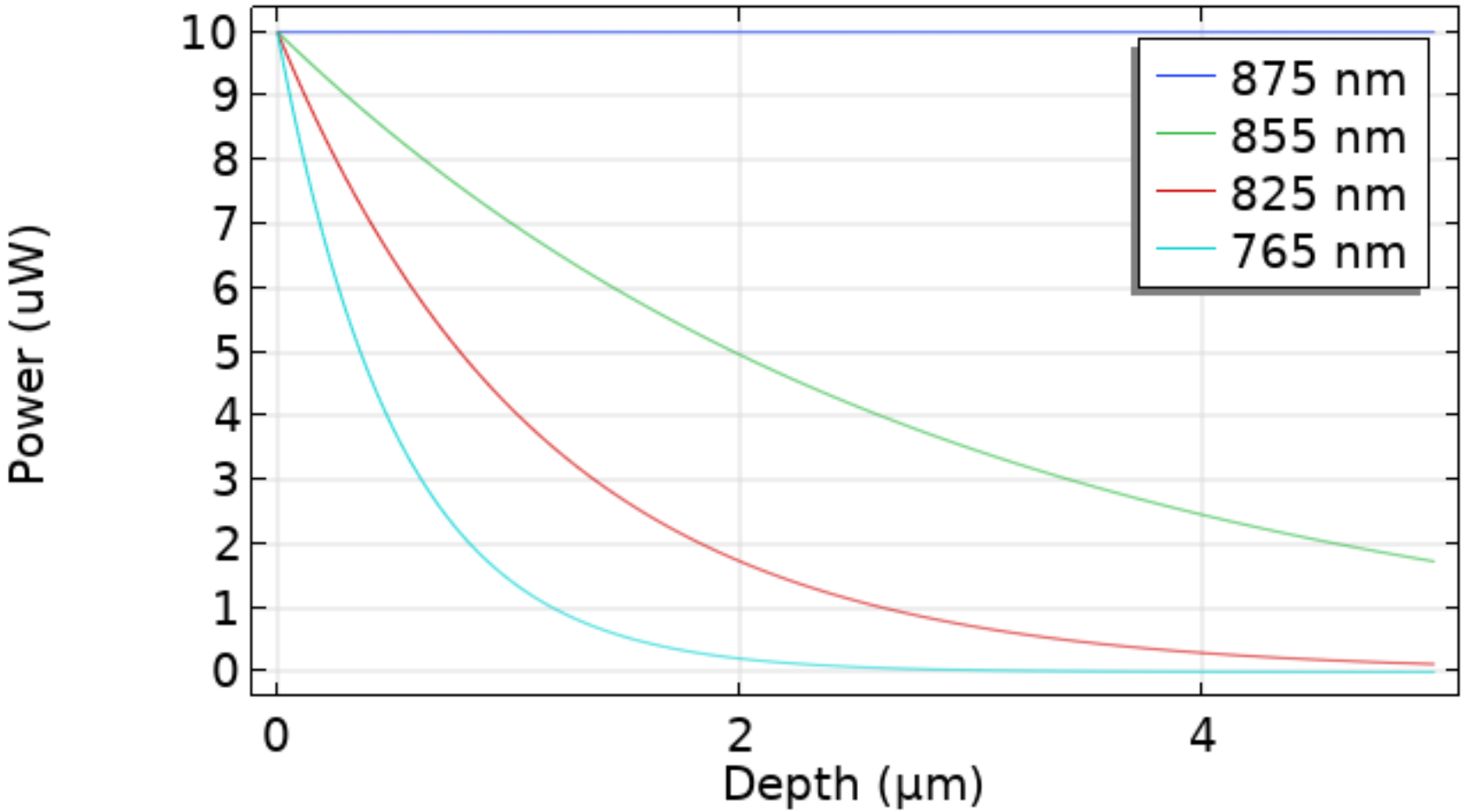
Geometry

Before I can discuss the actual calculation process we need to describe the geometry



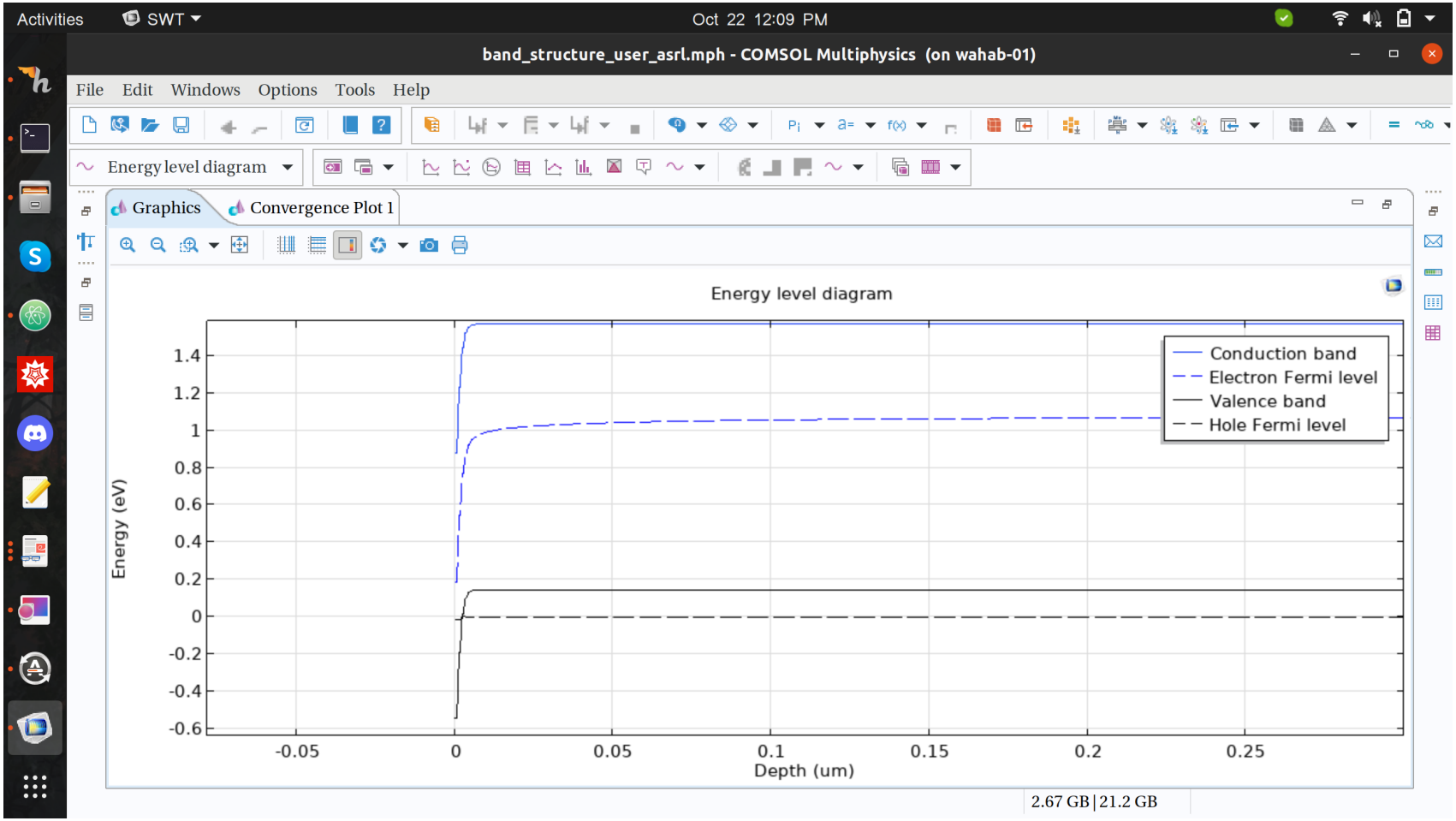
Absorption

Band bending requires manual absorption curves/coefficients



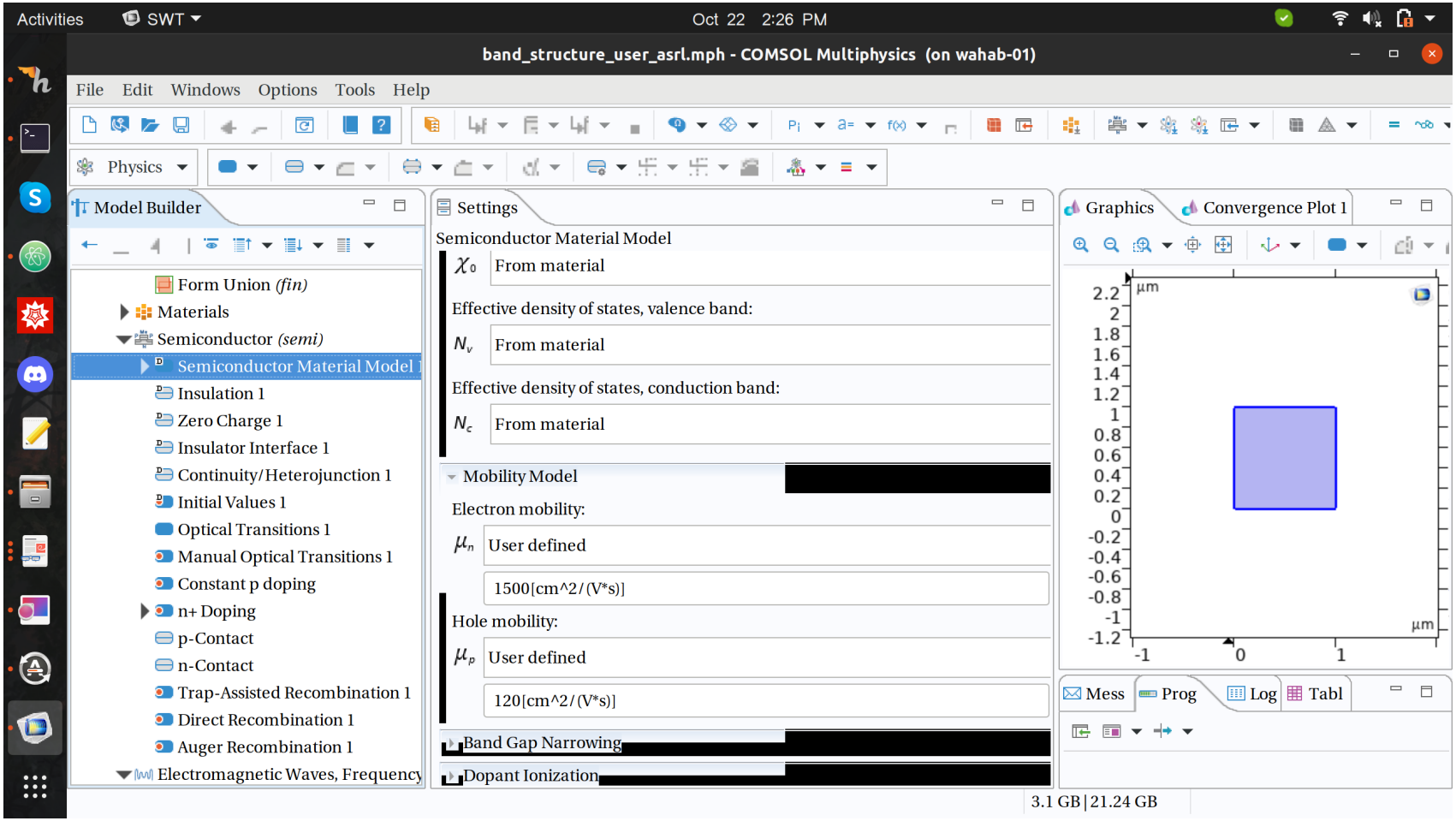
Band Bending

Surface "pinning" bends band down and scales with bulk doping



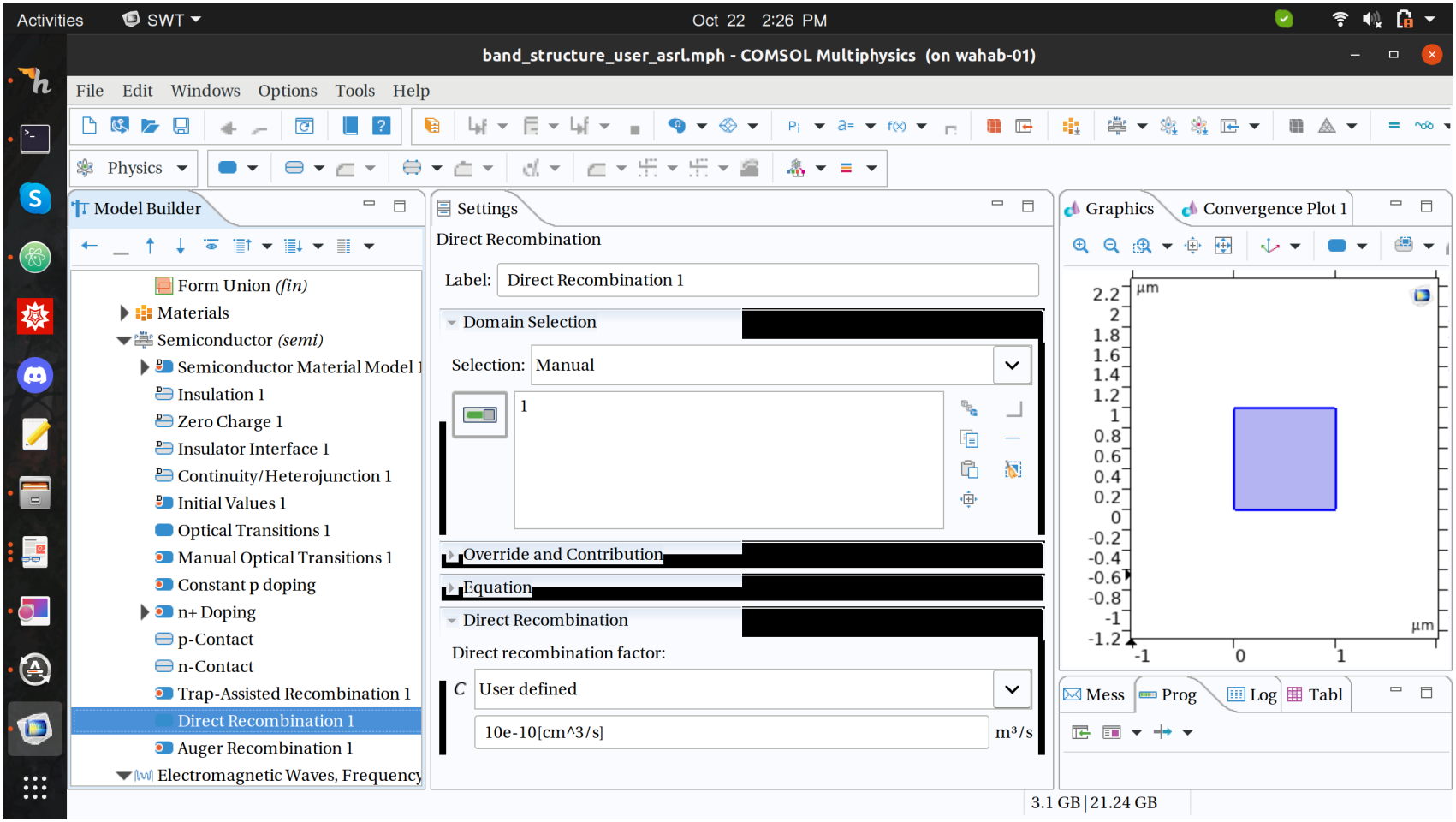
Mobility

User-defined μ for doped material... one variable includes ALL effects



Recombination

All built in types are included - values set to bulk GaAs (needs work)



The physics I think are working!

So, its clear absorption is intended to be a clear Beer-Lambert law ignoring doping effects. Difficult to check but I believe optical transitions are well suited

$$P = P_0 e^{-\alpha z}, \alpha \neq f(z)$$

Electron mobility is defined manually! We have the mobility for a given doping!

Band Bending is performing very well - magnitude is correct and width a user defined! https://doi.org/10.1063/1.4794822

Recombination is on correctly, just scaling needs optimization

All in all the semiconductor module is the most well understood...

And some I am not so sure...

There are some concerns I have still with a number of the physics. I am working to understand and debug them!

Namely, the incident light for stimulated absorption. There is an out of plane thickness as well as a number of propagation constants that needs to be better understand. They can easily impact magnitude of the QE curve.

The ray-optics package is less travelled by me so far!

Additionally, meshing. I am not sure that my meshing does not impact the results yet. It shouldnt but it needs to be verified!

I would really enjoy being able to see laser power as we travel through the material... I am close, but there are close to 500 variable to work with!

Emission and WKB

So we get a current... what percentage of the current gets through to the vacuum? We use WKB approximation to estimate the probability! Recall,

$$|T|^2 = e^{-2\gamma}, \gamma = \int_0^x \frac{\sqrt{2m(V(x) - E)}}{\hbar} dx$$

We have three variables to control $x, V, andE$. It is easier to reconfigure this integral by definition a form of the barrier potential

$$V(x) = Ae^{-x}$$

We can then rewrite our integral in terms of peak barrier height A and the percentage of the barrier height that electrons reach the surface with

$$\gamma = \int_0^x \frac{\sqrt{2mA(e^{-x} - P_E)}}{\hbar} dx$$

Emission and WKB continued

We can now bind the range of our emission! We can choose a minimum and maximum value for x, A, P_E and observe our probability.

I choose the barrier thickness to be between 1-2 nm, the barrier height to be 1.5-2.5 eV, and the percentage of max energy between 60 and 90 %

This process gets us a max value transmission at 1,1.5,90, and a minimum at 2,2.5,60 for the obvious reasons

The results probabilities are 10^{-3} to 10^{-11}, which agrees with expectation on the mid-higher end. I use 10^{-6}

Opening a can of worms...

If the peak transmission probability is 0.001, an internal QE of 1000 % is required to have 1 % external QE...?

Does this make any sense? Typically internal QE refers to "per absorbed photon" which is why it exceeds external QE which includes all incident photons. However, if 100 % of photons are absorbed inside 5 um, say at 720 nm, then the internal QE and external QE are only separated by magnitude of emitted current. This means the internal current must be at least 3 orders of magnitude larger than external!

Assuming it makes sense...

We must assume that without emission our QE can exceed 100 %

We can then scale this high QE by our emission probability

$$\eta = |T|^2 \frac{hc}{\lambda q} \frac{I}{P}$$

which is the number I report in all results currently... Of course there are caveats!

For example, I do not yet know if the laser power is reporting correctly (see earlier) or that the recombination is scaled correctly. These could alter the QE.

A reminder: This is not a finished model - the goal of this progress so far is to demonstrate we have access to the variables that impact QE

Recombination