FFI

Master projects in Semiconductor Physics and Condensed Matter Theory 2015/2016

Our research in Computational Materials Science and Computational Optoelectronics is focused on fundamental photon, phonon and charge carrier interactions in semiconductors and on development of numerical simulation tools and methods for quantitative description of semiconductor materials and devices.

FFI is located at Kjeller near Oslo. The projects can all be carried out in Trondheim. Travel expenses between Kjeller and Trondheim are refunded by FFI.

If you are considering any of our projects, please feel free to send us an email with your CV and a few words describing your research interests.

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Project 1

Higher Order Quantum Processes in Semiconductors

Approximate expressions describing basic phenomena occurring in materials of technological importance are usually readily available. Unfortunately, they are often of a more or less empirical nature, with a high degree of uncertainty. Improvement can be obtained by numerical calculations and by introducing higher order corrections.

Recombination mechanisms represent a typical case where such corrections are needed. They decide how fast the charge carriers in the valence and conduction bands reach their equilibrium values after a disturbance. For every recombination mechanism there is also a corresponding generation mechanism to consider.

Ordinary band-to-band recombination, either direct (by emitting a photon) or indirect (via trapping levels or by emitting a phonon and a photon) are probably the most well-described textbook cases because they are usually very fast. However, ordinary thermal generation, for example, often require the energy of many photons to excite a charge carrier from the valence band to the conduction band and is a slow, but actually very complicated process.

Other mechanisms, like Auger recombination, can be both fast and complicated. Here a single particle description is not sufficient. The inverse of Auger recombination is impact ionization. Being non-radiative transitions, the Auger mechanisms are detrimental to semiconductor laser operation, as the population in higher energy levels is depleted without producing radiation. Other higher order effects can be mixed into the bare Auger processes, such as virtual phonon emission, which may influence Auger recombination rates by as much as 30% or more.

Impact ionization is very important in ultra-sensitive Avalanche Photodiodes. Often impact ionization can be coupled to band-to-band tunneling if the reverse bias electric field of the avalanche photodiode is sufficiently strong.

Generation mechanisms decide the dark current of photodiodes, and should therefore be minimized. Carrier-carrier scattering affects the operation of Quantum Cascade Lasers, and effects of finite collision times (intracollisional field effect) are important in modern Field Effect Transistors.

Although many of these mechanisms are qualitatively well known, there are huge uncertainties in 3D and 2D systems, and experimental verification without more theoretical guidance is often difficult. This situation may in turn affect the direction of future technologies.

We have developed a rudimentary **kp** based software for calculating some of the mechanisms. The project will consist of further development of this software, but now based on first principles band structure codes with main emphasis on Auger recombination, impact ionization and generic carrier-carrier scattering.

Project 2

FEM Poisson Solvers for Monte Carlo Transport Simulators

When modeling devices where free charge carriers are involved, solution of the Poisson equation becomes a central task.

If the solver is to be used in a Monte Carlo (MC) particle simulator, the basic timestep must be chosen sufficiently small so that all scatterings of the particles are resolved. Solution of the Poisson equation may be done with larger timesteps than the basic timestep however, but this “Poisson”- timestep should still be small enough to resolve the collective excitations of the electron gas (plasmons).

Large devices can often be described by solving the Poisson equation in 2D, but new field effect transistors currently require a 3D solver due to the intricate shape of the gate electrode, while nano-scale devices often demand 3D modeling because of a need for modeling also the surrounding environment.

Likewise, large area optoelectronic devices would benefit from 3D simulation when the optical beam destroys an otherwise electrical 2D symmetry.

Nonlinearities may be introduced by changing material properties as excess electronic charge is injected electronically or optically.

Although there are faster solvers available, Finite Element Solvers (FEM) are more flexible and they are therefore the first choice when complex geometries or fine details are to be modeled in any device, large or small.

The project focuses on experimentation with and development of FEM Solvers adaptable to our Full Band MC code, but it is also desirable that the solvers can operate as generic stand-alone software.

Project 3

Simulation of Quantized Semiconductor Structures

This project deals with those cases where quantization in low dimensional systems plays a major role. Typically, the degree of confinement depends on the energy of the charge carrier, where the low energy charge carriers can obey 2D transport and scattering whereas high energy carriers obey 3D processes. Confinement then occurs typically either normal to or parallel to the direction of transport.

As the dimensions of the structures shrink below 20 nm, electron transport becomes (quasi-) ballistic, and the entire physics of electronic devices changes. Remote phonon scattering and intracollisional field effects, finite collision duration times and uncompleted collisions must all be taken into account. Impurities can no longer be treated as a continuum background distribution but should be treated as single scattering objects.

Device performance now becomes much more influenced by the carrier injection process. Development of accurate particle boundary conditions for the highly doped electrical contact regions is therefore required. High doping is usually necessary in order to establish good ohmic contact to metal interconnects. The standard injection model for semi-classical Monte Carlo (MC) simulation is based on adapting the injection rate of electrons so as to achieve charge neutrality at the ohmic contacts, i.e. no capacitive charge buildup is allowed. This injection model is not particularly accurate for highly doped degenerate contact regions, because it neglects Fermi correlations between the injection of consecutive electrons. For small devices this inaccuracy becomes critical, but we have also observed irregularities for very large area devices when studying charge carrier with large effective masses (holes).

Today’s transistors have already entered the transition regime where semi-classic transport begins to fail and the wavelike properties of the charge carriers become important. It is therefore desirable to increase our understanding of this region by working out a set of algorithms that can treat the device physics in a unified manner.

The project aims to develop and integrate quantum correction algorithms into an existing MC computer code that enables study of devices with active regions smaller than 20 nm.

Project 4

Charge Transport based on first principles Electronic Structure Codes

User friendly and openly distributed electronic structure codes and the ever increasing computer power now make the calculation of band structures even for relatively complex materials more and more straightforward.

Clearly, any quantitative simulation of materials properties should be based on an accurate description of the material, as provided by the first principles codes. However, the description of non-equilibrium systems is still a hard problem.

What is needed then is a method capable of describing non-equilibrium cases, and this leads us to consider Monte Carlo (MC) particle simulators. However, it has turned out over the last decades that this computationally expensive method is rarely used beyond the most technologically important semiconductor materials, whereas first principles electronic structure codes are currently put to use for virtually any material.

As different electronic structure codes operate with different basis sets, it becomes necessary to adapt a MC code to a particular electronic structure code. Any limitation of the electronic structure code will then automatically become a limitation of the MC simulator, so ideally the MC simulator should be adapted to several first principles electronic structure codes.

Traditionally, MC simulators have been adapted to more primitive empirical pseudopotential codes. This has to do with the relative ease of adaptation, the ability to study technologically important disordered alloys with empirical pseudopotential codes using the “Virtual Crystal Approximation”, and the simple calculation of phonon modes within the rigid pseudo-ion model.

Today, available first principles codes have possibilities for much more sophisticated phonon model calculations and possibilities for transforming the calculated wavefunctions into standardized Wannier functions, which is expected to increase the portability of an MC code between different first principles codes. Furthermore, the recent introduction of automated Brillouin zone “backfolding” software for an alternative treatment of disordered alloys is expected to make it possible for us to use a broader range of more appropriate first principles codes as input to our MC simulator.

Students interested in this project will work with leading first principles electronic structure codes and develop adaptations of these codes to MC simulation.

Project 5

Wave propagation with FEM methods

Novel optoelectronic devices require modeling of propagating electromagnetic (EM) fields while simultaneously solving an electronic transport problem. For example, modern trends towards more precise imaging technologies with reduced pixel dimensions can lead to severe diffraction effects in infrared detectors. Some of these effects are directly related to the contact metallization, but in more sophisticated structures made up of layered materials delineated by deep trenches (MESA structures), the problems become more difficult to handle. Here the propagation solver must be able to deal with light diffraction and reflection in several interface layers and on slanted MESA walls.

Solving this involves a two-step calculation where the two steps may be strongly or weakly coupled, and the problem can be more or less nonlinear. First the electromagnetic (EM) calculation has to be carried out on a 2D (or 3D) domain, and then the next step would be an electrical simulation.

The coupled EM/transport problem is also central in experimental techniques which probe materials with laser pulses to study laser-matter interactions and carrier dynamics.

In this project the aim is to construct new effective FEM algorithms that includes both device physics and FEM methods and so this project is well suited for students with interests in either or both of these fields.