DFT and MD simulations of oxygen migration and domain walls

Motivation:
Domain walls exhibit a wide variety of interesting physical phenomena. Recently, the colleagues at Materials Science (IMA) have investigated domain walls in manganese oxides where oxygen migration towards the interface appears to play a crucial role, see the figure below.

The density functional theory (DFT) of electronic structure provides a powerful method to calculate materials properties at the atomistic level. Here, we are interested in coupling DFT with molecular dynamics (MD) as we aim to investigate the atomic motion of oxygen defects while moving across the sample towards the domain wall.

What the student will do in the project:
The student will study profoundly the DFT and MD methodology. Firstly, he/she will perform benchmark DFT simulations for crystalline manganese oxides and domain walls with different DFT approximations (exchange correlation functionals). Secondly, the student will carry out simulations for oxygen migration by modelling the oxygen migration paths based on static simulations (nudged elastic band method) and molecular dynamics algorithms with an external history-dependent bias at different temperatures (“metadynamics”). The DFT simulations will be performed on local supercomputers using existing codes (VASP and CP2K). The generation of model geometries with domain wall interfaces and analysis of results will require using modelling tools and/or scripts. Input to the simulations will come from close experimental collaboration with other researchers and students working in the Department of Materials Science (IMA).

Required from the student:
Background in materials physics (solid state physics), and interest in materials science will be an advantage. We need a student interested in modelling and programming, and working independently in a larger group of scientists. An interest in using and developing simulation tools is required. Experience with C++ or Python is essential. Previous knowledge with the basics of DFT will provide a good starting point for further learning.

Other aspects:
This topic is a collaboration with the Department of Materials Science (IMA). As part of the DFT training, the student may visit theory collaborators in the Tampere University of Technology and Aalto University (Finland). We shall also consider ways to incorporate machine learning as part of the simulations.

Contact persons: Jaakko Akola, Dennis Meier (IMA), and Sverre Magnus Selbach (IMA)

Figure: Experimental images of the corresponding domain walls (from IMA).
DFT simulations of precipitate formation in titanium alloys

**Motivation:**
For metal alloys there are challenges when it comes to establishing relations between the nanostructure and the mechanical properties, as for example strength and ductility. *Titanium has interesting alloys with a broad use - in aerospace, medical, marine, chemical processing and sport industries.* The crystal structure of titanium at ambient temperature and pressure is close-packed hexagonal (α). At about 890°C, titanium undergoes an allotropic transformation to a body-centered cubic β phase, which remains stable to the melting temperature. alloying elements can be categorized according to their effect on the stability of the α or β phase. Most alloys are α + β alloys, and have high-strength and formability. A common alloy, called ‘the work horse of Ti alloys’, is the *Titanium Grade 5,* - this is alloyed with 6% Aluminum and 4% Vanadium and known as Ti 6Al-4V. Here aluminum is an α-stabilizer and Vanadium is a β-stabilizer, allowing substantial amounts of β to be retained on quenching from the β → β + α phase fields. During additive manufacturing the metal experience cyclic cooling and reheating which strongly affect the phases formed.

The goal of our group is to develop a computational platform for studying metal alloys at atomistic level and with high accuracy (DFT level) which will enable efficient simulations and investigations of different intermetallic compositions. The proposed MSc work on titanium alloys is part of this larger scheme.

**What the student will do in the project:**
The student will perform benchmark DFT simulations for Ti-based alloys and the resulting data will be used by machine-learning algorithms to obtain a Cluster Expansion (CE) model for interatomic interactions. In addition, the student will perform migration path mapping (by DFT) for selected atomic transitions. The obtained information (energetics, migration barriers) will be fed into kinetic Monte Carlo (KMC) simulations. The DFT simulations will be performed on local supercomputers using an existing code (GPAW). Input to the simulations will come from close collaboration with other researchers and students working experimentally with transmission electron microscopy at NTNU.

**Required from the student:**
Background in materials physics (solid state physics), and interest in materials science will be an advantage. We need a student interested in modelling and programming, and working independently in a larger group of scientists. An interest in using and developing simulation tools is required. Experience with C++ or Python is essential. Previous knowledge with the basics of DFT will provide a good starting point for further learning.

**Other aspects:**
There are several people working on titanium alloys at NTNU, and we have an ongoing external project with Norsk Titanium. As part of the DFT training, the student may visit theory collaborators in the Tampere University of Technology and Aalto University (Finland). We shall also consider ways to incorporate machine learning as part of the simulations.

**Contact persons:** Jaakko Akola, Randi Holmestad, Jesper Friis (SINTEF)
DFT simulations of the inoculation effect in cast iron

Motivation:
For metal alloys there are challenges when it comes to establishing relations between the nanostructure and the mechanical properties, as for example strength and ductility. In cast iron, the presence of carbon and its segregation into graphitic layers affects the overall morphology and mechanical properties of the end product. Inoculation is a way of controlling the structure and properties of cast iron by minimizing undercooling and increasing the number of graphite nodules during solidification. An inoculant is a material added to the liquid iron just prior to casting that will provide a suitable phase for nucleation of graphite nodules during the subsequent cooling. We wish to investigate the interplay between carbon and several other additive elements within the iron host material, such as Mg, Si, Ca, Al, O and S. Their presence or absence will define the microstructure in the final cast iron material, see figures below.

The goal of our group is to develop a computational platform for studying metal alloys at atomistic level and with high accuracy (DFT level) which will enable efficient simulations and investigations of different intermetallic compositions. The proposed MSc work on cast iron is part of this larger scheme.

What the student will do in the project:
The student will perform benchmark DFT simulations for Fe-based alloys which will be used for training the Cluster Expansion (CE) method for interatomic interactions. In addition, the student will perform migration path mapping (by DFT) for selected atomic transitions. The obtained information (energetics, migration barriers) will be fed into kinetic Monte Carlo (KMC) simulations. The DFT simulations will be performed on local supercomputers using an existing code (GPAW). Input to the simulations will come from close collaboration with the researchers at Elkem Foundry Productions.

Required from the student:
Background in materials physics (solid state physics), and interest in materials science will be an advantage. We need a student interested in modelling and programming, and working independently in a larger group of scientists. An interest in using and developing simulation tools is required. Experience with C++ or Python is essential. Previous knowledge with the basics of DFT will provide a good starting point for further learning.

Other aspects:
This topic is a collaboration with the Elkem Foundry Products. As part of the DFT training, the student may visit theory collaborators in the Tampere University of Technology and Aalto University (Finland). We shall also consider ways to incorporate machine learning as part of the simulations.

Contact persons: Jaakko Akola, Leander Michels (Elkem)

Ductile Iron: Mg treated and inoculated with Si, Ca, Al and Ce showing graphite nodules.

Gray Iron: no Mg treatment but inoculated with Si, Ca, Al showing a flake graphite structure.
Spintronics (spin+electronics) is the science of using spin of electrons instead of their charge. Two main challenges of spintronics are manipulation of spins and long-range spin transport. The bit of data (0’s and 1’s) could be encoded in the spin degree of freedom. Finding efficient ways to write the data (i.e. switching the direction of spins) and read-out of the data (i.e. detecting the spin direction) are vital for designing novel information storages and processors. So far, several methods have been proposed and successfully experimentally realized for manipulation of magnetization direction such as applying magnetic fields, spin-currents, spin-orbit torques and spin waves.

The ultimate goal is to design devices which work faster, dissipate lesser energy, and are smaller in size.

In the centre for quantum spintronics (QuSpin), our focus is on the study of different magnetic materials and exotic magnetic textures such as topological domain-walls, skyrmions, etc. We are also interested in heterostructures such as magnetic material/superconductor, magnetic material/heavy metal, etc. We investigate these systems both analytically (using either microscopic or phenomenological approaches) and numerically.

The aim of project is to offer a taste of research in one of the hot topics in condensed-matter physics and show how simple mathematical models, are able to describe the real and complex world.

**Pre-knowledge requirements:** Basic courses in solid-state physics, quantum mechanics and mathematics. Programming ability is an advantage.

**Supervisors:** Prof. Arne Brataas and Dr. Aireza Qaiumzadeh

For more information, contact Dr. Alireza Qaiumzadeh (alireza.qaiumzadeh@ntnu.no), office: E5-147.
Student Projects in Materials Physics – 2018/2019

Prof. Dag W. Breiby

All the projects outlined here can be suitably modified to be suitable as 15, 30 or 45 ECTS projects. Some of these projects may be co-supervised by Prof. Ragnvald Mathiesen, who is the other head of the X-ray Physics Group, and with whom the X-ray facilities are shared.

The projects suggested here are all closely linked to well-funded on-going research projects, ensuring that the MSc students will be part of an active and stimulating research environment with PhD students, postdocs and international collaboration. We regularly receive funding from industry, the Norwegian Research Council and other funding agencies. We are also closely connected with SFF PoreLab.

If you are interested in one or more of these projects, please contact Dag.Breiby@ntnu.no

Fall 2018: 1-3 project students welcome!

We expect that you –
- enjoy experimental work
- enjoy testing, refining and applying theoretical models
- enjoy (and are good at!) computer programming
- can work independently (yet under regular supervision)

Dag W. Breiby
PhD in physics at NTNU, 2003. Permanent staff at Dept. of Physics NTNU since 2007, full professor since 2013. Adjoint Prof. in microsystems at University College of Southeast Norway (USN).

Teaching: Solid State Physics, Materials Physics, Measurement and Characterization (MEA4000, at USN), General Physics, Optics.

1. Computational Microscopy

Considering that the fundamental design of standard light microscopes has not changed much since the first one was constructed about 400 years ago, it is quite refreshing that many research groups these days work actively on both miniaturization and how the performance can be radically improved when computers are employed as active elements in the imaging process. The last few years a computational revolution relating to the imaging process itself, i.e. not simply post-processing, has been taking place. This technology is promising for example for point-of-care healthcare diagnostics and wide field-of-view high-resolution screening.

Modern microscopy techniques rely heavily on computations, with keywords being compressed sensing, machine learning & artificial intelligence, tomography, and sub-diffraction-limit imaging. Our specialty in this field is that we are working mainly in the X-ray regime, which gives additional challenges, but also possibilities like non-destructive internal imaging. We are currently attacking these challenges from several directions, including instrumentation, visual-light test-rigs, high-performance computing (in collaboration with the Dept. of Computer Science (IDI)), synchrotron experiments, and simulation efforts.

X-ray imaging is a rapidly developing field, spurred by both experimental (e.g. improved coherence, better detectors) and theoretical developments (e.g. improved phase-retrieval algorithms). By exploiting different contrast mechanisms (absorption, phase-change, scattering), the resolution and contrast can be tailored and the dose reduced.
### 1.1 Fourier-ptychographic microscopy

*Fourier ptychography* [Zheng 2013, Tian 2014] is a microscopy technique based on a standard microscope where the traditional sample illumination has been replaced by a 2D array of partially coherent LED lamps, see figure. From each single LED, used one at a time, the light enters the sample with a unique direction. By taking one moderate-resolution exposure for each LED sequentially, one gets a set of images that can be used to reconstructed both the amplitude and the phase of the imaged object. In other words, one single high-resolution wide field-of-view (gigapixel) image is obtained after the numerical manipulations.

In this project you will
- Review & understand the physics of Fourier ptychography
- Implement Fourier ptychography on a standard light microscope (this includes construction, LED controller programming, and writing code for image synthesis).
- Optionally: Construct a microscopy extension including an *app* for your smartphone
- Optionally: Monitor the curing of paint or epoxy in collaboration with industry.

This project requires outstanding programming skills and an interest in photonics.

**Co-supervision:**
The project will be carried out in close collaboration with the University College of Southeast Norway, Prof. Muhammad Nadeem Akram [Muhammad.N.Akram@usn.no](mailto:Muhammad.N.Akram@usn.no)

**References:**
Tian et al, Biomedical Optics Express, 2014: [https://www.osapublishing.org/boe/abstract.cfm?uri=boe-5-7-2376](https://www.osapublishing.org/boe/abstract.cfm?uri=boe-5-7-2376)
See also this link, [http://cellscope.berkeley.edu/technology/](http://cellscope.berkeley.edu/technology/)
1.2 Numerical simulations of X-ray propagation

The scattering of electromagnetic radiation by spherical objects played an important role in the development of physics, with early highlights including Descartes’ understanding of the rainbow 400 years ago, Rayleigh scattering by small particles, and Mie’s exact solution to the scattering of a plane wave by a sphere. In this project, we will study X-ray scattering from densely (hexagonal) packed monolayers of absorbing spherical particles deposited on a multilayer thin film. The particles are of diameter $D \gg \lambda$, where $\lambda$ denotes the wavelength. X-rays typically have an index of refraction $n = 1 - \delta + i\beta$, with $\delta \sim 10^{-5} - 10^{-6}$ and $\beta \sim 10^{-6} - 10^{-8}$ for condensed matter, emphasizing the common knowledge that X-rays are highly penetrating.

We have already developed numerical software for solving the related problem of scattering from a single absorbing sphere under different approximation levels. Extending this software to include the case of scattering in reflection geometry is a first task. Secondly, for the case of 2D hexagonally packed layers of non-absorbing spheres, analytical solutions exist in the X-ray (short $\lambda$) regime. It is however a challenge to modify the software to deal with the 2D dense layer of absorbing spheres. Ultimately, the project aims at modeling experimental synchrotron data, and is thus of both theoretical and applied interest.

![Figure 1. Modeling the light scattering from a single spherical object.](image-url)

Project tasks:
1. Study the relevant models and approximations for light (and X-ray) scattering.
2. Implement an efficient computer program for calculating the reflected intensity distribution for a single sphere on a smooth surface
3a) Extend to the case of a hexagonally densely packed 2D layer of spheres, and/or
3b) Extend to the case of (spherical) core-shell structures
4. Verification towards existing analytical solutions for limiting cases.
5. Optional: apply machine learning to extract information about the scattering objects from the measured intensity distribution (inverse problem).

Co-supervision:
The project will be carried out in close collaboration with Prof. Alain Gibaud at Le Mans Université in France.
1.3 4D-CT and multiphase flow in porous media

Computed tomography (CT) retrieves 3D images from a series of projection images obtained at different sample orientations. For “dynamic” objects that change during the data acquisition, special precautions must be made to avoid reconstruction artefacts. A key example is patients moving during CT-measurements at hospitals. In other cases, as in this project, precisely the movements taking place within certain sub-volumes of an otherwise stationary sample are the point of interest. 4D-CT, or dynamic CT, aims at resolving in 3D structures that change with time. In collaboration with SFF PoreLab, we offer a project on multi-phase flow in porous media. More specifically, we will consider the drainage of a high-contrast fluid out of a well-defined static porous matrix. The project will involve some experimental work, but the demanding part of the project is to work on computer algorithms to exploit a priori information about the object under study. In this case, the a priori knowledge is that the synthetic porous material matrix will be fully static during the drainage. The scientific goal is to optimize the measurement strategy with respect to temporal and spatial resolution of the receding liquid/air interface. So-called Haines jumps and snap-off represent particular challenges in this regard.

The project requires strong computer programming skills and will be done in collaboration with partners at the Dept. of Computer Science and at SFF PoreLab. Several possibilities for extending the project exist, including machine learning.

1.4 Deep Learning object recognition in 3D image data (EXTERNAL)

This project deals with testing out methods based on «Machine Learning» that will teach a machine («robot») how to recognize and localize parts of a scene. This is particularly relevant for objects where a 3D-model of a rigid object cannot be used (e.g. for food, fish, or other objects that do not always look exactly the same). The project will be carried out in collaboration with Zivid Labs in Oslo (see www.zividlabs.com). The 3D data will be provided by Zivid, and the project will be based on openly available software (e.g. TensorFlow, Theano, Caffe, etc.).

The project requires strong computer programming skills, and some knowledge of artificial intelligence would be helpful.

Co-supervision:
The project will be carried out in close collaboration with Zivid Labs, by Dr. Øystein Skotheim.
2. Quantitative CT Study of Bone and Cartilage

Computed tomography (CT) is routinely applied to biological and medical samples, and of course patients, in the hospitals. We offer this project in collaboration with the Division of Biophysics and Medical Technology. CT will be used to study bone and cartilage. The aim is to better distinguish the hierarchical structures found in these materials by exploiting contrast differences in Dual Energy Computed Tomography (DECT) acquisitions, as described below.

The physics of CT can be described in short terms as follows: X-rays are passed through the sample, and are attenuated by the material. From a series of projection images based on beam attenuation, one can calculate the absorption properties for the 3D volume of the sample. For each voxel in the reconstructed volumes a linear attenuation coefficient $\mu$ is usually assigned. The attenuation is element specific, but it also varies with the material density and the photon energy. Distinction between elements can be made by using a tunable monochromatic X-ray energy. However, in most CT-scanners the “white” polychromatic beam is used to have a high flux and thus short exposure times. By combining information from CT scans obtained with different beam energy distributions (“Dual Energy CT”; DECT), the CT images can be interpreted quantitatively in terms of chemical composition and density.

![Figure. Micro-CT image of the bone-cartilage interface in a foal. Lateral trochlear ridge of tarsus, distal view. Tubular structures are barium-stained cartilage canals, found in the growth cartilage of young individuals (The cartilage itself is not visible).](image)

If the calcified cartilage, the cartilage canals and the bone can be distinguished by DECT, this can help to gain a better understanding of how calcification of cartilage canals (blood vessels in growth cartilage) is related to vascular failure and cartilage necrosis.

Tasks:
- Literature study of DECT: How does the technique work? What are the common reconstruction algorithms and how do they work? What are the limitations of the technique?
- DECT measurements on dummy samples. Quantitative modelling.
- DECT measurements of a bone/cartilage sample from a mammal, with critical data analysis in terms of resolution, contrast, time consumption and dose (relevant for future in vivo experiments).

Co-supervision:
Post doc Basab Chattopadhyay, email basab.chattopadhyay@ntnu.no
PhD student Fredrik K. Mürer, email fredrik.k.murer@ntnu.no
3. In-situ ultra-fast annealing

Organic photovoltaics is an emerging technology with the prospects of cheap, flexible and easy mass-production of solar cells. However, there are several challenging before reaching that goal, perhaps most fundamentally related to the chemical and morphological stability of the organic materials involved. It is a fact that different heat treatments of the polymer (“plastic”) materials gives solar cells with widely different performances. While the fundamental reasons for this behavior are gradually becoming clear, much remains to be done also in the microscopic studies of such materials.

In this project, you will be modifying our modular optical microscopy setup, and work on implementing flash heating and fast scanning calorimetry (FSC) for in situ studies of the morphology changes triggered by thermal annealing. Flash heating allows heating/cooling rates of $>10^4$ K s$^{-1}$ (!) for sufficiently small sample volumes.

![Figure 1. Example of electronic chip used for fast scanning calorimetry.](image)

Possible project tasks:
1. Optimize microscopy setup for video-rate imaging. Possible extensions: computational imaging by using structured illumination and scattering contrast.
2. Design and build a flash heating setup, including PID-control, compatible with future synchrotron experiments
3. Describe quantitatively the measured crystal growth of various polymer mixtures under different thermal annealing schemes.

Co-supervision:
Post doc Basab Chattopadhyay, email basab.chattopadhyay@ntnu.no
4. Project with SINTEF: CuttingEdge*

*Nanoscale Geophysics!* Understanding claystone shales ("skifer"), which are ubiquitous sedimentary capping rocks, is of high importance both to the oil industry and for future CO₂-storage. To evade the necessity of extracting expensive borehole core samples, SINTEF and our group have recently been granted the *CuttingEdge* project for developing nanoscale methods for understanding porosity and permeability in shale cuttings ("borkaks").

*Are you keen on saving the environment while employing state-of-the-art nanoscale methods?* The approach taken here will be to use focused ion beam microscopy (FIB-SEM) in NTNU NanoLab combined with in situ X-ray CT & diffraction measurements (mechanical and flow properties), atomic force microscopy (AFM) and nanomechanical indentation to understand shales. A key approach will be to do in situ studies of shale cuttings using CT to get 3D images for better understanding the complex chemo-mechanical reaction pathways.

Possible project tasks:
1. Acquire the necessary knowledge on shale mechanics.
2. Learn to use the CT machine, collect data. Reconstruction, segmentation of volumetric data, visualization, analysis.
3. Learn to use FIB-SEM.
4. Nanoscale-mechanics
5. Study the effects of CO₂ exposure on fractured cement

Special remark: *Excellent opportunity to write an environment-oriented project in close collaboration with Norwegian industry!*

Co-supervision:
The project will be carried out in close collaboration with SINTEF and Prof. Alain Gibaud at Le Mans University in France.

* Project funded by the Norwegian Research Council.
This project combines research from the fields of spintronics, material research and nanoscience. We will use molecular beam epitaxy (short: MBE – for a description see below) to develop a synthesis process for high quality antiferromagnetic materials. We will especially focus on the growth of copper pyrite, CuFeS$_2$. CuFeS$_2$ is an antiferromagnetic semiconductor with a very high Néel temperature $> 800$K and thus very interesting for investigations and applications in spintronics research. The research field of spintronics aims at using the spin degree of freedom for data storage and manipulation. Recently especially research into Antiferromagnetic materials has become a focus in this field since antiferromagnets have no magnetic stray fields and very high resonance frequencies in the THz regime. This makes these materials very interesting for data storage and manipulation at frequencies that are orders of magnitude higher than those used in present day electronics. Additionally, the absence of stray fields eliminates one of the key reasons limiting the minimum size and stability of present magnetic components. In this project, we will grow CuFeS$_2$ using MBE and investigate its properties using crystallographic methods (for example X-ray and TEM) and electronic transport studies.

**Molecular beam epitaxy** is a technique used for the growth of ultrapure crystals in the form of thin films or nanostructures (e.g. nanowires and quantum dots). The MBE growth technique aims at building up crystals atomic layer after atomic layer and thus enables the synthesis of very high quality single crystals. This is achieved by using ultra high vacuum chambers and evaporating materials at very low pressures in combination with precise temperature control of the crystal. The high amount of control on the crystalline properties, when using MBE, allows custom tailoring of many material properties down to the nano-level. Especially, the dimensionality, interface properties and strain state of a material can be controlled very precisely. MBE growth also enables the combination of materials into heterostructures and superlattices, where different materials can be stacked in thicknesses of a few nanometers or less, down to single atomic layers. In this way, the (quantum mechanical) properties of a material can be influenced to build materials with specific behavior or to access new physical phenomena.
Multifunctional nanoparticles and ultrasound to improve cancer therapy
Contact: Catharina Davies, Catharina.davies@ntnu.no
Web page https://www.ntnu.edu/physics/biophysmedtech/drugdel

Background: Ultrasound mediated delivery of NPs in tumour tissue

Nanotechnology has started a new era in engineering multifunctional nanoparticles (NPs) for improved cancer diagnosis and therapy, incorporating both contrast agents for imaging and therapeutics into so called theranostics NPs. Encapsulating the drugs into NPs improves the pharmacokinetics and reduces the systemic exposure due to the leaky capillaries in tumours. In most normal tissue the blood vessels are not leaky and the NPs are constrained to the blood, thereby reducing the toxicity to healthy tissue. Although the NP can extravasate from the blood to the extracellular matrix, the NPs do not to travel far away from the blood vessels. Thus, only a small population of cancer cells located close to the blood vessels will be exposed to the cytotoxic drugs as shown in the figure. A prerequisite for successful cancer therapy is that the therapeutic agents reach their targets and limit the exposure to normal tissue. To ensure high drug payload, the NPs have to be relatively large (100-200 nm) and therefore the NPs face severe problems reaching the target cells. The delivery depends on the vasculature, the transport across the capillary wall, through the extracellular matrix (ECM), and if the final target is intracellular the NPs also have to cross the cell membrane.

Although the NPs may pass the tumour capillaries rather easily, the uptake and distribution of NPs and the released drugs are low and heterogeneously distributed in the tumour tissue. The drug has to penetrate the ECM which consists of a protein network of collagen embedded in a gel of glycosaminoglycans and proteo-glycans.

In order to improve the distribution of NPs the delivery should be combined with a treatment facilitating the delivery. Ultrasound (US) has been reported to be able to improve drug delivery by different mechanical mechanisms, acoustic radiation force and cavitation. High frequency and highly focused US can induce acoustic radiation force pushing the NP across the capillary wall and through the ECM. Cavitation is the oscillation of gas filled microbubbles in the acoustic field. Such oscillations can be stable and generate mechanical shear stress on the capillary wall thereby increasing the vascular permeability or the microbubbles can collapse in a violent process generating jet streams that also increase the vascular permeability, improve the transport through the ECM and increase the cellular uptake of NP. The overall aim this project is to characterize NP and microbubbles to be used in therapy and study how ultrasound can be optimized to improve the delivery of distribution of NP in tumour tissue.

We are mainly working with two different microbubble concept. In collaboration with SINTEF Material and Chemistry, we study polymeric NPs forming a shell around a gas bubble. We hypothesise that having NP on the microbubble surface make this a very efficient platform for delivery of NP to tumors, and we have successfully shown that these NP-microbubbles can be used to treat tumors growing in
In collaboration with the company Phoenix Solution AS we study the concept of Acoustic Cluster therapy (ACT) which is a novel microtechnology drug delivery platform based on clusters of microbubbles and microdroplets. After intravenous injections, focused ultrasound is applied to the target tissue whereby the microbubbles transfer energy to the microdroplets, which undergo a gas-to-liquid phase shift. Growing in size, these large bubbles transiently block blood flow at the capillary level. Further exposure of ultrasound causes these large bubbles to oscillate and induce biomechanical effects enhancing the transport of drugs or nanoparticles across the capillary wall. We have successfully shown that this concept can be used to treat tumors growing in mice.

**Projects for the fall 2018 - spring 2019:**

1. **Mechanical properties of nanoparticles**
   Supervisors Catharina Davies [Catharina.davies@ntnu.no](mailto:Catharina.davies@ntnu.no), Astrid Bjørkøy [astrid.bjorkoy@ntnu.no](mailto:astrid.bjorkoy@ntnu.no)

   SINTEF material and Chemistry has developed a new polymeric nanoparticle which has the ability to form a shell around a gas bubble. We have successfully used this nanoparticle-microbubble to improve the delivery of nanoparticles to tumors in combination with focused ultrasound. The nanoparticles need to be further characterized to understand the effect of ultrasound on the nanoparticles. It is necessary to have knowledge about the mechanical properties of these nanoparticles, i.e., their elasticity/stiffness.
   **Aim:** Measure the elasticity/Young modulus of nanoparticles using atomic force microscopy.

2. **Distribution of nanoparticles in tumors exposed to focused ultrasound**
   Supervisors Catharina Davies [Catharina.davies@ntnu.no](mailto:Catharina.davies@ntnu.no), Andreas Åslund [andreas.aaslund@ntnu.no](mailto:andreas.aaslund@ntnu.no), Einar Sulheim [Einar.sulheim@ntnu.no](mailto:Einar.sulheim@ntnu.no), Marieke Olsman [marieke.olsman@ntnu.no](mailto:marieke.olsman@ntnu.no); Sofie Snipstad [sofie.snipstad@ntnu.no](mailto:sofie.snipstad@ntnu.no)

   Ultrasound increases the uptake of nanoparticles in tumor tissue and improves the distribution of nanoparticles throughout the tumor. We are optimizing the delivery of various nanoparticles using different ultrasound parameters. Tumors growing in mice have been exposed to ultrasound after injection of nanoparticles.
   **Aim:** Characterize quantitatively the uptake and distribution of various nanoparticles in frozen sections from tumors exposed to ultrasound. Confocal laser scanning microscopy will be used to image the frozen sections, and image analysis to quantitate the uptake and displacement of nanoparticles from blood vessels. Typical confocal laser scanning image is shown in figure 1.

3. **Use the chicken chorioallantoic membrane (CAM) model to study effect of ultrasound on nanoparticle behaviour in tumor tissue**
   Supervisors Catharina Davies [Catharina.davies@ntnu.no](mailto:Catharina.davies@ntnu.no), Andreas Åslund [andreas.aaslund@ntnu.no](mailto:andreas.aaslund@ntnu.no), Melina Mühlenpfordt [melina.muehlenpfordt@ntnu.no](mailto:melina.muehlenpfordt@ntnu.no)

   We have recently established the chicken embryo model to study tumor development and angiogenesis (vascularization). The model has the advantage of having functional blood vessels already 3 days after fertilization of the egg and the eggs can be grown in petri dish in an incubator (Figure 3). Tumor cells can be implanted into the CAM and used an ex vivo tumor model.
**Aim:** To use the CAM assay to study behaviour of microbubbles and nanoparticles during ultrasound exposure (SINTEF NP-Microbubbles and ACT-bubbles).

![Image of CAM assay](image)

**Fig. 3:** The figure depicts injection of the dye Evans blue into a CAM.

4. **Study behaviour of microbubbles using artificial blood vessels**  
Supervisors Catharina Davies [Catharina.davies@ntnu.no](mailto:Catharina.davies@ntnu.no); Melina Mühlenpfordt [melina.muhlenpfordt@ntnu.no](mailto:melina.muhlenpfordt@ntnu.no); Sofie Snipstad [sofie.snipstad@ntnu.no](mailto:sofie.snipstad@ntnu.no)

We have recently established microfluidics channels and coated them with endothelial cells thereby forming artificial blood vessels.  
**Aim:** We want to use this system to study the behavior of the various microbubble platforms we are using (SINTEF NP-Microbubbles and ACT-bubbles) under the exposure of ultrasound.
Coarse-grained modelling of nanoparticle-polymer interactions

Supervision: Assoc. Prof. Rita Dias (rita.dias@ntnu.no) and Ph.D. student Morten Stornes (morten.stornes@ntnu.no)

Systems comprising of nanoparticles (NPs) and oppositely charged polyelectrolytes are common components in formulations used in food, pharmaceutics and drug delivery. In such applications, the presence of polymer chains that bridge two or more NPs can induce the aggregation of the NPs and consequent destabilization of the formulations.

Within the class of charged polymers, weak polyelectrolytes present very interesting properties. Their charge can be tuned by variations in pH resulting in systems that can, in principle, respond to such external stimulus.

In this work we study systematically the effect of charge mobility (quenched vs. annealed) on the adsorption of polyacids (PAs) to NPs, also possessing titratable surface charge groups. Novel data analyses will be implemented throughout the project for evaluating complex system involving many NPs and chains.

Students that have worked or are currently working in this project:
Binamra Shrestha, MSPHYS
Development of novel methodologies to quantify turgor pressure levels in plant cells

Supervision: Assoc. Prof. Rita Dias (rita.dias@ntnu.no) and Assoc. Prof. Thorsten Hamann (Department of Biology, thorsten.hamann@ntnu.no)

All plant cells are surrounded by cell walls. They form an exoskeleton that provides protection from the environment and support during growth and development. At the same time the (turgor) pressure in a plant cell is similar to the one in a car tire and is contained by the cell wall. By coordinating turgor pressure and cell wall composition / structure the plant cell regulates cell morphogenesis during development.

Recent novel unpublished data from our research group has shown that turgor pressure seems to also coordinate cell wall formation with cell cycle activity. The available evidence suggests that turgor pressure has a very important function in different biological processes and could be very dynamic. However the problem is that no methods exist to quantify turgor pressure levels in plant cells in vivo, non-invasively.

This project aims to develop novel methods to detect changes in turgor pressure and quantify their extent during development. The work will involve different wet lab activities like tissue culture, use of fluorescent reporters, confocal laser scanning microscopy, and/or molecular dynamic computer modelling.

Literature:


Students that have worked or are currently working in this project:

Eskil Nodeland Indregard, MSPHYS
Nanoparticles for tissue nanobridging and wound healing

Supervision: Assoc. Prof. Rita Dias (phone: 73593422, rita.dias@ntnu.no), Co-supervision: Assoc. Prof. Maria Benelmekki, IMA and Assoc. Prof. Brita Pukstad, IKOM/St. Olav Hosp.

Tissue gluing driven by nanoparticles (NPs) has enormous application potential. This concept relies on the fact that the macromolecules in the biological tissue form multiple interaction points with the NPs that serve as a nanobriges between the tissues, and has been used to efficiently heal wounds in mice, showing a healing process that was equivalent to sutures and better than Dermabond, a glue using in medicine [1].

Preliminary results conducted in our labs using equivalent NPs to glue a wound in an in vitro human skin model were, on the other hand, disappointing: the applied NP solutions did not bridge the tissue. Differences in morphology between the skin of rats and humans could explain this result. Keeping in mind the enormous potential of NP-induced tissue gluing, the aim of the project is to design hybrid nanostructured particles for tissue bridging and wound healing applications.

Different types of NPs will be synthesized, characterized, and tested regarding tissue adhesion. NPs presenting good adhesion will additionally be screened according to their cytotoxicity and biocompatibility. To assess NP-driven nanobridging and healing of human skin, the in vitro human skin model will be standardized towards deep wounds and used to assess the healing abilities of a wound in the presence of NPs.

We are also interested in the molecular aspects of the nanobridging, such as strength of the interaction, diffusion of nanoparticles from the complex interface, and macromolecule diffusion across the interface. For this we will also use gels to mimic tissue, and use confocal microscopy, atomic force microscopy, and tensile and adhesion tests.

In addition, we would like to implement coarse-grained gel-gel systems and study the interaction of NP with the gel polymers and NP diffusion into the gels using computer modelling.


Students that have worked or are currently working in this project:

Nicholas Christiansen, MTFYMA
Christian Sundby, MTFYMA
Corinna Dannert, MSPHYS
**Synergistic effects in DNA condensation**

Supervision: Assoc. Prof. Rita Dias (phone: 73593422, rita.dias@ntnu.no)

The genome of E. coli has about 6.4 million base pairs, corresponding to a circumference of 1.6 mm. In order to fit inside the small volume of the cell (ca. 0.65 μm³), the DNA needs to be folded. In eukaryotic (e.g. humans), DNA condensation is done by proteins called histones. This type of proteins does not exist in bacteria. Instead, there are a few different types of proteins, such as H-NS proteins, that modulate the genome. In addition, and contrary to eukaryotic cells, bacteria have no nuclear membrane, and the fact that the cytoplasm has a very large number of macromolecules (RNA and proteins) is believed to help DNA condensation, by the so-called molecular crowding effect.

Despite the extensive study in this area during the past years, the mechanistic details and their relative contribution to DNA condensation is still unclear.

In this project we assess the characteristics of the crowding environment (charge and topology) on DNA condensation and protection towards DNase digestion. In addition we look at how crowding affect the binding of small molecules that mimic proteins to DNA.

We use a range of biophysical techniques, including fluorescence spectroscopy, fluorescent correlation spectroscopy, and gel electrophoresis, to evaluate the binding of various DNA binding agents in the presence of crowding agents to DNA and DNA condensation. Coarse-grained molecular modeling, using simple model systems can also be explored.

**DNA foot printing assay.** Left-hand side: Agarose gel electrophoresis of linear DNA with increasing H-NS concentrations in the absence and presence of PEG. Right-hand side: same samples as in the first gel but now in the presence of NdeI, a restriction enzyme for AT-rich regions. We can see that sufficiently large concentrations of H-NS hinder the DNA digestion, and that the presence of PEG lowers the concentration of H-NS needed to protect DNA towards enzyme activity. Experiments and figure by Sravani Keerthi Ramisetty (PhD student)

Students that have worked or are currently working in this project:

Šárka Sovová, Master student from Brno University of Technology, Czech Republic

Lars Martin Furunes, MTFYMA
PROJECT/MASTER PROJECTS 2018 IN LABORATORY FOR SOFT AND COMPLEX MATTER STUDIES

The Laboratory of Soft and Complex Matter Studies has a focus on natural materials (clay, cellulose, carbon, iron-oxide etc.), their properties and functionalities (like structural, optical, electronic), the fundamentals of soft matter (colloids and particle-particle interactions), active matter, and cross disciplinary topics (such as medical drug release, CO₂ capture). Depending on the studied problem, our work includes everything from hands-on work with simple experiments using in-house equipment to top-end experiments at international synchrotron radiation facilities. The project descriptions below are aimed at both 5-year and 2-year Master students, of physics, chemistry, materials science, nano-technology, or bio-physics.
PROJECT 1:
STRUCTURAL COLOURS – MAKING COLOUR WITHOUT PIGMENTS

Motivation
Nature can produce various wonderful physical colours without use of chemical pigments, as we can see when looking at butterflies, birds, beetles, reptiles or bacteria. How is it possible that no dye is needed to make such a nice effect? Periodic structures on the surface can cause constructive or destructive interference of incoming light and as a result, colour perception with no dye included is observed. One motivation of the current project is to go beyond the traditional ways of making colours, and use structure of surface itself to reflect light with desired wavelength.

Left: Butterfly. Middle: Mesoporous SiO$_2$ film reflecting in red. Right: Polystyrene-clay layer reflecting in green.

Role of the student in the project
The Master student will focus on preparation of the structural colour samples. The actual work will depend on the student’s interest and preferences. Materials used for sample preparation can be polystyrene and glass nanobeads, single layer clay sheets, cellulose, carbon black particles and their combination. Projects involve making the extended colour palette using monodispersed polystyrene or glass nanobeads and clay, preparing mesoporous glass films combined with cellulose and/or clay, changing colour tone selected structural colour sample, preparation of multilayered structures combining effect of structural colour and multi-layer reflectivity or others. The Master students will work on their own specific projects in the NTNU home lab and in case of interest, participate on experimental work performed on synchrotron facilities and laboratories of collaborating partners.

Requirements
Interest in science and experimental work. Background in the soft matter, condensed matter, material physics or chemistry is of high advantage. Ability to work independently under the supervision and in the larger experimental group.

Other aspects
There are several ongoing projects in the lab. Students can participate in the experiments carried at the synchrotron/neutron facilities and experiments in external collaborating laboratories (NOVA University Lisboa, Portugal or Univ. Cambridge, UK).

Contact person(s)
For further details of project description, please contact Ana Trindade (ana.c.trindade@ntnu.no), Ville Liljeström (ville.v.liljestrom@gmail.com) or Jon Otto Fossum (jon.fossum@ntnu.no).
PROJECT 2:
GRAPHENE-CLAY HETEROSTRUCTURES

Motivation
Two dimensional (2D) structures belong to the new class of materials exhibiting completely new and exciting physical properties. With this class of materials, we have the experimental access to phenomena that were either just predicted theoretically or their existence was even not postulated before. Inspired by the variety of studied 2D (semi)-conductors and insulators, we work on 2D systems based on layered silicates and graphene, with the focus on their potential use in electronics.

Role of the student in the project
The Master student will study different types of 2D materials and heterostructures, with focus on preparation and selected characterizations. The actual work will depend on the student’s interest and preferences. Possible projects involve preparation and characterization of mechanically exfoliated single sheets of natural or synthetic clays; development of various methods for conversion of graphene oxide to graphene and/or investigation of its structure and electrical transport properties; preparation and selected characterizations of multi-layered structures of graphene and clay; development of methods for preparation of macroscopic layers with desired functionality, combining clay and graphene and others. Master student will work on its own specific project in the home NTNU lab and in case of interest, participate on experimental work performed on synchrotron facilities and laboratories of collaborating partners. Master work is related to the project Graphene-Clay systems.

Requirements
Interest in science and experimental work. Background in the condensed matter physics is of high advantage. Ability to work independently under the supervision and in the larger experimental group.

Other aspects
There are several ongoing projects in the lab. Students can participate in the experiments carried at the synchrotron/neutron facilities and experiments in external collaborating laboratories (Univ. Manchester, UK; Chalmers University, Sweden; Univ. Bayreuth, Germany).

Contact person(s)
For further details of project description, please contact Barbara Pacakova (barbara.pacakova@ntnu.no), Paulo Brito (paulo.h.m.brito@ntnu.no) or Jon Otto Fossum (jon.fossum@ntnu.no).
PROJECT 3: NANOFLUID EMULSIONS

Motivation

Nanofluids are fluids that contain one or multiple nanosized components such as metal, polymer, or mineral nanoparticles. Colloidal nanoparticles can be used to modulate the carrier fluid properties. Typical examples include improving the thermal or flow properties. Nanoparticles can also be used to stabilize emulsion drops (Pickering emulsions). In a complex material such as the three-phase system of water-oil-clay particles, the water-oil interface will additionally take part in the governing of the self-assembly, since the particles will be trapped by capillary forces and confined in a film at the liquid-liquid interface, as illustrated below. We focus on environmentally friendly nanoparticles. Such can be applied for example in medical applications, food industry, cosmetics, and improved oil recovery. The properties, distribution, and diffusion of nanoparticles within emulsions are studied in this project. The research utilizes microfluidics to produce uniform emulsions with controlled composition.

Schematic (not to scale) representation of clay particle structure on an oil drop in water, without salt (left), and with salt (right), respectively. For the system without salt, a repulsive “Wigner” colloidal glass is formed at the interface. For the system with salt, a particle network is formed at the interface, leading to a gel state. In the schematic representation, each thick line represents a Laponite clay nano-disk, while the ellipsoids around them represent the range of electrostatic repulsions. From A. Gholamipour-Shirazi, M. S. Carvalho, M. Huila, K. Araki, P. Dommersnes & J. O. Fossum SCIENTIFIC REPORTS BY NATURE 6, 37239 (2016)

Role of the student in the project

The student will carry out microfluidic experiments, which will be initially monitored using optical microscopy. The student will take part in the planning and design of the experiments. Further characterization of nanofluid emulsions can be carried out using X-ray scattering or rheometry. The student will work together and be instructed by a post-doctoral researcher or a doctoral candidate.

The project is in collaboration with international partners and the planned research allows for a shorter or longer stay (one week to several weeks) at a partner organization. The partner organizations in this project are the École supérieure de physique et de chimie industrielles (Paris), Pontifical Catholic University of Rio de Janeiro (Brazil), Chalmers (Sweden).

Requirements

Enthusiasm and curiosity about materials science and soft materials. Any knowledge in chemistry and experience in micro- or nanofabrication is considered a plus.

Other aspects/ or Supplementary specifications

The project can include travelling to international synchrotron facilities (voluntary).

Contact person(s)

For further details of project description, please contact Paul Dommersnes (paul.dommersnes@gmail.com), Ville Liljestrom (ville.v.liljestrom@gmail.com) or Jon Otto Fossum (jon.fossum@ntnu.no).
PROJECT 4: ELECTROHYDRODYNAMIC SELF-ASSEMBLY OF NANOPARTICLE STRUCTURES

Motivation
Nanoparticles, both synthetic and biological (e.g. proteins) can be viewed as functional building units. Recent studies show that such nanoparticles can be self-assembled into functional aggregates with a well-ordered structure. Also the macroscopic shape (submillimetre range) of such assemblies can be controlled. For practical application such materials need to be further manipulated, processed, and integrated into a device. This project focuses on understanding and controlling the electrostatic self-assembly of facetted multicomponent nanoparticle crystals, which can in a later stage be assembled into larger structures using external fields i.e. electrohydrodynamic self-assembly (EHD).

The relationship between the observed face centred cubic structure and the macroscopic crystal habit.


Role of the student in the project
The student will work hands-on with in-house equipment. The student will participate in most of the experiments included in the project. The project includes microfluidic experiments that will be initially observed with optical microscopy and eventually small-angle X-ray scattering (SAXS) will be used to analyze the resulting structures. The project is in collaboration with international partners and the planned research allows for a shorter or longer stay (one week to several weeks) at a partner organization. The partner organizations in this project are Aalto University (Finland), the École supérieure de physique et de chimie industrielles (Paris), Pontifical Catholic University of Rio de Janeiro (Brazil), Chalmers (Sweden).

Requirements
Enthusiasm and curiosity about materials science and soft materials. Any knowledge in chemistry and experience in micro- or nanofabrication is considered a plus.

Other aspects/ or Supplementary specifications
The project can include travelling to international synchrotron facilities (voluntary).

Contact person(s)
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PROJECT 5:
ACTIVE MATTER

Motivation
The objective is to investigate and model experimentally and theoretically how dynamic activated colloidal (such as clay) particle assemblies can be used to mimic common structures found in nature, such as bird, fish or insect flocking, or even human or traffic crowding behaviors. Active matter (https://en.wikipedia.org/wiki/Active_matter) is currently itself a very active area in soft matter statistical physics, and we will initiate student projects looking at active processing of novel soft materials structures based on natural materials such as clay, zeolite, cellulose, graphite, etc.

Role of the student in the project
The Master student will work together with a PhD candidate or a postdoc, and will study cooperative behaviors of activated particles, and aid in modeling the cooperative mechanisms. The experimental techniques involved are optical microscopy and subsequently image analysis. At a later stage we will study such phenomena using nanoparticles and employ (synchrotron or NTNU home-laboratory based) X-ray scattering, neutron scattering (at Institute for Energy Technology) at Kjeller, or at international neutron facilities. International collaboration is integrated in the activities, and the Master project can be designed to contain from weeks to months stays with external partners. The main international partners in these activities are: Aalto Univ. Finland, IPGG/ESPCI-ParisTech in France, Oxford Univ. in UK (numerical studies), and Harvard Univ. in USA.

Requirements
It is advantageous with an enthusiastic interest and course background in material physics, condensed matter physics, materials science, materials chemistry, nano-science.

Contact person(s)
For further details of project description, please contact:
Paul Dommersnes (paul.dommersnes@gmail.com), Ville Liljestrøm (ville.v.liljestrom@gmail.com), Etien Martinez (etien.martinez@ntnu.no) or Jon Otto Fossum (jon.fossum@ntnu.no).
PROJECT 6:
ADSORPTION AND DESORPTION FROM DOPED CLAY SURFACES

Motivation
Studies of absorption in clay minerals are relevant for sequestration of greenhouse gases, as well as for clay-supported catalysts which may be used in a variety of chemical reactions. The objective is to investigate and tune adsorption properties of metal nanostructures on clay substrates.

![Temperature programmed desorption of CO from Ni-doped muscovite mica clay](image1.png)

**Left:** temperature programmed desorption of CO from Ni-doped muscovite mica clay. **Right:** Sample holder assembly inside the ultra-high-vacuum chamber.

Role of the student in the project
Clay minerals are materials that contain two-dimensional stacks of inorganic layers. A negative charge on each layer is balanced by cations between the layers. In smectite clays, molecules may be intercalated into the interlayer spacing. These are swelling clays where the lattice parameter perpendicular to the layers increase as more molecules are absorbed. In this project, adsorption of CO, CO$_2$ and CH$_4$ on the surface of muscovite mica, which is a non-swelling clay, will be studied by use of X-ray photoelectron spectroscopy (XPS), temperature programmed desorption (TPD), and atomic force microscopy (AFM). Different metals will be deposited on the mica substrates surfaces prior to adsorption of gases. These nanostructured samples serve as model systems for studying doped clay surfaces by surface analytical tools. The student will perform sample preparation, data acquisition and analysis with assistance from other members of the research group.

Contact person(s)
For further details of project description, please contact Steinar Raaen (steinar.raaen@ntnu.no) or Kristoffer Hunvik (kristoffer.hunvik@ntnu.no)
PROJECT 7: CAPTURE MECHANISMS OF CO₂, METHANE OR DRUG MOLECULES BY NANO-LAMELLAR CLAY SYSTEMS: FROM GREENHOUSE GAS CAPTURE TO DRUG-DELIVERY

Motivation
A large variety of molecules may adsorb onto nano-silicate clay surfaces by means of different mechanisms. The objective of this activity in our laboratory is to understand active fundamental molecular interaction mechanisms at nano-confined clay surfaces. We put particular emphasis on capture of CO₂, methane (CH₄) or drug molecules. In this context clays represent lamellar nano-“container” systems (capturing/transport/release elements). Nano-lamellar clays are unique as molecular carrier “vehicles” due do their large effective surface area with more than 1000 square kilometers of effective surface area contained in one cubic meter, coupled to their tunable surface charge (order of magnitude 1 electron charge per square nm). Actual relevance here is for capturing and sequestration of green-house gases such as CO₂ or methane, or for medical drug delivery by means of clays etc. Our group has already a considerable experience in studies of the nano-fluidics of H₂O and CO₂, as well as in drug capture, and we wish to develop this further using several experimental methods.

Left: Intercalated cations in between the lamella of a stacked nano-layered clay particle may capture and retain CO₂ molecules. This results in an expansion of the structure that can be measured by means of standard X-ray scattering methods. See: Intercalation and Retention of Carbon Dioxide in a Smectite Clay promoted by Interlayer Cation, L. Michels, J. O. Fossum, Z. Rozynk, H. Hemmen, K. Rustenberg, P. A. Sobas, G. N. Kalantzopoulos, K. D. Knudsen, M. Janek, T. S. Plivelic & G. J. da Silva, SCIENTIFIC REPORTS BY NATURE 5, 8775 (2015)


Role of the student in the project
The Master student will work together with a PhD candidate or a postdoc, and will study molecular adsorption, and retention in synthetic nano-silicate clay particles, and aid in modeling the capturing mechanisms. The experimental techniques involved are (synchrotron or NTNU home-laboratory based) X-ray scattering, neutron scattering (at Institute for Energy Technology) at Kjeller or at international neutron facilities. Thermodynamic methods such as TGA or calorimetry will also be employed. International collaboration is integrated in the activities, and the Master project can be designed to contain from weeks to months stays with external partners. The main international partners in these activities are: Institute for Energy Technology at Kjeller, University of Copenhagen (neutron scattering), Texas Tech. University USA (on numerical modeling), Univ. Bayreuth Germany (sample preparation).

Requirements
It is advantageous with an enthusiastic interest and course background in material physics, condensed matter physics, materials science, materials chemistry, nano-science.

Contact person(s)
For further details of project description, please contact: Kristoffer Hunvik (kristoffer.hunvik@ntnu.no), Leide Cavalcanti (leide.cavalcanti@gmail.com) or Jon Otto Fossum (jon.fossum@ntnu.no)
Description

It is of considerable fundamental interest, and potentially of great technological importance, to investigate the transport of charge, spin, and heat on the nanometer scale. On such small length-scales, the laws of quantum mechanics governs the physics and leads to surprising phenomena when it comes to how matter behaves.

One example is superconducting materials. These materials are characterized by the fact that electric currents can flow through them with exactly zero resistance and the fact that they expel magnetic fields. It goes without saying that the prospect of generating electric currents without energy loss is of high interest when it comes to technologies ranging from computers to medical imaging.

It has recently been realized that superconductors not only carry electric currents in an exotic fashion, but that they also transport spin and even heat in a way that exceeds the performance of non-superconducting materials. This occurs when they are combined with another type of material known as ferromagnets – systems that are magnetized.

Picture taken from the work of present M.Sc student Morten Amundsen depicting the theoretical prediction of supercurrent flow in a superconductor/ferromagnet structure.

Through hard work, he managed to publish his work in one of the Nature-journals, which are among the most prestigious scientific peer-reviewed journals in the world.

At first glance, this might seem like a contradiction: didn’t we just state that superconductors expel magnetic fields? If so, how can one combine
superconductors with magnetic materials and as a result obtain superior quantum transport of charge, spin, and heat?

I invite you to take a journey into the **fascinating world of quantum condensed matter physics**, which is the largest of all fields in physics. What makes this exciting is that you will not only find answers to questions such as the one above, but you will discover new questions that we don’t know the answer to yet. And maybe – just maybe – you will be able to find the answer and thus move the frontier of what we know about nature forward.

**Qualifications**
The successful applicant is a motivated and ambitious student with good grades. The student should preferably have a solid background in quantum mechanics and some familiarity with software such as MATLAB and Maple.

**What you can expect from me and what I expect from you**
You will get a supervisor who is genuinely interested in the work of his students and who will invest his time in preparing and executing supervision of your thesis work. Several of my previous master students have through hard work managed to publish their thesis work in highly prestigious journals of physics and some students have also been offered to continue with a Ph.D degree.

If you are hardworking, ambitious, and passionate about discovering new physics, you will find a good match in me as your supervisor.

**Contact**
For more information, contact Professor Jacob Linder (jacob.linder@ntnu.no), room E5-123.

You can also read more on our group webpage [http://folk.ntnu.no/jacobrun/master.html](http://folk.ntnu.no/jacobrun/master.html) to see which topics previous master students worked on and what they accomplished.
Intermediate band solar cells

Solar cell materials with more than one bandgap offer the possibility to increase the efficiency of the solar cell beyond that of a single bandgap cell.

The intermediate band solar cell (IBSC) is one such possibility, where an intermediate energy band (IB) is placed in the otherwise forbidden bandgap of the solar cell material, see figure 1 [1].

Research on this device is motivated by high theoretical efficiencies [2-5]: The maximum efficiency of an IBSC, having the ideal bandgaps of $\varepsilon_L=0.71$ eV, $\varepsilon_H=1.24$ eV and $\varepsilon_G=1.97$ eV, is as high as 63.2 %. The single bandgap cell has an efficiency limit of 40.7%.

One attempt to realize the IBSCs relies on utilising quantum confinement of electrons in so-called quantum dots (QDs) to form the intermediate energy band, see figure 2 [1]. A QD is a nanometre sized semiconductor “particle” (made of e.g. InAs) embedded in another semiconductor with a higher bandgap (e.g. GaAs). Each QD then forms a potential well for the electrons in the conduction band, and the energy level of the confined electrons is determined by the well depth and lateral size. If the QDs are closely and evenly spaced in a three dimensional super-lattice, the confined energy levels will form an energy band; the needed intermediate band in the bandgap.

In order for such a QD-IBSC solar cell to reach its potential maximum efficiency, a high density of QDs with homogeneous sizes and shapes and a material system without defects, are some of the requirements that need to be fulfilled.

Intermediate band materials can also be realised without relying on quantum confinement effects, but instead the intermediate band is formed due to addition of (typically) metal atoms to the material. The new atoms modify the electronic energy band structure, so that an additional intermediate energy band forms in the bandgap intrinsically. Examples of such materials are Si doped with Ti, ZnS doped with Cr or the so-called highly mismatched alloys (HMAs) such as ZeMnTe:O, or GaAs:N [6].
At NTNU we are following several routes for the realization of IB materials: We are trying to make QD nano-materials for QD-IBSCs, by growing III-V based semiconductors (i.e. GaAs based materials) using molecular beam epitaxy (MBE) at the Department of Electronics and Telecommunication (IET). We also have a project on so-called III-V dilute nitrides as HMA for (bulk) IB materials, in collaboration with IET. These materials have an intrinsic IB, and might be easier to fabricate than the QD materials. A post doc and 1 PhD student are currently involved in the III-V materials activities.

We also have activities on other bulk IB materials, where the IB is formed by doping; i.e. doped ZnS, Cu$_2$O, TiO$_2$ and Si. Here we use pulsed laser deposition (PLD to deposit doped and undoped materials at IFY, or we use ion implantation for the doping of single crystals or thin films at external facilities. For the Si, TiO$_2$ and Cu$_2$O materials we collaborate with Sverre Selbach at IMT and Jon Andreas Støvneng at IFY, respectively, on simulations of the material’s band structure using DFT calculations. Three PhD students are currently be involved in these activities.

We fabricate simple devices using NTNU Nanolab, and test them using a solar simulator or a flash lamp. In addition we simulate solar cell performance, of both ideal and more realistic IBSCs.

**What the student will do in the project**
.. depends on the interest and qualifications of the student. It is possible to be involved in the growth; MBE, PLD, e-beam deposition or resistive evaporation, and the characterisation; atomic force microscopy (AFM), scanning or transmission electron microscopy (SEM/TEM), photoluminescence (PL), X-ray diffraction (XRD), ellipsometry etc, of the materials, as well as processing into solar cells (in NTNU Nanolab) and testing of the cells; current-voltage characteristics (IV) and spectral response (SR). Finally, it may also be possible to have a project on calculation of IBSC efficiencies.

**Required from the student**
Interest in experimental work and background in solid state physics or functional materials are an advantage.

**Other aspects**
There is a large activity at Gløshaugen on solar cell materials, and the student will get the possibility to join this activity.

**Contact persons**
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IET: Bjørn-Ove Fimland (bjorn.fimland@iet.ntnu.no) (room A381 / Elektro A)

**References**
Topics for project & master thesis works academic year 2018/2019

Biological polymers: Mesoscale structure formation and interactions.
Supervisors: Bjørn Torger Stokke and co-workers,

The webpage provide information on topics that we so far have published within. We are currently also working within additionally topical areas that can be suitable for project / master thesis topics, please contact me to learn about these.

Bioresponsive hydrogels as signal transducers
Supervisors: Bjørn T. Stokke (bjorn.stokke@ntnu.no), Eleonora Jonasova (eleonora.jonasova@ntnu.no)

Hydrogels adopt an equilibrium swelling state based on thermodynamic principles, where changes in ionic environment, pH, temperature, pressure etc., can induce various swelling states depending on the molecular properties of the polymers constituting the network. Within this project, we have recently developed a line of research for technological utilization of molecular interactions integrated in hydrogels to be applicable for biosensors. In addition to tailor-making of hydrogel materials to act as biological signal transducers, this line of research takes advantage of a high resolution (2 nanometer) interferometric technique for the characterisation of optical length of responsive gels. This technology providing a 100 fold improved resolution compared to diffraction limited optical imaging, is currently being applied for the characterisation of developed, bioresponsive (various components) hydrogel materials aiming at sensor development. The 50-60 µm radius, hemispherical hydrogel manufactured at the end of an optical fiber constituting the environmental sensing element makes up a Fabry-Perot cavity for high resolution interferometric detection of the optical length. The interference of light guided by the optical fiber and reflected at the fiber-gel and gel-solution interfaces enables detection of the optical pathlength within the gel and thus the swelling degree of the gel (Figure 1a).

Both the amplitude and phase of the interference wave reflected back through the optical fiber contains signatures that can be used to deduce changes of the optical properties of the responsive hydrogel material, but the phase represents the highest resolution information. The function of the miniaturized bioresponsive hydrogel material is both to embed specific biological recognition event and to transduce this to changes of the hydrogel that readily can be read-out by the interferometric platform.

Figure 1. (a) Shematic illustration of optical detection of changes of a hemispherical hydrogel. (b) Schematic illustration of glucose induced reduction of equilibrium swelling volume of a glucose-selective hydrogel.
The technique has been applied to characterize various developed hydrogel matrices to explore the potential resolution of the technique and for demonstration of biospecific sensing transduction. A glucose sensor is realized on this platform by utilizing glucose sensing functionality incorporated into the hydrogel matrix (Figure 1b). The interaction between glucose and a recognition element, changes the driving forces for gel swelling thus inducing a glucose sensitive hydrogel swelling. The properties of the responsive hydrogel as a glucose sensor were determined in more detail with respect to swelling kinetics and equilibrium swelling degree for the physiological relevant range of glucose. Results showed there was a good degree of reversibility, both for equilibrium swelling and swelling kinetics.

Within this topical area, the aim for a project work/thesis will be to design a recognition element for a selected biological (macro) molecule, prepare such sensor and to characterise it. Part of the work can be developed within NTNU NanoLab infrastructure.

**Symmetry breaking in responsive hydrogel membranes**

Supervisors: Bjørn Torger Stokke (bjorn.stokke@ntnu.no), Eleonora Jonasova (eleonora.jonasova@ntnu.no)

Hydrogels are three-dimensional networks consisting of polymers. They can absorb large quantities of water and swell to several times their size in dry state. The combination of polymer strands and a large volume of water gives them properties of both solids and liquids.

A subgroup of hydrogels, called responsive or smart hydrogels, has the ability to change their shape and/or structure in response to external stimuli (pH, temperature, a specific molecule). This change is often the change in swelling equilibrium, meaning the gel swells or shrinks as a result of being exposed to a trigger. This makes hydrogels particularly interesting for fabrication of label-free biosensors, as they translate a change in their environment into easily observable swelling. Other applications include preparation of drug-delivery agents. In this case, the gel particles would change their shape or other properties and release the drug at the desired location in the body.

Hydrogels can be prepared in various geometries and our activities include preparing semi-hemispherical responsive hydrogels. The proposed project would consist of preparation and characterization of patterned hydrogel membranes, similar to those described by Wu et al, which can be seen (fig. 2)

![Figure 2](image)

*Figure 2 Hydrogel membranes equilibrated at two different pH values. The round holes at pH 2, due to swelling and subsequent buckling, have changed their shape at pH 4. Image taken from Wu.*

The swelling of these gels creates stresses and strains and consequently changes in geometry and symmetry of the pattern. The layers can be prepared with holes of various sizes and shapes. During the swelling the size and shape of these holes is changing and buckling and breaking of symmetry is observed. The patterned surfaces can be used to study the mechanical aspects of hydrogel swelling and (in case the stimulus is a molecule) relate these mechanical aspects to the migration and binding of the trigger molecule within the gel. The patterned gels could also be eventually used as biosensors.
The project will require preparation of patterned hydrogels using soft lithography and studying the influence of various geometric factors, such as the ratio of the hole size to the distance between the holes, the shape of the holes, thickness of the gel layer, etc. The visualization of the gels will be carried out using various imaging techniques, including e.g. quantitative phase contrast microscopy. Parts of the soft lithography process, such as preparation of PDMS molds, may be carried out in NTNU NanoLab.

**Optimizing biomarker mass transfer in Lab-on-a-Chip biophotonic sensor platform**  
Stokke (bjorn.stokke@ntnu.no), Ingrid Haga Øvreeide (ingrid.h.ovreeide@ntnu.no)

The ability to accurately detect a specific biomolecule in the body using small sample volumes and time is progressively becoming more important in health care. One way in which this can be achieved is through the use of a Lab-On-A-Chip device, which will produce an output signal where the wavelength intensity of the light will change if the biomolecule reaches the active sensing surface. For this to occur the biomarkers must be efficiently transported to the specific sensing area, which is achieved using microfluidic channels. The parameters of the microchannel play an important role regarding the overall efficiency of the integrated sensor device, where the main challenge regarding the microfluidic channel design originates from mass transfer limitations, which is linked to the parameters involved.

Although the microfluidic channels are partnered with sensors to limit sample consumption, make the analysis quicker and reproducible in Lab-on-a-chip sensor platform, it also introduces challenges. The main challenge is that the laminar flow in the microfluidic channel limits the efficient exposure of biomarker to the active sensor area. The topic can be within selected areas of this overarching topic, e.g:

Tasks:
- Identify limitations, and characterize means to enhance the mass transfer
- Experimental – Soft lithography – imaging; numerical

**Side-view microscope - biomarker mass transfer in Lab-on-a-Chip biophotonic sensor platform and determination of soft biomaterials deformation**  
Supervisor: Bjørn T. Stokke (bjorn.stokke@ntnu.no); Ingrid Haga Øvreeide (ingrid.h.ovreeide@ntnu.no); Astrid Bjørkøy (astrid.bjorkoy@ntnu.no)

Characterization of flow lines to optimize biomarker mass transfer in integrated microfluidic – biosensor devices are not always easily characterized using conventional confocal microscopes. Examples of this include the need to determine curvature of flow velocity profiles induced by ceiling structures in the microfluidic flow channel in the vertical direction. This is limited by the acquisition time for the z-stack image series in a typical 20 µm channel height. Similarly, z-stacking will not be the preferred acquisition mode to study gel microbeads deformation experiments in a flow channel where the gel bead is kept in proximity to an adhesive surface by gravitation (and the nature of the adhesion is expected to induce deformation depending on the gel bead mechanical properties and flow parameters). In both these examples, a horizontal alignment of the optical axis is preferred as compared to the conventional vertical alignment of the optical axis. In the present project, we will optimize the microscope design, the image acquisition and the design of sample geometries for a selected realization.
The system will be tested for a particular application, either for the characterization of fluid flow in microfluidic channels related to the Lab-on-a-chip biophotonic activity, or for the determination of effects of adhesion on deformation of soft gel beads. This activity is planned to exploit various interaction mechanisms, e.g., electrostatic or specifically interaction molecular partners with known energy landscapes. The soft gel beads will be synthesized using microfluidics and exploiting a recently established workflow for preparation of Ca-alginate gel beads we expect to be tunable with respect to Youngs modulus in the range 10 kPa to above 100 kPa, e.g., in the range reported for some cancer cells (1kPa) to collagenous bone (100 kPa), and with various surface densities. Thus, the combined effect of possible cooperative nature of the interaction supported by several individual binding partners and compliance of underlying support, similar to cells, will be determined.

Macromolecular interactions at the single-molecule level - fluctuation analysis of bound states
Supervisor: Bjørn T. Stokke (bjorn.stokke@ntnu.no); Nina Bjørk Arnfinnsdottir (nina.arnfinnsdottir@ntnu.no); Ingrid Haga Øvreeide (ingrid.h.ovreeide@ntnu.no)

Macromolecular interactions are underpinning signal-recognition, biocatalysis, hybridization and soft materials assembly. Such interactions can be characterized at different level of detail, from thermodynamics, to identification of specific atomic groups involved in recognition, binding and eventual catalysis. In the present project we will develop a strategy for the determining characteristic properties of selected macromolecular interactions using equilibrium fluctuation analysis of single binding events. This will be conducted by applying total internal reflection fluorescence microscopy, combined with immobilization one of the components and implement image processing strategies for the fluctuation analysis.

In total internal reflection, there is generated an evanescent wave on the low-refractive index side that decays with the distance from the interface as:

$$I(z) = I_0 e^{-z/d}$$

where $I_0$ is the intensity at the interface, and $d$ the characteristic distance for penetration depth of the evanescent wave. The parameter $d$ depends on the optical properties of the materials and the angle of incidence. Typically $d$ is of the order of 100 nm, but can be tuned by varying the incident angle of the light. The exponentially decaying evanescent field at the sample side in TIRF will be exploited for selective observation of fluorescently labelled molecules in this thin section. The fluctuation characteristics will be affected by binding to the surface. Analysis of the time dependent trajectory of individually fluorescent macromolecules that is bound specifically to its binding partner (immobilized on the surface) forms the basis for characterization of the interaction at the single molecule level.

The project include various subtopics for the particular macromolecular pair to investigate (to be decided among those in the laboratory: e.g: competitive displacement in dsDNA,):

- Implement immobilization protocol on glass surface and characterize the functionalized surface (AFM, fluorescence)
- Spatiotemporal observation of fluorescent labelled ligand by TIRF; specificity and characteristics. (Observations on TIRF will be carried out using an EMCCD camera supporting up to 24 frames/second in full frame (1024x1024 pixels) or faster for selected / binned area. Sensitivity: photon counting in each pixel)
- Analysis of spatiotemporal behavior at the single-molecule level to extract fluctuation parameters
The goal of the project is to establish procedures for a single-molecule sensitive interaction assay and its application of a particular macromolecular pair. The principles of the assay is expected to be transferable to numerous applications.

**Microfluidic based projects:**

*NTNU Microfluidics Group*  
([http://www.ntnu.edu/microfluidics/](http://www.ntnu.edu/microfluidics/))

Within microfluidics, we explore application of droplet-based and continuous flow microfluidics for molecular assemblies, separation. We have recently established platforms that enable production of various polysaccharide microstructures (single and multi layered microparticles, microfibers, egg-shaped particles etc). Some applications include:

- Cell encapsulation for bone mimicking materials
- Biocompatible drug delivery systems (we are currently working on producing sub-micron particles)
- Characterization of mechanical properties of particles using force probing techniques (optical tweezers and atomic force microscope)
- Encapsulation of bacteria to study colony growth in 3D scaffolds

In continuous microfluidics, our focus is on lab-on-a-chip devices for applications in diagnostics. We are currently developing a platform for isolating exosomes from blood samples. Exosomes are nanoparticles secreted from many cell lines, including tumor cells. The information enclosed in exosomes may be used for early diagnosis of various diseases, including tumor metastasis. We believe a lab-on-a-chip device can revolutionize this field.

Current projects builds on a fundament including the following strategy:

- AutoCAD/Clewin for design of microfluidic devices (masks for fabrication)
- Working in the NanoLab for fabrication of devices
- Microfluidics experimental setup. This includes using an inverted microscope with mounted high speed camera and applying new high persistency syringe pumps

Some projects will include:

- Nanoscale patterning using electron beam lithography
- Characterization using scanning electron microscopy (SEM)
- Optical tweezers and/or AFM
- Confocal microscopy to characterize produced particles

Note that training will be given on all activities. There are no requirements on previous lab/cleanroom experiences.

**Micron Sized Polysaccharide Particles**

**Supervisors:** Bjorn T. Stokke

Gel beads can be exploited for various purposes, e.g., immobilization of cells as supported by gel bead generation technologies such as electrostatic, core-shell particles, and microfluidic. All of these strategies explore only one type of polymer constituents at the time. In the present project, we aim at designing uniform populations of gel bead particles and surface functionalize these for controlling adhesion properties. Control of adhesion properties are important on various length
scales from molecular to mesoscale for e.g., cell adhesion, but also for organizing soft materials. The synthesis of the homogeneous gel bead populations with size in the range 20 – 50 micrometer will be based on a recently developed process to include Ca-induced polysaccharide gelation in microfluidics.

The project will include fabrication of microfluidic devices and on-chip polymer gel bead synthesis, their characterization, eventual further surface functionalization, and assessing how gel bead mechanical properties influences deformation geometries under adhesion processes (observed e.g., side-view microscope, and others)

**Dissecting the impact of cellulose production on the elastic modulus of epidermal cells in Arabidopsis seedling roots**

Supervisors: Bjørn Stokke and Thorsten Hamann

Thorsten.hamann@ntnu.no Bjorn.Stokke@ntnu.no

Plant cell walls represent the first line of defense against environmental stress as well as form key elements during plant cell morphogenesis and plant growth. During these different biological processes the walls have to maintain their functional integrity to perform their activities. The available evidence shows that plant cells have evolved a mechanism to monitor the functional integrity of their cell walls by modifying cell wall composition and structure as well as cellular metabolism in order to compensate for cell wall damage (CWD) impairing the integrity. Plant cell wall composition/structure influence the quality of plant biomass and the yield of food crops. Understanding the mode of action of the cell wall integrity maintenance mechanism could therefore generate novel strategies to facilitate bioenergy and food production.

The Hamann lab has established a model system to study the mode of action of the cell wall integrity maintenance mechanism. Arabidopsis seedling roots are being used as biological material while cellulose biosynthesis inhibition is used to simulate CWD. Cellulose was chosen because cellulose microfibrils are the main load bearing elements in plant cell walls. The Hamann lab has previously shown that different signaling molecules are required to mediate the response to CWD and several genes have been implicated. However, it is not known how quickly and in what way the inhibition of cellulose production changes the mechanical characteristics of the cell wall.

The Stokke lab is in the process of establishing nanomechanical mapping of soft materials as mode for using atomic force microscopy. This mode, different from more conventional known ones such as contact, non-contact or tapping mode, potentially allows correlations between the morphological features (height variations) and the resulting mechanical (elasticity) properties of cells. The elastic properties are obtained by using the maximum indentation force as the feedback signal for each pixel in the scanning process. Elastic properties are deduced using a model for the
deformation geometry induced by the tip of the cantilever. Elastic maps can potentially be obtained with lateral resolution in the order of 10 nm.

The Hamann and Stokke labs have teamed up to offer a project with the aim to apply atomic force microscopy to determine changes in the mechanical characteristics of plant cell walls induced by manipulation of cellulose production. This will provide the foundation to understand how plant cells perceive CWD and translate a physical stimulus into quantitative biochemical signals regulating adaptive downstream responses.

Below preliminary results are shown where the mechanical characteristics of a seedling root tip have been examined with AFM.

Fig. 5
Hamann et al., Plant Journal 2009
Denness and Hamann, Plant Signaling and Behavior 2011
Milani et al., Plant Journal 2011
Peaucelle et al., Current Biology 2011
The transmission electron microscopy (TEM) allows for resolving structures well below 1 nm and is an important technique in nanotechnology. The TEM Gemini Centre has three state-of-the-art microscopes including the most sophisticated technology available. It allows for advanced materials characterization, novel experimental solid state physics and practically doing nanotechnology. As a student in the TEM group, you will have a unique opportunity to use some of the world’s most advanced scientific instrumentation yourself!

As a project or diploma student in the TEM group you can take an active part in one of the exciting research projects which require nanoscale material characterization. You work together with a PhD student, a SINTEF research team or one of our external collaborators to achieve a common goal. The work can have an applied character and be very practical, or theoretical to support experimental activities within the group. Also a combination of practical and theoretical work is possible. In all projects the TEM or input from TEM is used to understand the structure of a material down to the atomic level and relate this to macroscopic properties of the materials.

Examples of student projects which are available:

- Development and characterization of new aluminium alloys
- Study of nanoparticles and nanowires to optimize synthesis
- Simulations and advanced data processing
- Studies of thin film oxides for use in electronics
- Studies of solar cell materials (Si, thin films, quantum dots & nanowires)

These projects are described in more detail in the next pages. Earlier, several student projects have led to publications [1-6]. Due to high demand on the research facilities and the intensive supervising we give, we can take in max 6 students in the group in the coming semester.
We offer:

- Choice of a project that fits your interests and background.
- Training in operating advanced and modern scientific equipment or/and simulation and quantification software (theoretical/modelling). Use of cleanroom can be included.
- Weekly meetings with a supervisor during the project.
- Being part of a large and dynamic scientific consortium.
- Possibilities in extending the project to a diploma or a PhD.

You are encouraged to contact one of us if you like to hear more details on a specific project, other available projects, options in academia or industry after a diploma in TEM or possibilities to incorporate own research ideas related to TEM. For more information on the current activities within the group, group members, equipment and recent publications, see the TEM Gemini Centre homepage: http://www.ntnu.edu/geminicentre/tem.

Also take a look at our video! https://www.youtube.com/watch?v=BuLqv4_cIMU

Contacts:

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References:


Nano-structure characterization or atomistic modelling for aluminium alloys development

Motivation:

In studies of light metal alloys there are challenges when it comes to establishing relations between the nano-structure and mechanical properties, as for example strength and ductility. Aluminium alloys are industrially relevant due to their superior mechanical properties (high strength/weight ratio and good corrosion properties). The hardness increase is due to precipitation of nanometre-sized metastable phases that are formed during heat treatment. The TEM group has for several years worked closely with Hydro and other companies in studying microstructure/precipitates in these alloys.

What the student will do in the project:

The student will do experimental testing of properties (hardness, conductivity, strength ..) with different heat treatments and/or alloy compositions, and learning and using different TEM techniques (such as BF/DF imaging, diffraction, EELS, SPED and EDS) to study the corresponding nanostructure. This year we have several proposed projects from collaborating companies, also involving summer jobs. In addition we have other ‘local’ projects – so please come and talk to us! We also welcome students interested in programming in Python to work on aluminium alloys! Projects can be related to the direction nanomaterials. Alternatively, the project could be pure theoretical, focusing on atomic modelling of the early stages of precipitation.

Required from the student:

Background in materials physics (solid state physics) and interest in materials science would be an advantage. We need a student interested in experimental work, and working independently in a larger group of scientists. For the modelling project experience and interest with coding is a pre.

Other aspects:

There are many people working on aluminium alloys at NTNU, and we have several ongoing external projects, including two Centres of innovation (CASA and SFI Manufacturing) where we work in close collaboration with SINTEF, Hydro and other companies producing aluminium products. Some of the companies involved are, in addition to Hydro Aluminium, Benteler Automotive, Steertec, Neuman Aluminium, Nexans and Gränges. See the video made in CASA here! The students will participate in project meetings with the companies in Trondheim or/and at industry sites. Students get their own problem which fits well into the rest of the work. Within this field there are possibilities for continuation as a PhD student and for a summer jobs. We also work closely with Professor Jaakko Akola who is doing atomistic modelling of these alloys (see his announcement elsewhere). We have an ongoing collaboration with two Japanese universities in Japan (University of Toyama and Tokyo Tech.). Contact us for more information if you are interested in doing something with Aluminium!

Contact person:

Randi Holmestad, IFY (randi.holmestad@ntnu.no) Other people currently working on Aluminium in the group: Calin Marioara, Sigurd Wenner and Jesper Friis at SINTEF and Emil Christiansen, Jonas K. Sunde, Marat Gazizov, Adrian Lervik, Tina Bergh and Jonas Frafjord, all PhD students and postdoc at IFY.
Structural characterization of heterostructured semiconducting nanowires

Motivation:
III-V semiconductor nanowires with high quality are grown Department of Electronics and Telecommunications (IET) for future application in optical devices (EDs, lasers) and solar cells. Because of their small size, nanowires have to be studied by characterization techniques with a high resolution as for example TEM.

What the student will do in the project:
You will study a specific batch of nanowires with interesting optoelectric properties. Your task is to help with optimizing the growth condition (to be specific GaN grown on a new MBE) or understanding the relation between optical & electric properties to the crystal structure / lattice defects/composition as determined by TEM. You will learn to use basic TEM techniques as electron diffraction and high resolution imaging techniques. SEM, STEM or FIB work within NTNU Nanolab could be part of the project. Your own characterization results are relevant to optimize growth and nanowire-based devices. An alternative project is making nanowire-based circuitry using FIB. The project is related to the direction nanomaterials and/or nanoelectronics.

Required from the student:
Interest in experimental work using the TEM. Join weekly project meetings with academics and other project students that grow the nanowires. You should be able to clearly communicate and relate your results to others in the project and understand what feedback they expect from your TEM work.

Other aspects:
The field of semiconductor nanowires, fundamental understanding and application of them in devices had an enormous growth in the last years. We had already 12 project/diploma students working on TEM of semiconducting nanowires. Results of students’ work are published afterwards. The research is interdisciplinary and a key example of fundamental & applied nanotechnology at NTNU. The obtained practical skills can be applied in the study of other nanostructures.

Contact persons:
Ton van Helvoort (IFY, a.helvoort@ntnu.no) Other key people in the project: Julie Stene Nilsen (IFY), Aleksander Mosberg (IFY), Helge Weman (IES) and Bjørn-Ove Finland (IES).
ADVANCED PROCESSING OF ELECTRON SPECTROSCOPY DATA

Motivation:
Determining the composition with high spatial resolution is important for many technological and academic projects. Of the two main spectroscopy techniques available in TEM, energy dispersive and electron energy loss spectroscopy (EDX and EELS respectively), EDX is the most used. Quantification is in general based on a dated empirical method with drawbacks. The Centre has been working on an alternative method (called zeta-method) that yet not available in commercial EDX packages. The zeta method gives more accurate compositional analysis than the currently used approach. However, further developing work is required before it can be used by all TEM operators. Developing the code base ourselves allows linking EDX to other data types and implementation of new technologies such as machine learning.

What the student will do in the project:
The student will collected own EDX data or work with data acquired in other projects. Important is understanding the characteristics of the EDX technique & data format and make use of code developed by previous students. Depending on the chosen material system at the start of the project, the focus will lie on extending the zeta calibration table or implementation of refinements such as absorption and crystal orientation corrections (see figure). The results will be compared to the conventional EDX quantification routine. The project is related to the direction nanomaterials and/or nanoelectronics.

Required from the student:
An interest in using and further developing Python-base software tools is required. The student needs to have interest in parallel aspects beside his/her own specified focus, such as technical details of the detection system or material specific issues. The skill and interest to work both practically and theoretical can be a bonus. Good communication and interaction with collaborating scientific and academic staff and PhD students as well as being able to work independently are important.

Contact person:
Ton van Helvoort (a.helvoort@ntnu.no)

Others involved: PhD students Adrian Lervik, Tina Bergh, Julie S. Nilsen and senior engineer Bjørn Soleim

(a) Zeta constant for Ga as function of tilt angle and crystal zone. (b) Intensity detected O_K radiation as function of tilt angle. Deviation compared to model (grey line) due to absorption and detector shadowing.

Other aspects:
This project offers the opportunity to become familiar with code development, experimental techniques (mainly TEM, but SEM-EDX could be included) and a specific material system. This broader spectrum might be beneficial for selectin of a master project and an asset in future job applications.
MACHINE LEARNING APPLIED TO EXPERIMENTAL NANOTECHNOLOGY

Motivation:
The advances made in data technology have made the terms “big data” and “Machine learning” more than just buzz words. In daily life are Big Data & machine learning algorithms steering us in the background (e.g. search engines) and will be even more in the future (e.g. google car). Also in nearly all research fields a disruptive transformation is ongoing due to these advances. In TEM both the growing amount of data and the conceptual different data analysing approach giving new insight in the structure of materials at the nm-scale. Previous projects have proven that students dedicated to data handling can add value to ongoing research projects and international projects.

What the student will do in the project:
The student will work with existing TEM data sets (primarily scanning diffraction data) and test new machine learning routines. Depending on the progress, new data might be acquired and the students can be active in planning and running the additional session. Collaboration with the data-owner and understanding the physics behind the material studied and diffraction technique used will be important. The data is related to crystal phase or orientation quantification in III-V semiconductors or Al-alloys. The developed data analysis routines should be made available and accessible to other people in the community (i.e. open-access). This means that the whole process of development, implementation and documentation need to be addressed.

Required from the student:
An interest in using and further developing software tools is required. Experience with Matlab, C++ or preferable Python is essential. Good communication and interaction with scientific and academic staff and PhD students involved as well as the skill to work independently are important.

Other aspects:
The intention is that final results will form a part of ongoing research and contribute to publishable result. “Big data” and data mining useful information from ever growing data set sizes are hot topic in today’s and future research. The skills learned might be attractive for jobs outside the field of material physics. The project is related to the direction nanomaterials and/or nanoelectronics.

Contact persons:
Ton van Helvoort (a.helvoort@ntnu.no) and Randi Holmestad (randi.holmestad@ntnu.no)

Others involved: PhD students Jonas Sunde, Julie S. Nilsen and Håkon W. Ånes from IFY and IMA.

(a) PCA scree plot, (b) RGB image constructed from 3 out of 6 NMF components from a larger scanning electron diffraction set of a GaAsSb nanowire, and (c) corresponding components.
TEM CHARACTERIZATION OF SOLAR CELL MATERIALS

Motivation:
At NTNU there are several ongoing projects working on solar cell materials. These include development of new materials and better understanding of microstructure in established materials. The new materials can consist of single- or multi-layer thin films on a crystalline substrates, ion implanted or highly doped structures etc. Traditional materials include multicrystalline silicon where defects formed during solidification and cooling will be studied. Another aspect is the interfaces and contacts in the produced cells. TEM plays an important role in all these studies as defects, interfaces, size/shape and composition variations at the nm-scale can determine the overall efficiency of the solar cell.

What the student will do in the project:
The student will study the crystal structure and different phases in the thin films and bulk using TEM, and correlate this to process parameters and other material properties and/or device performance. The actual work will depend on the type of material and the interest of the student. Possible projects include studies of defects, grain structure, particle density, strain, development of a specimen preparation routine that allows efficient characterization of grain size, crystallinity and defects and studies of the effect of doping in relation to the electro-optical properties. The project is related to the direction nanomaterials and/or nanoelectronics.

Required from the student:
We seek students with background from physics or nanotechnology. Interest in solid state physics and nanoscience or solar cell physics is needed. We need a student interested in experimental work, working independently and being able to collaborate with the research groups synthesizing the materials/devices.

Other aspects:
There is a large activity at Gløshaugen on characterization and on solar cell materials, and the student will get the possibility to join these activities, with participation in weekly lunch meetings etc. It is possible that the student projects will lead to important findings which may be included in scientific publications. SEM and STEM work within NTNU Nanolab could be part of some of the suggested projects.

Contact persons:
Randi Holmestad (randi.holmestad@ntnu.no) and Per Erik Vullum (per.erik.vullum@sintef.no)

Others involved in the projects; Turid Dory Reenaas (IFY), Marisa Di Sabatino (Department of Materials Science and Engineering) and Hogne Lysne (IFY).
TEM CHARACTERIZATION OF OXIDE THIN FILMS MADE BY CHEMICAL METHODS

**Motivation:**

Ferroic materials constitute a unique class of materials possessing either ferromagnetism, ferroelectricity or ferroelasticity. Two or more of these properties are found in so-called multiferroics. These materials have many applications in information and communication technology as well as in energy and in medical technology. Applications include sensors, transducers, actuators, etc. Lead-free materials such as K$_{0.5}$Na$_{0.5}$NbO$_3$ (KNN) and Bi$_{0.5}$Na$_{0.5}$TiO$_3$ (BNT), ferroelectric tungsten bronzes such as Sr$_1$–xBaxNb$_2$O$_6$ and multiferroic materials such as BiFeO$_3$ and YMnO$_3$ have been central to the research in the last decade. At Department of Materials Science and Engineering, NTNU they have many years of experience in developing these materials and the characterization of their structural and functional properties. TEM investigation allows the determination of the detailed structure which can be related and compared to first principles calculations and functional properties.

**What the student will do in the project:**

The student will prepare samples (using Nanolab FIB or other routes) and examine them in the TEM, to support and complement other analyses being performed, and will work in close collaboration with others synthesizing the materials or studying the same materials with other techniques.

**Required from the student:**

We seek students with background from physics, materials science or nanotechnology, interested in solid state physics/chemistry and/or nanoscience. If you are interested in experimental work, working independently and collaborating with the research groups synthesizing the materials/devices, please contact the advisors listed below. The project is related to the direction nanomaterials.

**Other aspects:**

There is a large activity at Gløshaugen on characterization of functional materials, and the student will be included in these activities, with participation in weekly lunch meetings etc.

**Contact persons:**

Randi Holmestad ([randi.holmestad@ntnu.no](mailto:randi.holmestad@ntnu.no)) and Per Erik Vullum ([per.erik.vullum@sintef.no](mailto:per.erik.vullum@sintef.no)).

This project is in collaboration with Mari-Ann Einarsrud and Tor Grande from Department of Materials Science and Engineering. Ragnhild Sæterli is involved in the project.
TEM CHARACTERIZATION OF NOVEL SiGe-CORE FIBRES FOR OPTOELECTRONIC APPLICATIONS

Motivation:
Glass fibres with silicon cores have emerged as a versatile platform for all-optical processing, sensing and microscale optoelectronic devices. Using GeSi in the core extends the accessible wavelength range and potential optical functionality because the bandgap and optical properties can be tuned by changing the composition. However, Si and Ge segregate unevenly during non-equilibrium solidification, presenting new fabrication challenges, and requiring detailed studies of the alloy structure from the atomic to the mm scale.

(a) Back scattered electron (BSE) image that show a cross-section of the glass fibre with the SiGe core. (b) TEM image of the grain and defect structure in the SiGe core.

What the student will do in the project:
The student will prepare samples and examine them primarily by TEM, but also by SEM, to support and complement other analyses. TEM and SEM will be used to characterize chemical composition, crystal structure, defect structures and grain morphology. These properties will be used to fundamentally understand and tailor the new and exciting properties of these novel materials.

Required from the student:
We seek students with background from physics, materials science or nanotechnology, interested in solid state physics and/or nanoscience. If you are interested in experimental work, working independently and collaborating with the research groups synthesizing the materials/devices, please contact the advisors listed below. The work will involve state-of-the-art instruments located in the national infrastructures NORTEM (TEM) and NORFAB (FIB, SEM).

Other aspects:
There is a large activity at Gløshaugen on characterization of optical materials, and the student will be included in these activities, with participation in weekly lunch meetings etc. It is expected that the student project will lead to scientific publications. The project is related to the direction nanomaterials and/or nanoelectronics.

Contact persons:
Randi Holmestad (randi.holmestad@ntnu.no) and Per Erik Vullum (per.erik.vullum@sintef.no). Professor Ursula Gibson's group makes the samples and studies processing of these materials.
TEM CHARACTERIZATION OF BEAM-SENSITIVE CALCIUM PHOSPHATE MINERALS

**Motivation:**

New equipment, novel routines and advanced data processing allows TEM study of beam-sensitive materials that was previous not possible. In this project crystalline and amorphous calcium phosphates will be studied, first by conventional TEM and later by novel TEM techniques. Calcium phosphates (CaP) material are relevant for biomineralization and for bioinspired material synthesis. For example, bone tissue is a composite consisting of a calcium phosphate mineral (hydroxyapatite, HAp) and collagen. A complex, hierarchical design, combining the stiffness of brittle mineral crystals and the toughness of the soft organic matrix, is responsible for the mechanical properties of bone. Understanding crystallization and transformations of CaP is therefore of key importance. The project should establish how to best study these materials by state-of-the-art TEM techniques, map crystal phases and possibly composition variation at the nm-scale.

**What the student will do in the project:**

The student will learn basic TEM, determine the critical dose for the different phases, study the crystallography and composition in calcium phosphates and develop a more robust TEM characterization routine. The results will be discussed from a TEM and a materials science point of view.

**Required from the student:**

We seek students with interested in experimental work at the TEM and to work across different field (experimental solid state, biophysics, crystal growth and biomaterials). The project is related to the direction nanomaterials and/or bionano.

**Contact persons:**

Ton van Helvoort ([a.helvoort@ntnu.no](mailto:a.helvoort@ntnu.no)).

Others involved in the project are Pawel Sikorski and Ragnhild Sæterli at IFY, and Jens-Petter Andreassen at the Department of Chemical Engineering.
TEM CHARACTERIZATION OF OXIDE THIN FILMS MADE BY PHYSICAL METHODS

Motivation:
Oxide materials show superior optical, magnetic, dielectric, piezoelectric, and electric conduction (superconductivity, ionic conductivity, semi-conductivity) properties, as well as excellent mechanical performance, which make them an important and promising class of functional materials. In the oxide electronics group at Department of Electronics and Telecommunications they have currently large focus on the effect of interfaces on (anti-) ferroelectric and piezoelectric materials. The goal is to understand how interfaces can be used to control properties for applications within sensor technologies. The system currently studied is (La,Sr)MnO$_3$. The thin films are grown by the Pulsed Laser Deposition (PLD) technique.

What the student will do in the project:
Study the crystal structure, domains and interfaces in the thin films using TEM and correlate this with properties. An important aspect here is to make good cross section samples, and TEM sample preparation will be a considerable part of the work.

Required from the student:
We seek students with background from physics or nanotechnology. Interest in solid state physics and electronics is needed. We need a student interested in experimental work, and working independently. Accuracy and patience are needed for the sample preparation work. The project is related to the direction nanomaterials and/or nanoelectronics.

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This project is in collaboration with Thomas Tybell from Department of Electronic Systems.