FFI

Master projects in Semiconductor Physics and Condensed Matter Theory 2017/2018

Our research in the fields of Computational Materials Science and Computational Electronics is focused on fundamental photon, phonon and charge carrier interactions in solid state materials and on development of new numerical simulation methods and software. Application targets are current and future electronic devices including infrared photodiodes, resonant tunneling diodes, solar cells, light emitting diodes, quantum cascade lasers, Thz sources, infrared quantum well and quantum dot detectors and lasers, Field Effect Transistors (FETs) for power electronics, RF microwave, and FinFETS for processor electronics.

Some of the projects listed below are focused on studying and describing various carrier interaction processes. Here, pen, paper and basic physical knowledge will be the main tool. Others are more 'hands on' and devoted to the study of specific devices, while the last 3 projects require good skills in numerical physics. Familiarity with Linux environments is preferable, but not mandatory.

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, or have own ideas for a project, please feel free to send us an email with your CV and a few words describing your research interests.

Contact:

Trond Brudevoll

Tel. 63 80 73 00

trond.brudevoll@ffi.no

Asta Storebø

Tel. 63 80 72 94

asta-katrine.storebo@ffi.no

PHYSICS AND APPLIED PHYSICS:

Project 1

Modelling Strategies for Quantum Cascade Lasers

Quantum cascade lasers have become important components in military platform defense systems and they are also used as sources for laser spectroscopy. These unipolar semiconductor lasers now cover a wide range of the infrared and terahertz spectrum. Lasing is achieved via optical intersubband transitions between quantized states in multiple-quantum-well heterostructures. Improvement of their performance with respect to operating

temperature, efficiency, and spectral range requires detailed modeling of all physical processes involved. As their diversified physics is also paralleled in other nanostructured semiconductor systems, quantum cascade lasers have become a veritable ‘melting pot’ for the development and improvement of simulation techniques in nano- and optoelectronics. Other devices involving similar physics include, to name a few; Field Effect Transistors, Resonant Tunneling Diodes, and Quantum Dot Infrared Photodetectors (QDIPS).

Modeling of carrier transport in the nanostructured gain medium and simulation of the optical cavity is manly to be carried out with adaptations of existing in-house numeric codes. Transfer matrix and finite difference or finite element methods for solving the Schrödinger equation and Schrödinger-Poisson systems will provide the quantized states in the multiple-quantum-well active region. Modeling of the optical cavity is carried out using basic waveguide resonator theory.

Simulation methods include empirical rate equation and related Maxwell-Bloch equation approaches, self-consistent rate equation and ensemble Monte Carlo (MC) methods, as well as quantum transport theories, in particular the density matrix and non-equilibrium Green’s function formalism. In the simplest cases, derived scattering rates and self-energies will generally be valid for n-type devices based on one-dimensional quantum confinement, such as quantum well structures.

Candidates interested in this project should have a keen interest in theoretical physics and some familiarity with Greens Function techniques applied to solid state manybody problems.

Project 2

Higher Order Quantum Processes

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 carrier populations 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 and strong interactions. Transitions within ions placed in a crystalline or glassy host rely on similar theories. However, ordinary thermal generation, for example, requires the energy of many phonons/photons to excite a charge carrier and is a slow and intricate process.

Other mechanisms, like Auger recombination, can also be fast, but 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%.

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.

Photon and phonon assisted tunneling can occur between superconductors, in quantum dot systems but also as band to band tunneling in semiconductors. Band to band tunneling may also occur as a result of closely spaced bands and requires specialized approaches when describing transport.

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.

We have developed software for calculating some of the mechanisms. The project will consist of further development of this software, based on first principles band electronic structure codes with main emphasis on one or more of the following mechanisms: Laser transitions in rare earth systems, Auger recombination, impact ionization, phonon and photon assisted tunneling and generic carrier-carrier scattering.

Project 3

Monte Carlo Simulation of Quantized Semiconductor Structures

The project aims to develop and integrate specific quantum correction algorithms into an existing semi-classical MC computer code that will enable it to be used in the study of devices with active regions smaller than 15 nm.

We shall deal 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, so that the low energy charge carriers may 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 15 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.

The project shall work out a set of algorithms that can treat the device physics for medium and small structures in a unified manner.

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 lead 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 wavefunction 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 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 packages.

Students interested in this project will work with first principles electronic structure codes and develop adaptations of these codes to MC simulation, emphasizing the main scattering mechanisms.

Project 5

Disordered Semiconductor Materials

In this project we shall study methods for dealing with materials having a certain degree of disorder.

Electronic energy eigenstates of periodic solids are usually represented by Bloch waves with a wave vector **k** describing the translational periodicity of a given state. Existence of a sharply defined wave vector in periodic structures determines their optical and transport properties which are manifested as selection rules for inter- and intraband transitions.

However, the ideal translational periodicity of technologically important solids is often (willingly) disturbed by disorder and defects, and there can be fluctuations of the chemical composition in compound alloys, as well as magnetic disorder or even the lack of long-range order in non-crystalline solids. Disorder can significantly alter the electronic properties of solids resulting either in new, wanted properties or in unwanted side effects in a device. For example, electronic states associated with substitutional impurities can facilitate optical transitions in otherwise indirect gap semiconductors.

Modeling of disordered structures requires construction of supercells greatly exceeding the size of the primitive basis cell. In **k**-space, Brillouin zones associated with a supercell are much smaller than the corresponding Brillouin zones of the primitive basis cell. Although downsized in **k**-space, the small Brillouin zone of the supercell apparently contains more bands than the larger Brillouin zone of the primitive cell. If the primitive cell and the supercell both describe the same material, we can say that the few bands of the primitive Brillouin zone have been “folded into” the smaller Brillouin zone of the supercell. As a result of the

zone folding associated with the supercell, recovery of a dispersion relation E(**k**) into the original primitive cell Brillouin zone becomes difficult. What is needed is a systematic way to "unfold" the supercell bands into the larger primitive cell Brillouin zone, thus making a link between the two. Within the supercell there is now further room for breaking the original symmetry by introducing various defects and disorder, thus weakening this link.

Linking the supercell band structure with the primitive basis cell relies on defining a Bloch spectral density or "spectral weight" which is normalized to 1 and represented as a delta function for crystalline materials. In supercells with a broken symmetry, the properties of a given energy eigenstate are characterized by a broadening of the spectral weight. For fully localized states, the uncertainty in the **k**-vector approaches a fundamental limit which is determined by a certain localization radius.

Spectral weights for local basis functions can be obtained by a Fourier transformation of the relevant atomic orbitals. With non-local basis sets, such as plane waves, spectral weights can be extracted from the Fourier expansion coefficients by collecting them in groups associated with a particular Bloch wave vector. This is the most direct route for implementation in solid-state *ab initio* electronic structure codes, as the plane wave expansion coefficients are readily available in pseudopotential or full-potential packages.

Basis for the project will be an existing Monte Carlo transport simulator which already uses band structures generated from atomistic *ab-initio* codes. Challenges will be to investigate how these zone folding techniques might be introduced into the description of electronic transport in semiconductor alloys.

Project 6

Detection of weak signals in Infrared Photodetectors

Avalanche photodiodes (APD's) have a considerable range of applications, serving as key components in fiber optic and quantum cryptographic communication systems, in nuclear instrumentation and medical imaging detectors, as well as in several broader areas including defense and space systems, night-vision devices and as imaging detectors for LADARs.

Although the basic operating principles of such diodes have been largely unchanged for many decades now, the recent attention drawn to these diodes is certainly not undeserved, not only because of their impressing performance, but also because of the many physical effects contributing to their inner workings. HgCdTe (MCT) electron initiated APD (e-APD) provide the best performance as they are characterized by high sensitivity and gain combined with low multiplication noise. In particular, the high performance of the HgCdTe (MCT) electron initiated APD's (e-APD's) in the infrared region make them almost ideal for many purposes.

In addition to the study of the physical processes that make the devices work, the project will pay special attention to the case of detecting weak signals with few incoming photons in a large device. Usually photodetectors in the infrared region are made very wide because the long wavelength dictates a large diffraction limited radiation spot in the focal plane. Furthermore, poor absorption due to the band structure of low-gap materials requires a deep absorption region. Describing both the avalanche charge multiplication in full detail and the various collective, ambipolar and screening behaviors of 'passive' background carriers in these large devices requires quite special methods to retrieve the small fluctuations that constitute the signal. Recent developments in such methods will be the main focus of the project.

NUMERICAL PHYSICS:

Project 1

3D FEM and FD Poisson Solvers

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

If the particle picture is used in the modeling of the charge carriers in a Monte Carlo (MC) simulator, the basic timestep must be chosen sufficiently small so that all scatterings of the particles are fully 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 version 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 are usually introduced as material parameters change when excess electronic charge is injected electronically or optically.

Finite Element Solvers (FEM) are very flexible due to their unstructured grids 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 introducing new 3D FEM and FD Solvers adaptable to our development of a Full Band MC code, but it is also a requirement that the solvers can operate as generic stand-alone software which can serve as a basis for dealing with more complex problems at a later stage.

Project 2

Wave Propagation Solvers

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.

Project 3

Coupled Nonlinear Equations and Multiscale Simulation

In the simulation of physical processes there are often different timescales and length scales involved. To obtain an efficient simulation, this would normally require very specialized methods at each scale. With the advent of powerful parallel computing however, it is possible to do calculations that consider different scales simultaneously. For the present project in the field of semiconductors, we shall try to reconcile particle based Monte Carlo (MC) simulation which normally and ideally operates at timescales up to some hundred ps and length scales from 10 nm up to 10 µm with a continuum model represented by the nonlinear Hydrodynamic semiconductor equations which can operate at larger length scales, albeit with less detail.

The present MC model involves the use of a specialized atomic model for providing the material properties; then there is a jump in scale up to the 10 nm – 10 um level where the inclusion of a continuum model is required to replace the particle model. To reconcile these two latter scales, solving coupled transport equations is necessary. Other equations, like Maxwells equations or the Poisson equation can be transferred more fluently, and does not pose this scaling problem. This project is currently of great interest for ongoing research into solar cells and future infrared detector technology.