FFI

Master projects in Semiconductor Physics and Condensed Matter Theory 2016/2017

Our research in the fields of Computational Materials Science and Computational Electronics is focused on fundamental photon, phonon and charge carrier interactions in semiconductors 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 (QWIPs) and quantum dot detectors (QDIPs) and lasers, Field Effect Transistors (FETs) for power electronics, RF microwave, and FinFETS for processor electronics.

Many of the projects listed below are focused on studying and describing various carrier interaction processes. Here, pen, paper and mathematics 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 mathematics. 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, please feel free to send us an email with your CV and a few words describing your research interests.

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PHYSICS AND APPLIED PHYSICS:

Project 1

Manybody Techniques for Small Scales and High Fields

Current Field Effect transistor technology operates with a feature length of 14 nm. At scales below 15 nm we enter a region where the quantum nature of carriers will strongly influence carrier transport. For a proper description we must therefore use appropriate theoretical methods. Finding the best way of solving such problems has been a major achievement over the last decades, and the area is still rapidly progressing.

The project includes work on a new quantum transport simulator that involves both a representation of the energy bands and electronic states of the charge carriers and the description of major processes involved in the transport.

The candidate interested in this kind of 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 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 carrier population in the valence and conduction bands reaches 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, require the energy of many photons to excite a charge carrier and is a slow, but actually very intricate 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%.

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.

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 also based on first principles band structure codes with main emphasis on one or two of the following mechanisms: 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 quantum correction algorithms into an existing MC computer code that enables study of devices with active regions smaller than 15 nm. The range of applications is similar to those in Project 1, but the methods are different, less specialized and not limited to nanostructures only.

We 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 generic set of algorithms that can treat device physics for both small and medium scale structures.

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 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 first principles electronic structure codes and develop adaptations of these codes to MC transport simulation.

Project 5

Field Effect Transistors

Field effect transistors (FETs) used in microprocessors have a complex geometry around the gate electrode. In the FinFET layout, a finned gate electrode is used for controlling the channel current. Whereas the electric field configuration in older transistors were essentially 2D and the charge carrier transport was in 3D, modern FinFETs invariably require that the electric field is calculated using 3D Poisson solvers.

Future transistors will be further scaled down, and it is expected that the active current leading channel will consist of more or less genuine 2D materials. The 2D conducting material can be either inorganic (MOS_2) or organic (e g graphene, small molecules such as rubrene, or polymers such as poly(3-hexylthiophene) (P3HT)). Electron withdrawing or donating groups can be attached thus facilitating hole or electron transport, but most OFETS are based on p-type conductivity. The n-type OFETs are yet poorly developed and are usually based on perylenediimides, fullerenes or their derivatives, and show electron mobilities below 2 $cm^2/(V \cdot s)$. Rubrene-based p-type OFETs have the highest carrier mobility at around 20–40 $cm^2/(V \cdot s)$.The mode of conduction in organic transistors is usually hopping conductivity, but band-like conduction is possible.

For nanoscale inorganic MoS_2 transistors the study of contact-dependent behaviors is still at an early stage. Here, the type of contacts and their quality can significantly affect the performance.

The project will investigate various alternatives for 2D channel materials, but the main focus will be on developing software with the necessary functionality for different classes of materials and explore how the available simulation methods can be applied at the smaller scales.

Project 6

Solar Cells

In this project one of the major challenges will be to adapt methods originally intended for micro and nanostructured systems to devices that may have much larger dimensions. Solar cells can basically be divided into two very different subtypes:

Organic: Not all aspects of generation, transport and extraction of charge carriers in polymer photovoltaic devices are well understood. Basically, the cell has layers of organic polymer materials acting as donors and acceptors, e g poly(3-hexylthiophene) (P3HT) as donor polymer with [6,6]-phenyl-C61 butyric acid methyl ester (PCBM) serving as acceptor material. Incident light is absorbed in the organic materials and leads to the generation of strongly bound excitons. These excitons separate at a donor-acceptor interface into electrons and holes, and the charges drift to the electrodes under the influence of an internal electric field. Photogenerated electrons and holes basically move by hopping conduction.

Semiconductor: These solar cells have more conventional charge carrier conducting processes with electrons and holes.

Basis for the simulation of both types of cells will be an existing Monte Carlo transport simulation code. Challenges will be to introduce hopping condition into the code and adapt the existing Poisson solver software to boundary conditions suitable for photovoltaic operation.

Combining MC and larger scale transport methods is a prominent issue both for organic and inorganic types, and can be included as a part of the project. Wave propagation in these structures can also be addressed.

Project 7

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 APDs (e-APDs) 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 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 subject matter of detecting weak signals with few incoming photons in a large device. Usually photodetectors in the infrared region are made very wide because of the 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 and the behavior of background carriers

in the resulting large device requires quite special methods to retrieve the small fluctuations that constitute the signal. We have just begun to explore and develop methods that address this question, and the much of the project will therefore be devoted to these kinds of activities.

NUMERICAL MATHEMATICS:

Project 1

FEM and FMM Poisson Solvers for Monte Carlo Transport Simulators

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 perfect 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.

“Gridless” solvers such as the FMM (Fast Multipole Moment Method) can be used in some special cases where computational speed is more important than accuracy, and the project should therefore do an introductory study testing this method.

The project focuses on introducing new FEM and FMM 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 other 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 becomes important to explore the possibilities of doing 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 Hydrodynamic 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.