

# Project work / Master / Diploma topics in the TEM Gemini Centre, 2022/23

## TEM Gemini Centre

The TEM activity in Trondheim is centered around the TEM Gemini Centre, which consists of professors, engineers, postdocs and students at Dept. of Physics (IFY), NTNU and researchers in SINTEF Industry.

We have in total three TEM instruments and are part of the national infrastructure NORTEM. One of these is one of the most advanced available.

In 2021, we have at IFY 3.4 (assoc.) professors, 2 engineers, 5 SINTEF researchers, 3 Postdocs, ~7 PhD students and several MSc students with TEM as their main activity.

Our research extends through various fields of solid state physics and materials technology, from cooperation with industry on aluminum, solar cells, nano-materials and data analysis.

<http://www.ntnu.edu/geminicentre/tem>

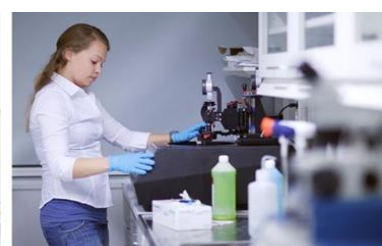
**The transmission electron microscopy (TEM) Gemini Centre has three state-of-the art microscopes. These TEMs include the most sophisticated technology available and give new possibilities for advanced materials characterization, novel experimental solid-state physics and nanotechnology down to the atomic scale. 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 or work with data from them!**

As a project or diploma student in the TEM group you can take an active part in one of the exciting research projects which requires nanoscale material characterization. You work together with a PhD student, SINTEF researchers 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 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:

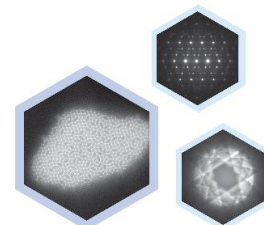
- Development and characterization of new aluminium alloys
- Study of nanoparticles and nanowires to optimize synthesis
- Simulations, atomistic modelling and advanced data processing
- Studies of thin film oxides for use in electronics
- Studies of multi-materials and joints
- Contribute to open-source code for data analysis

These projects are described in more detail in the next pages. Earlier, several student projects have led to scientific publications [1-8]. Due to high demand on the research facilities and the intensive supervising we give, we can take in max 8 new students (5 experimental) in the group in the coming semester.



The TEM Gemini Centre is a strategic collaboration between NTNU and SINTEF. We work within the fields of solid state physics, materials science and metallurgy, and study a broad range of materials down to the atomic level. Our lab hosts some of the most advanced transmission electron microscopes (TEM) in the world.

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## 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).
- Weekly meetings with a supervisor during the project.
- Being part of a large and dynamic scientific consortium.
- Possibilities in extending the project to a Master or a PhD.

Within the Aluminium projects we this year offer a summer job through SFI PhysMet at NTNU. There is also a possibility to stay one month in Japan in an aluminium company as a part of the project/MSc (covid permitted!) – We also offer a summer job in the In-Sane project!. - Ask us about details!

All topics can be adjusted to 15,30 or 60 ECTS. 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](https://www.youtube.com/watch?v=BuLqv4_cIMU)

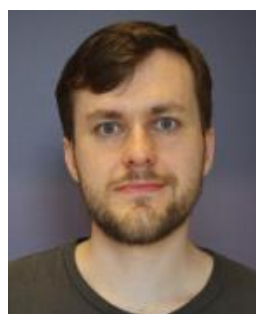
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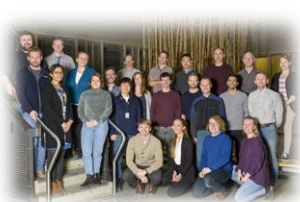
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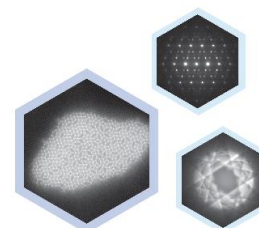
## References: (master students in bold)

- [1] T. Bergh, D. N. Johnstone, P. Crout, S. **Høgås**, P. A. Midgley, R. Holmestad, P. E. Vullum, and A. T. J. van Helvoort, "Nanocrystal segmentation in scanning precession electron diffraction data", Journal of Microscopy, doi.org/10.1111/jmi.12850, 2020.
- [2] N. H. Gaukås, S. M. Dale, T. M. Ræder, A. **Toresen**, R. Holmestad, J. Glaum, M.-A. Einarsrud, and T. Grande, "Controlling Phase Purity and Texture of  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  Thin Films by Aqueous Chemical Solution Deposition", Materials 12, 2042, 2019.
- [3] J. **Busam**, S. Wenner, A.M. Muggerud and A.T.J. van Helvoort, Structural Characterization of Natural Quartz by Scanning TEM, Microscopy and Microanalysis 24(S1), 2044-2045, 2018.
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- [7] F de la Peña et al, Hyperspy 1.6 Zenodo. <https://zenodo.org/record/4294676#.YD0tkuhKg2w> and D. Johnstone et al, pyXem 0.13, Zenodo, <https://zenodo.org/record/4436723#.YD0p2ehKg2w> [Open-source software]
- [8] E. Thronsen, H. **Mørkeseth**, C.D. Marioara, K. Minakuchi, T. Katsumi, K. Marthinsen, K. Matsuda, and R. Holmestad "The effect of small additions of Fe and heavy deformation on the precipitation in an Al-1.1Mg-0.5Cu-0.3Si at.% alloy, Submitted 2022.



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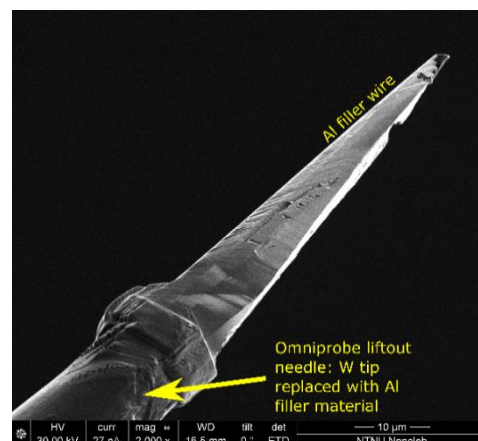




## Joining for a Multi-Material Future

### Motivation

The development of lightweight multi-materials in vehicles is inevitable to reduce the environmental impact and to increase fuel efficiency. This also counts for battery power packs, where replacement of Cu with Al wires can have a weight saving potential. However, welding dissimilar metals can be challenging since they often have large differences in thermo-physical properties, different solid solubility, and new phases can form on the interface. Hybrid metal extrusion & bonding (HYB) is a novel, patented solid-state joining technique developed by [HyBond](#). HYB can join dissimilar (or similar) metals at temperatures below the melting point of the most commonly used metals and alloys (cold welding), using a filler wire. Structural characterization on the nanoscale of multi-material joints and of the filler wire before and after joining is important to understand both the technique and the mechanical properties of the resulting joints. In project [In-Sane](#) we want to perform cold microjoining using a focused ion beam (FIB) instrument. In this project we offer a **summer job to work on the FIB to prepare samples for this project** (see figure).



replaced with Al (AA6082-T4) using a focused ion beam. The tip will subsequently be used for cold pressure microwelding. (image by Ambra Celotto).

### Your project

The summer job will be on working in NTNU NanoLab preparing samples to establish an efficient way to prepare the Al filler wire. Further, the student will characterize joints with transmission electron microscopy (TEM), possibly made using FIB. Thorough training will be given; the student will learn how to use the TEM, and to analyze and understand the results of different electron microscopy techniques, such as energy dispersive X-ray spectroscopy, electron diffraction and scanning TEM (STEM). The project can be adjusted to 15, 30, 45 or 60 ECTS.

### Requirements

For the summer job, a nanotechnology student with experience in using FIB is preferred. The student should be interested in materials physics, electron microscopy and electron diffraction, as motivation for the project work is the most important requirement. Experience with programming, preferentially Python, is an advantage. The most relevant courses are Nanotools, Solid State Physics and Materials Physics. It is important to be willing to work both independently and in cooperation with other researchers in the project. The student will collaborate closely with PhD candidates and SINTEF as part of the TEM group and the NANO2021 project In-Sane. The results will complement other work and will likely be part of scientific publications.

### Contact persons

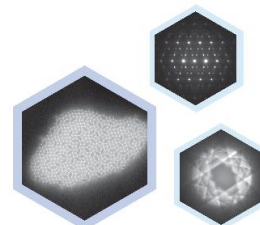
Associate Professor II/SINTEF scientist Per Erik Vullum ([per.erik.vullum@sintef.no](mailto:per.erik.vullum@sintef.no)), Professor Randi Holmestad ([randi.holmestad@ntnu.no](mailto:randi.holmestad@ntnu.no)) and PhD student Jørgen A. Sørhaug, ([jorgen.a.sorhaug@ntnu.no](mailto:jorgen.a.sorhaug@ntnu.no)), Department of Physics, NTNU.

The project is a collaboration with professors Filippo Berto, Jan Torgersen and Øystein Grong and PhD student Ambra Celotto Department of Mechanical and Industrial Engineering



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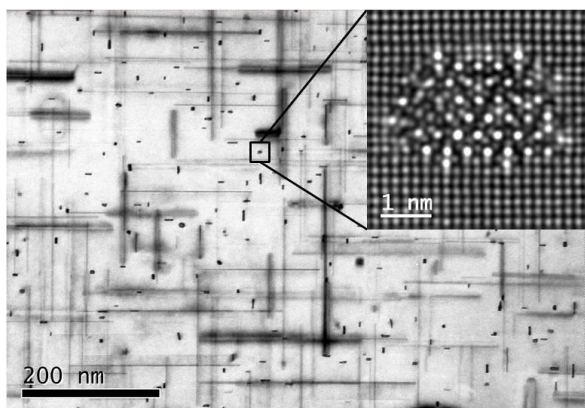
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## TEM investigations of aluminium alloys in collaboration with industry



### Motivation

In the studies of light metal alloys there are challenges when it comes to establishing relations between the nano-structure and the mechanical properties, as for example strength and ductility. In Al-Mg-Si-Cu alloys, the strength increase is due to precipitation of nanometer-sized metastable phases that form from solid solution during heat treatment. These so-called precipitates are studied by transmission electron microscopy (TEM), see image to the left.

NTNU (Departments of Physics and Materials Science and Engineering) and SINTEF have several ongoing collaboration

projects with Norwegian (and international) aluminium industry. Within this collaboration, we offer specialization projects/masters within characterization of microstructure in aluminium alloys. The work will contribute in the development and design of new aluminium alloys, mainly for the automotive industry. This work can be connected to the [SumAl](#) project or the [SFI PhysMet](#) centre, where we work in close collaboration with SINTEF, [Hydro](#), [Benteler Automotive](#) and [Neuman Aluminium Raufoss](#) and other industry partners. The student will be invited to internal aluminium meetings as well as to project meetings in Trondheim or/and at industry sites. **This year we offer a summer job at NTNU in Trondheim for a kick-start of the project/MSc work!** Within this field there are also possibilities for internships in Japan and continuation as a PhD student.

### Your project

In [SumAl](#) we have currently a project with Benteler Automotive where we want to combine accurate TEM measurements with tensile tests. The aim of the project is to change and control the precipitate growth process, hence adjusting the overall material performance. The student(s) will here run different heat treatments and do metallurgical characterization of properties (such as hardness, strength, ductility and conductivity). Afterwards the student will study the corresponding nanostructure (precipitates) in the TEM, supervised and in collaboration with PhD students and SINTEF researchers (who can help with more advanced microstructure characterization if needed).

### Requirements

Background in materials physics (solid state physics) and an interest in material science would be an advantage. We want students interested in doing experimental work and working independently in a larger group.

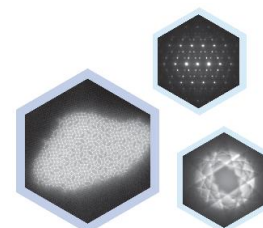
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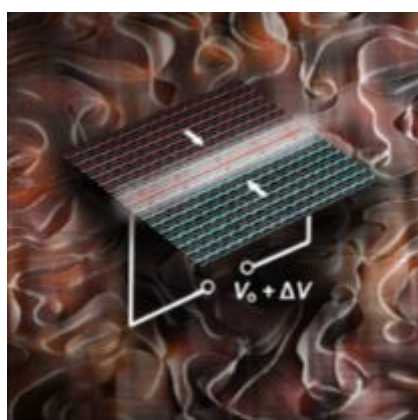




## Domain imaging in ferroelectric oxides

### Motivation

Ferroelectric materials exhibiting a spontaneous electric order that can be switch. This class of materials is now in the spotlights because of interesting solid-state physics phenomena, already finding application in state-of-the-art non-volatile data storage. In addition, these materials hold great potential for the realization of conceptually new concept for nanoelectronics devices. The unique electric properties of ferroelectric materials are related to the structure at the atomic scale and, hence, controlling structure means controlling electronic functionalities. At NTNU, there are several research groups working on the forefront in ferroelectrics research. This student project is part of a collaboration between the departments of physics and materials, where the ferroelectrics are studied in order to enable next-generation nanotechnology. Transmission Electron Microscopy (TEM) is an indispensable technique to understand the electric order across all relevant length scales down to the atomic scale.



### Your project

Your task will be to image the electric domain and domain-wall structure in functional ferroelectrics by TEM at different scales. The atomic-scale properties of the candidate materials fall into a largely uncharted territory, offering an ideal playground for high-resolution TEM studies. You will learn to prepare TEM specimens starting from millimeter-sized single-crystals, study the microstructure at different length scales, including lattice defects and how these interact with the domain structure. The same materials will be studied by PhD students using complementary techniques, such a scanning probe and scanning electron microscopy techniques. You can have a vivid exchange and scientific discussion with your colleagues. In the project you will learn basic TEM, including lattice imaging and diffraction techniques. In a follow-up master, the work might be extended with scanning electron microscopy (SEM), scanning electron diffraction and electron spectroscopy techniques (EELS fine structure data analysis). The project can be adjusted to 15, 30, 45 or 60 ECTS.

### Requirements

- Interest in experimental work, which here includes specimen preparation and operation of larger microscope units. Some data processing could be included.
- Have regular meetings with supervisors to link your TEM work to other activities on the same material. You should be able to clearly communicate and relate your own work to that of others in the group.
- Interest in doing research to understand how properties are related to the materials structure.

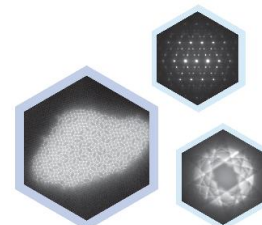
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# Extracting meaningful data from BIG electron diffraction data sets

## Motivation

The advances made in data technology have made the terms *big data* and *machine learning* more than just buzzwords. In daily life, big data and machine learning are steering us in the background (e.g. with search engines) and will be even more used in the future (e.g. Google car). In nearly all research fields a disruptive transformation is ongoing due to these advances.

In the TEM group we have been working on new ways to analyze scanning electron diffraction data (ie acquiring 2D diffraction pattern at each pixel). Group members on all levels, including project students, have contributed to recent progress. We have a state-of-the-art, special detector for electron diffraction. The new detector enables acquisition of datasets 10 to 100 times as big as what is commonly acquired today. New ways are needed to handle the growing amount of data and to extract the added information in it. Work on analyses of such data is part of ongoing research and international collaboration focused on achieving smart data acquisition and data handling.

## Your project

You will get TEM data sets, primarily scanning electron diffraction data, and develop and test new routines and algorithms for the analysis of the given data. The aim is to do crystal phase or orientation analysis over larger areas preserving nm-scale spatial resolution. The data could be from semiconductor material, nanoparticles, or aluminium-alloys. In addition, there is special interest in establishing routines for analysis of beam-sensitive non-crystalline materials, e.g. biomaterials and plastics. Collaboration with the data-owner, taking part of new experimental sessions, and understanding the physics behind the crystallography data can be important. The created digital tools should be made available and accessible to other people in the research community via open-source platforms, primarily by including developed code via Git into the repositories pyXem. This means that the whole process of development also must address implementation, version control, testing and documentation. The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Required from the student

You should have an interest in using and further developing software tools. Experience with Matlab, C++ or preferably 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 also important. The intention is that results will contribute to scientific publications. The expertise you will gain during this project should be attractive for jobs outside the field of material physics, as the tools and skills can be applied to challenges in several fields.

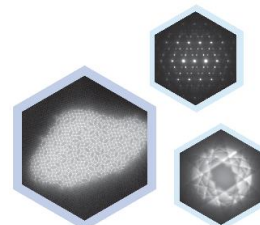
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# TEM studies of catalysts and membranes

## Motivation

Two specialization projects are available within a collaboration between the TEM and KinCat NTNU Gemini Centres with link to the centre [iCSI – industrial Catalysis Science and Innovation](#). Development of *state-of-the-art* research methodology is at the core of iCSI's activities and includes investigating catalysts and process materials at the nanoscale. You will study catalysts or membrane materials that are of high industrial and environmental relevance. The projects involve collaboration with several research groups and industry, and it is likely that your work will be a part of a publication.

## Your Project

You will get TEM training to become an independent user, and you will employ a combination of imaging, spectroscopy, and diffraction techniques to characterise your material system. *State-of-the-art* instruments at the Norwegian national infrastructures NORTEM (TEM) and NorFab (SEM and FIB) will be used. The project goals and experimental methodology will be tailored according to your interests. You will have the opportunity to both work on collection of big TEM data, and on data analysis and method development. For instance, the TEM group has specialised towards scanning electron diffraction data collection and data analysis routines, which are currently hot topics in the field. Additional investigations by spectroscopy (e.g. Raman, IR, XPS, Auger) or theoretical modelling (DFT) can be included depending on the relevance and interest. You will study on one of the two following material systems (both project can be adjusted to 15, 30, 45 or 60 ECTS):

1. **Silver (Ag) catalysts for partial oxidation of methanol to formaldehyde (MTF)** - characterisation of Ag restructuring and oxygen dissolution in Ag. Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate in the production of many fine chemicals. We collaborate with the formalin technology operator and licensor Dynea and the catalyst producer KA Rasmussen AS. The Ag catalyst restructures heavily under process gas at 650°C, and the restructuring is coupled to the interaction with and dissolution of oxygen. These phenomena again affect the selectivity to the desired product, CH<sub>2</sub>O. Better understanding of the crystalline structure and chemical interactions before, during and after the reaction may facilitate increased productivity in the MTF process.
2. **Pd alloy thin films for hydrogen separation membrane technology** – structural phenomena related to hydrogen transport and membrane stability. PdAg membrane technology is currently being commercialized by Hydrogen Mem-tech based on a sputtering fabrication process developed by SINTEF Industry. The idea is to enable Blue Hydrogen, i.e. hydrogen from natural gas with capture and storage of CO<sub>2</sub>. Investigating the structural properties and changes occurring during separation could yield information critical to performance and stability improvements.

## Contact persons

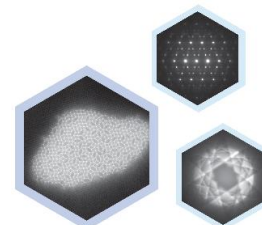
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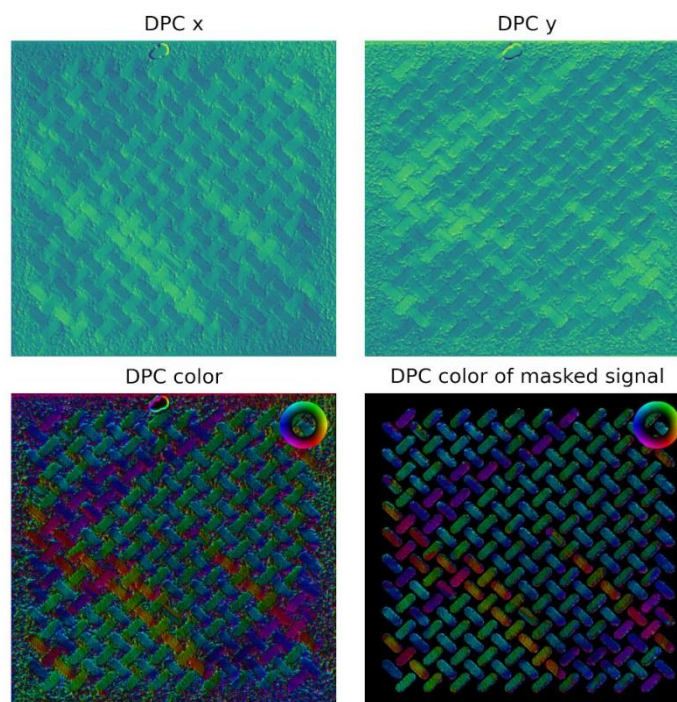




# Nanoscale imaging of ferromagnetic artificial spin ice structures using Transmission Electron Microscopy

## Motivation

Ferromagnetic materials are an important class of functional materials, with applications within data storage and sensing devices. A fairly recent development is nanostructuring of these materials, allowing for tailoring of the magnetic structure and properties. One such class of systems is artificial spin ice (ASI), shown in the figure. Here, nanostructuring techniques such as the Focused Ion Beam (FIB) or Electron-Beam Lithography (EBL) is used to make magnetic elements which acts as individual magnetic “spins”. When these elements are placed close together, they interact with each other, and form macroscopic magnetic “domains”. The structure and behavior of these “domains” depend on the size, angle, and distance between the elements.



## Your project

You will study the ferromagnetic domain structure of artificial spin ice structures using the TEM. This will involve using the Scanning Transmission Electron Microscopy – Differential Phase Contrast (STEM-DPC) technique, which gives the color maps shown in the figure. The aim will be to see how the ferromagnetic domains respond to external magnetic fields, which will be applied inside the TEM. You will learn how to operate and use the TEM, combined with the state-of-the-art of nanoscale magnetic imaging. This will be coupled with advanced data processing utilizing python libraries such as HyperSpy and pyXem. The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Requirements

The student should be interested in experimental work using the TEM, and programming using Python. The most relevant courses are Solid State Physics, Material Physics and Nanotools.

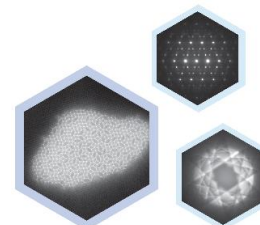
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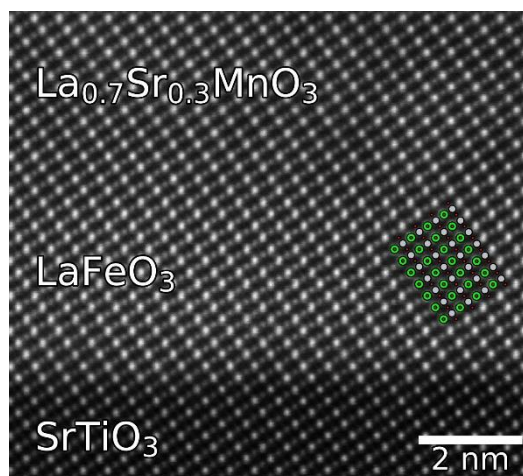




# Nanoscale structural and magnetic studies of perovskite oxide thin films using TEM

## Motivation

The perovskite oxide material family exhibit a wide range of functional properties, from ferromagnetism and ferroelectricity, to multiferroicity and colossal magnetoresistance. This range of properties is enabled by a strong structure-function coupling, where small changes in the structure can result in large changes in the functional properties. Through careful tuning of growth parameters, different types of perovskite oxides can be grown epitaxially, down to nanometer length scales. This thin film growth introduces a large range of parameters to fine tune the functional properties. To properly understand how these functional properties arise in these thin films, it is necessary to study them at the nanoscale: both the chemical composition, crystal structure, and functional properties.



## Your project

You will use the Transmission Electron Microscope (TEM) to study magnetic perovskite oxide thin film materials. The aim will be to characterize both the crystal structure and magnetic domain structure of the films, to better understand the coupling between the structure and functional properties. This will also be coupled with advanced data processing using Python, utilizing libraries such as HyperSpy and pyXem. The thin films will be made by Ingrid Hallsteinsen's group at IMA, and be made as TEM-samples via the Focused Ion Beam by her group. Thin film materials will include  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ ,  $\text{LaFeO}_3$  or  $\text{La}_2\text{NiMnO}_6$ . The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Requirements

The student should be interested in experimental work using the TEM, and programming using Python. The most relevant courses are Solid State Physics, Material Physics and Nanotools.

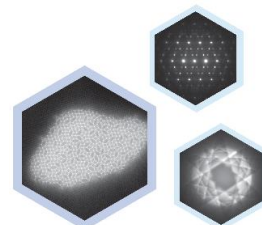
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# Electron microscopy of thin films for spintronics applications

## Motivation

Spintronics is an emerging field which connects theoretical physics, nanotechnology, materials science and computer science. It is a method for computation with low energy dissipation, where information is transmitted by spins rather than electric charge. Certain materials such as antiferromagnets are ideal for the transmission of spin waves at low temperatures. The Center for Quantum Spintronics (QuSpin) at NTNU has established a lab for growth of the antiferromagnetic thin film materials FeSn and CuFeS<sub>2</sub>. To assess whether growth conditions are ideal for creating a single phase, monocrystalline, defect free thin film, transmission electron microscopy characterization is essential.

## Your project

Your work will be focused on the atomistic structure of thin films and their connection with the growth substrate. High-resolution TEM imaging of the atomic lattice will be used to observe defects, compositional changes, and lattice misfits between the substrate and the thin film. Samples will be prepared by mechanical polishing, Ar ion milling or focused Ga ion beam milling. 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. The project can be adjusted to 15, 30, 45 or 60 ECTS.

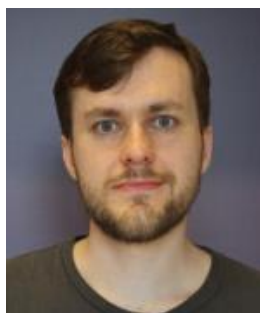
## Requirements

The student should have a background within physics or nanotechnology and have an interest in condensed matter physics and crystallography. You will work independently with a range of experimental methods and provide feedback to the thin film growers on film quality and growth parameters. Any experience with SEM/FIB will be useful for sample preparation.

## Contact persons

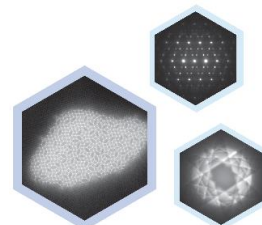
Magnus Nord, Associate Professor, Department of Physics, NTNU, [magnus.nord@ntnu.no](mailto:magnus.nord@ntnu.no) Ton van Helvoort, Professor, Department of Physics, NTNU, [a.helvoort@ntnu.no](mailto:a.helvoort@ntnu.no)

This project is in collaboration with Christoph Brüne from Center for Quantum Spintronics (QuSpin) - NTNU.



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# Mineralogy and TEM: nm-scale characterization of beautiful systems

## Motivation

While mineral specimens are spectacular objects for rock collectors and wearers of gems, they also are invaluable recorders of rock-forming processes in the earth's crust and its deeper interior. Their detailed chemical composition (nominal constituents as well as impurities), their crystal structure (including polytypes), and fluid-driven reactions transforming pre-existing minerals into new that better suit changing pressure and temperature conditions, provide insights in rock formation and ore-forming processes. TEM is an essential tool to study the nature and transformations within and between minerals at the smallest scale.

## What the student will do in the project

The student will learn how to operate a TEM to characterize mineral crystallographic and compositional properties. The project aims to link observations at different size scales (eg. optical microscopy/petrography – SEM – TEM) and different techniques (eg. microscopy, EDS, XRD). Consequently, sample and specimen preparation will be an important part of the study. The project will look at illite, a phyllosilicate (clay) mineral closely related to muscovite and other micas. The illite is formed during brittle deformation (*viz.* 'earth quakes') and is particularly challenging to study because of fine grain size, as well as variations in chemistry (Al,Si-ordering, interlayer content/vacancies), polytypism and morphology. The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Required from the student

The perfect applicant has an interest in interdisciplinary experimental work, and is creative, inventive, self-reliant, independent, pro-active, and able to communicate cross-disciplinary with researchers from different disciplines.

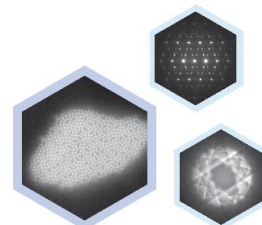
## Contact persons

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## Conductivity of aluminium at the nanoscale



### Motivation

There is recently huge industrial interest in using aluminium (Al) instead of copper (Cu) in cables and busbars for electrical vehicles, both because of favourable price and weight. One key challenge in further improving Al-alloys for conductor applications is to better optimize for high electrical conductivity while maintaining good mechanical performance at elevated temperatures. The main factors that cause improvements in strength are additions of alloy elements (solid solution and precipitate strengthening) and deformation

(reduction of grain size and work hardening). However, both lead to losses in electrical conductivity when compared to pure, undeformed Al. In this project we will establish a method for measuring conductivity in aluminium alloys from very small volumes based on studies of electron-phonon coupling phenomena in transmission electron microscopy and use the results from such measurements to extract data for the electrical conductivity of specific microstructure constituents at unprecedented spatial resolution.

### Your project

Electron resistivity can be estimated at the nanoscale by plasmon characteristics of electron energy loss spectra (EELS) in a transmission electron microscope (TEM). You will measure quantities that characterize the electron-phonon coupling by EELS at the nanoscale of different materials/phases/constituents, and fit theoretical conductivity models to the data extracted from the spectra. The studies will address the effects factors such as alloying, deformation, temperature, etc. have on the conductivity of individual microstructure components. You will make TEM samples, learn how to operate the TEM, do experiments, and analyze the results in Python. Thorough training will be given; in how to operate the TEM, and to analyze and understand the results of different electron microscopy techniques, such EELS and electron diffraction. The project can be adjusted to 15, 30, 45 or 60 ECTS.

### Requirements

We search for a student with background in materials physics/solid state physics, who is creative and interested in experimental work, method development, and programming/data analysis.

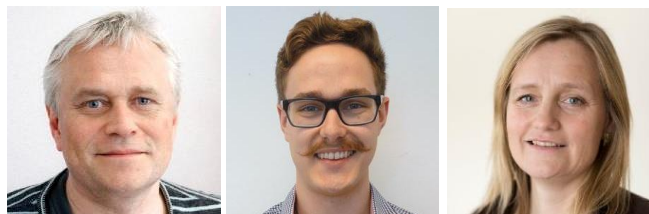
### Contact persons

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Senior engineer Emil Frang Christiansen,

[emil.christiansen@ntnu.no](mailto:emil.christiansen@ntnu.no)

Professor Randi Holmestad, IFY, [randi.holmestad@ntnu.no](mailto:randi.holmestad@ntnu.no)

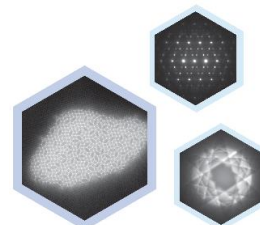


Materials will be provided by  
Hydro Precision Tubing through  
Dr. Jonas K. Sunde, [jonas.sunde@hydro.com](mailto:jonas.sunde@hydro.com)



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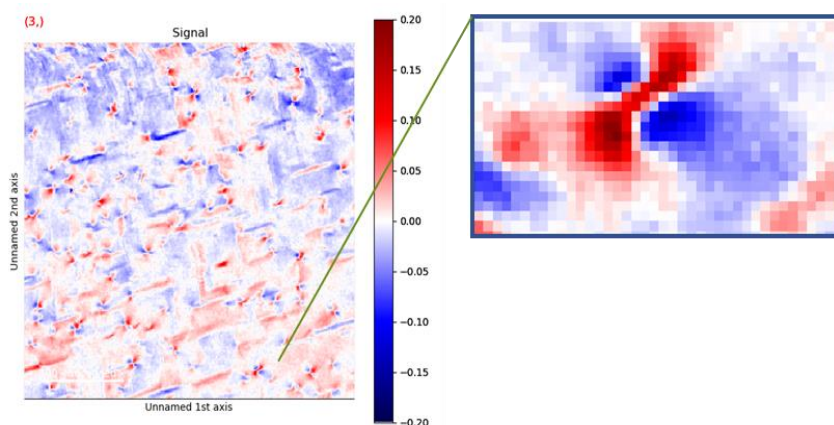




# Data analysis of strain around precipitates in Aluminium alloys

## Motivation

Production of aluminium alloys is an important industry for Norway. The strongest aluminium alloys are heat treatable, meaning that they gain strength from nano-sized precipitate phases during heat treatment. These precipitates have different crystal structures, that are coherent with the aluminium crystal lattice. The lattice parameters of precipitates and aluminium are generally slightly different, resulting in the precipitates pushing the aluminium lattice outwards, creating a strain field. This field is important for the growth of precipitates and how they hinder the deformation of the material.



The scanning precession electron diffraction (SPED) technique has proven to be very sensitive to changes in crystal structure and therefore also changes in lattice parameters (strain). The TEM Gemini Centre hosts a state-of-the-art system for SPED, using a direct electron detector that counts each diffracted electron for maximum sensitivity. This has been used to acquire datasets from alloy systems containing several different precipitate phases, and can be used to generate strain maps (see fig).

## Your project

The project concerns analysis of SPED datasets, with an emphasis of accurate strain quantification and comparison with physical models. As the datasets contain rich information, the strain distribution will be correlated to precipitate phase and orientation, producing statistical correlations across different alloys and heat treatment conditions. Python packages are available for advanced data analysis. The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Requirements

We search for a student with background in materials physics/solid state physics, with interest in doing programming/data analysis. Experience with Python is wanted.

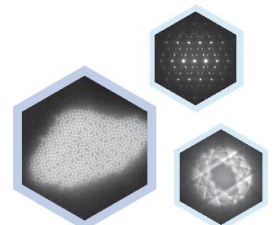
## Contact persons

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 Ruben Bjørge, SINTEF Industry, [ruben.bjorge@sintef.no](mailto:ruben.bjorge@sintef.no)  
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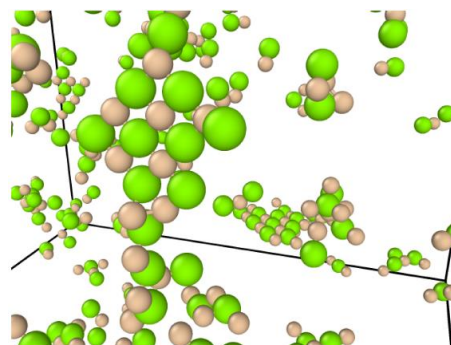
# Atomistic modelling of clustering in aluminium alloys

## Motivation

Precipitation hardening is the most important strategy for the aluminium industry to improve performance of both AA6xxx wrought alloys and foundry alloys. A key to control and manipulate nucleation and growth of hardening precipitates is to understand their formation, starting from clustering of solute atoms.

## Your project

The student will study the clustering of solute atoms and the initial formation of metastable particles using kinetic Monte Carlo (KMC). This will be done by using an existing off-lattice KMC code called k-ART. Input to the simulations will come from close collaboration with other researchers and students working experimentally with transmission electron microscopy (TEM) and theoretically with density functional theory (DFT) or cluster expansion.



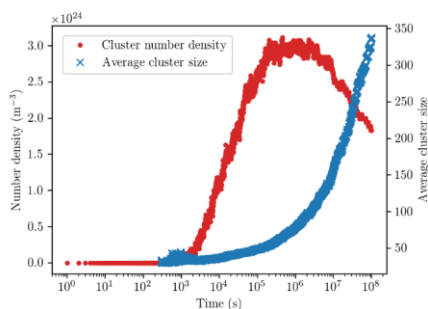
*Simulated clustering of Mg and Si in aluminium using kinetic Monte Carlo.*

## Requirements

Background in materials physics (solid state physics), and interest in materials science would 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. Programming experience is essential.

## Other aspects

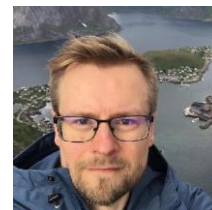
There are many people working on aluminium alloys at NTNU, and we have several ongoing external projects. This work will be connected to the SumAl project, where we work in close collaboration with SINTEF, Hydro, Benteler Automotive and Neuman Aluminium. The students will be invited to internal aluminium meetings as well as to project meetings in the SumAl consortium in Trondheim or/and at industry sites. Students get their own problem which fits well into the rest of the work done. Within this field, there are possibilities for continuation as a PhD student and summer job. This topic is also coupled to the NTNU Digital Transformation project "AllDesign" by Professor Jaakko Akola which builds a multiscale modelling platform for these alloys.



*Cluster evolution predicted på KMC.*

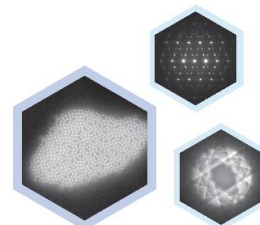
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# Calculation of energy barriers by cluster expansion

## Motivation:

The global demand for aluminium alloys is increasing along with the focus on more environmentally friendly materials in industrial applications. The advance of computer-driven alloy design requires better interatomic potentials to incorporate lower scale effects into the models. Nudge elastic band (NEB) method, Figure 1, is a routine method of finding minimum energy pathways for barrier calculations, but this is tedious work if you have many possible steps to consider.

An alternative way to calculate the energy barriers is to train a cluster expansion algorithm. This method can be used to efficiently calculate the energy barriers of a configuration based on parametrisation within a Bayesian framework. Accurate NEB calculations are used in the training set.

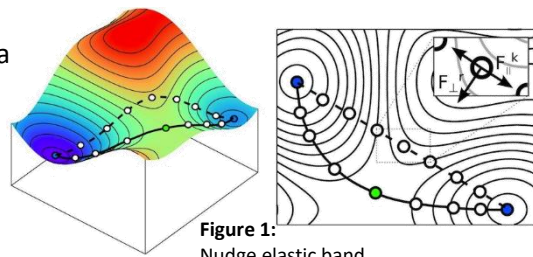


Figure 1:  
Nudge elastic band

## What the student will do in the project:

The student will study various configurations in a relatively simple aluminium alloys system (Al-Sc) to validate the calculations of the energy barriers by cluster expansion. The validation is conducted in an in-house kinetic Monte Carlo (KMC) framework. The precipitation of the Al-Sc clusters is one of the key outputs expected from the simulations. The student will also be part of a group of other researchers and students that are investigating aluminium with density functional theory, molecular dynamics, and transmission electron microscopy.

## Required from the student:

Background in material physics and interest in material science would be an advantage. We need a student which is interested in modelling and programming, thus some experience with numerical methods will help to quickly get started.

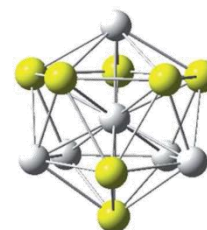


Figure 2:  
Al<sub>6</sub>Sc<sub>7</sub> (ref. doi.org/10.1039/D1RA06994B)

## Other aspects:

The use of cluster expansion to calculate energy barriers is a novel method developed by the joint modelling group of the TEM Gemini centre and SINTEF industry. Collaboration outside NTNU is ongoing, and a short exchange might be possible. Many people are working on aluminium alloys at NTNU, and we have several ongoing external projects. The student will be connected to the [SumAl project](#), where we work in close collaboration with SINTEF, Hydro, Benteler Automotive and Neuman Aluminium. The student will be invited to internal aluminium meetings as well as to project meetings in the SumAl consortium in Trondheim or/and at industry sites. Students get their own problem which fits well into the rest of the work done. Within this field, there are possibilities for continuation as a PhD student and summer job. This topic is also coupled to the NTNU Digital Transformation project "AllDesign" by Professor Jaakko Akola which builds a multiscale modelling platform for these alloys.

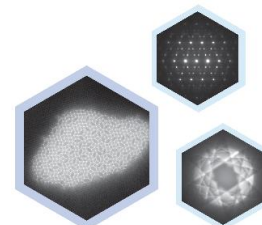
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# Advanced processing of electron spectroscopy data from nanostructures

## Motivation

Determining the composition with high spatial resolution is important for many technological and academic projects. The main spectroscopy techniques available in electron microscopy are catholuminescence (CL), energy dispersive and electron energy loss spectroscopy (EDX and EELS respectively). EDX is the most used as it is relatively easy to acquire data. However, accurate quantification is in general challenging. The most used method for quantification of EDX data is based on a dated empirical method with drawbacks and presumptions that often are not met. Crystal orientation, particle shape and statistics can affect the final quantification.

People in the TEM Centre have been working on an alternative method, termed the zeta method, that is not yet available in commercial EDX packages. The zeta method can give more accurate compositional analysis than the currently default approach. Group members have also developed a factor-less approach and have worked on calibration routines. These methodologies should be developed further before they can be used by all SEM and TEM users. Developing the quantification code base ourselves allows linking EDX to other data types such as diffraction patterns and EELS. In addition, implementation of new technologies such as machine learning to reduce data set sizes or noise levels has proven valuable.

## Your project

There are two possibilities: i) First collecting yourself EDX data by SEM (NanoLab) and TEM. Or ii) focus will be on the data analysis, and you will get data acquired in other projects, for example using internal calibrations. You must become familiar with the characteristics of the EDX technique and the data structure as well as code already developed by previous students which is made available via open-source projects. Depending on the chosen material system at the start of the project, the focus will lie on extending the zeta approach or automating the detector calibration so it can be implemented in the analysis to improve the overall accuracy in the final compositional analysis.

## Required from the student

Interest and skill in applying and further developing Python-based software tools are required. You will have to balance fundamental aspects, implementation of code and working on real material systems and problems, i.e. to work on practical and theoretical aspects in parallel. Good communication and interaction with collaborating scientific and academic staff and PhD students, also based abroad, is essential. The project will use and contribute to the open-source platform [HyperSpy](#). This project offers the opportunity to become familiar with code development for spectroscopy and could be extended in a master to other techniques and material systems.

## Contact person

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



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