# Project work / Master / Diploma topics in the TEM Gemini Centre, 2021/22

## 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, 1 Postdoc, ~8 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.

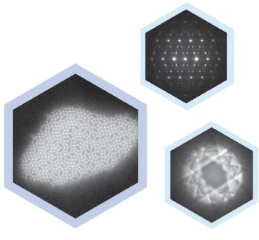
Examples of student projects which are available:

- 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.

https://www.ntnu.edu/physics/temgemini



## 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.

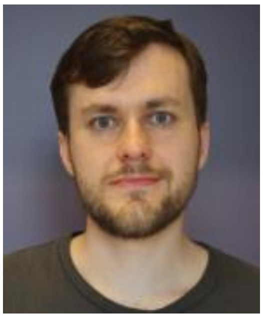
Within the Aluminium projects we this year offer a summer job through SFI PhysMet at NTNU. There is also a possibility to stay one month in Japan in an aluminium company as a part of the project/MSc (covid permitted!) – We also offer a summer job in the project with Elkem!. Ask us about details!

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

## Contacts





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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 $K_{0.5}Na_{0.5}NbO_3$ 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.

[4] H.W. Ånes, I.M. **Andersen** and A.T.J. van Helvoort, Crystal Phase Mapping by Scanning Precession Electron Diffraction and Machine Learning Decomposition, Microscopy and Microanalysis 24(S1), pp. 586-587, 2018.

[5] J.K. Sunde, Ø. **Paulsen**, S. Wenner and R. Holmestad, "Precipitate statistics in an Al-Mg-Si-Cu alloy from scanning precession electron diffraction data", Journal of Physics: Conf. Ser., 2017, 902, 012022. doi :10.1088/1742-6596/902/1/012022

[6] A. Mosberg, S. **Myklebost**, D. Ren, H. Weman, B. Fimland and van A.T.J. Helvoort, "Evaluating focused ion beam patterning for position-controlled nanowire growth using computer vision", Journal of Physics: Conf. Ser., 2017, 902, 012020. doi :10.1088/1742-6596/902/1/012020

[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] T. Bergh, **H. Fyhn**, L. Sandnes, J. Blindheim, Ø. Grong, R. Holmestad, F. Berto, P.E. Vullum "Microstructure and tensile and tensile properties of a multi-material aluminium-copper-steel-titanium butt joint made in one pass by hybrid metal extrusion & bonding" Submitted.

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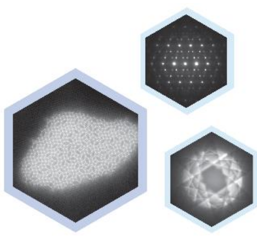
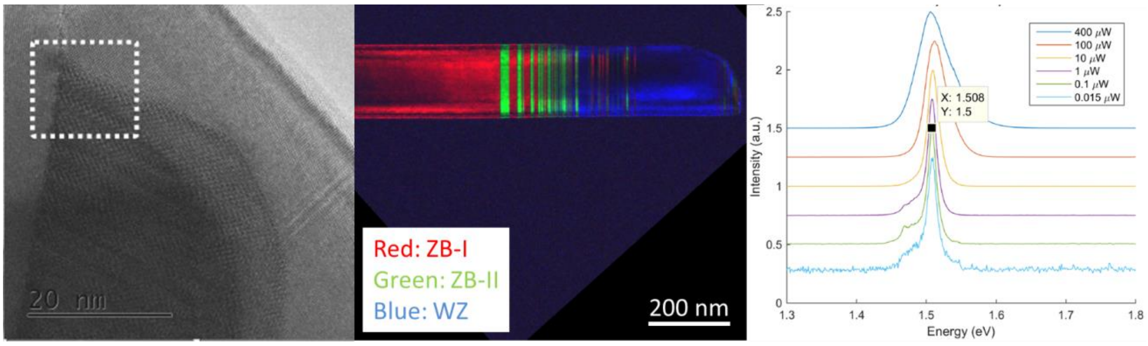


# Structural characterization of heterostructured semiconducting nanowires

## Motivation

III-V semiconductor nanowires with high quality are grown at Department of Electronic Systems (IES) for future applications in optical devices (LEDs, 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 optoelectrical 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 & electrical 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 can be adjusted to 15, 30, 45 or 60 ECTS.

## 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.

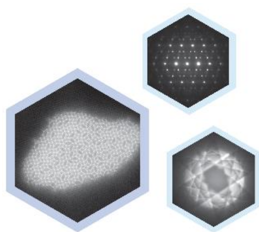
## Other aspects

The field of semiconductor nanowires, fundamental understanding and application of them in devices had an enormous growth in the last years. We had already 14 project/master 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: Helge Weman (IES) and Bjørn-Ove Fimland (IES).





TEM Gemini Centre

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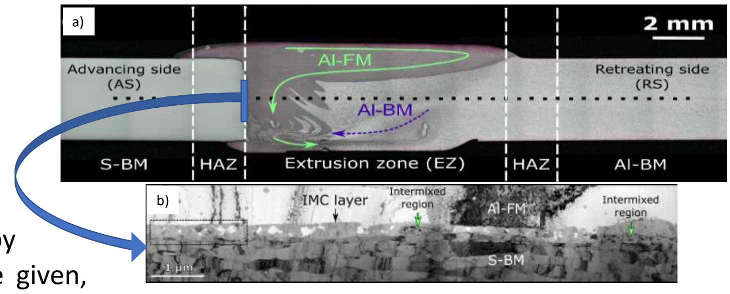
# Joining for a Multi-Material Future

## Motivation

The development of lightweight multi-materials in vehicles is inevitable to reduce the environmental impact and to increase fuel efficiency. Two examples here are 1) vehicle bodies, where aluminium-steel joints combine the low weight and formability of aluminium with the strength and low cost of steel and 2) battery power packs, where replacement of Cu with Al cables has enormous weight saving potential. To join or bond metals is challenging, since they often have large differences in thermo-physical properties, different solid solubility and new phases are formed on the interface. Hybrid metal extrusion and bonding (HyB) is a novel, patented solid-state joining technique developed by HyBond, where dissimilar metallic materials can be joined at low temperatures using a filler wire. Structural characterization on the nano-scale of the 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.




*The figure shows a) an optical macrograph of the Al-steel HYB butt weld and b) TEM characterization of the HYB Al-steel interface region (from Sandnes, Bergh, Grong, Holmestad, Vullum, Berto, Mat. Sci. & Eng. A, in press (2021) 140975. https://doi.org/10.1016/j.msea.2021.140975*

## Your project

The student will characterize multi-material joints with transmission electron microscopy (TEM). Thorough training will be given, and 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

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 electron microscopy or with programming, preferentially Python, is an advantage. The most relevant courses are 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. The results from the project work will complement research done by others and will likely be part of scientific publications. The student will be a part of the TEM group and connected to the SFI Manufacturing centre that has 15 industrial partners, and the NANO2021 project In-Sane where we want to do nano-joining inside the focused ion beam (FIB) instrument.

## Contact persons

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Randi Holmestad, Professor, Department of Physics, NTNU.
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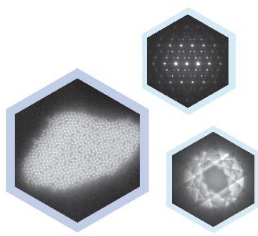
The project is a collaboration with Department of Mechanical and Industrial Engineering and professors Filippo Berto, Jan Torgersen and Øystein Grong.





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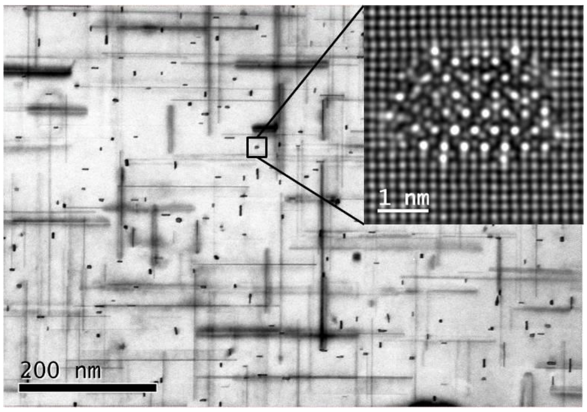
# TEM investigations of aluminium alloys in collaboration with industry




## 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 (see TEM image) that form from solid solution during heat treatment. These so-called precipitates are studied by transmission electron microscopy (TEM).

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. The students 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 SFI PhysMet we have currently a project with Hydro and Raufoss where we want to combine accurate TEM measurements with atom probe tomography (APT) measurements. The student(s) will here do experimental testing of properties (such as hardness, strength, conductivity..) with different heat treatments, and 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). We also have two specific project offers with Hydro Extrusions (see end of this document + contact us!)

## 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 of scientists.

## Contact persons

Randi Holmestad, Professor, Department of Physics, NTNU.
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Other key people in the project:
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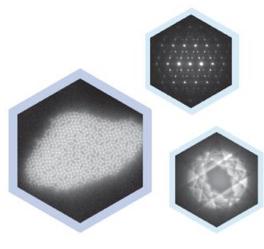


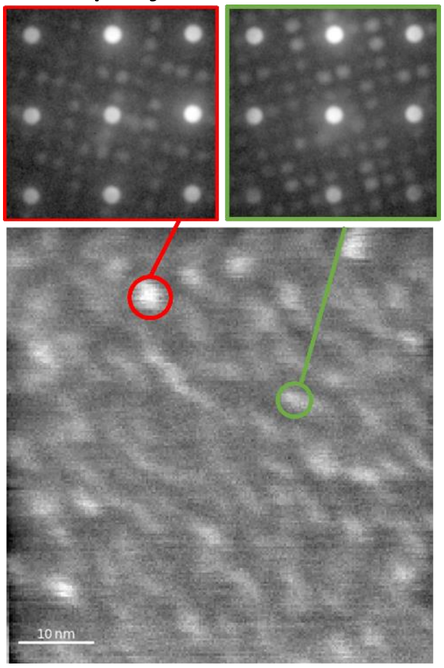


# Developing data processing routines for diffraction datasets from novel electron detectors

## Motivation

Electron diffraction is a crucial tool in characterizing different materials. At NTNU, the so-called scanning precession electron diffraction (SPED) technique has been extensively used for characterizing different Aluminium (Al) alloys to explain their macroscopic properties [1]. The goal is to understand the physics behind the strengthening mechanisms in Al alloys, by studying the early stages of industrial thermomechanical heat treatments at the nm scale. With the SPED technique, we obtain a 4D dataset comprised of a 2D real-space position and a 2D signal in reciprocal space (one electron diffraction pattern from each scanned position). Our facility has recently got one of the first new generation electron detectors, the so-called direct electron detectors. To fully use the potential of the new technology, there is a need to explore the detector settings and optimize the post-acquisition data analysis.

## Your project




We have acquired 4D datasets from the new detector, and an example dataset is shown in the figure to the left. In the image denoted VDF (virtual dark field), bright spots correspond to pixels where the diffraction patterns contain extra information compared to the Al surroundings. By adding the diffraction patterns inside the red and green circles in the VDF, we obtain diffraction patterns like the ones shown in the top of the figure. Here, the large bright spots are signal from Al, while we are interested in everything between the Al spots (clusters which are responsible for the materials strengthening). Your task will be to try out various data analysis techniques on the dataset to extract structural information from the small cluster regions. In addition, development of data processing routines for new datasets are planned.

## Requirements

The student will need programming experience (eg Python) and interest as well as knowledge within condensed matter physics.

## Contact persons

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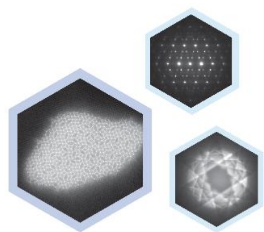
Others involved: Ton van Helvoort

[1] J.K. Sunde, C.D. Marioara, A.T.J. van Helvoort, R. Holmestad, The evolution of precipitate crystal structures in an Al-Mg-Si(-Cu) alloy studied by a combined HAADF-STEM and SPED approach, Mat. Char., 142, 2018, 458-469.

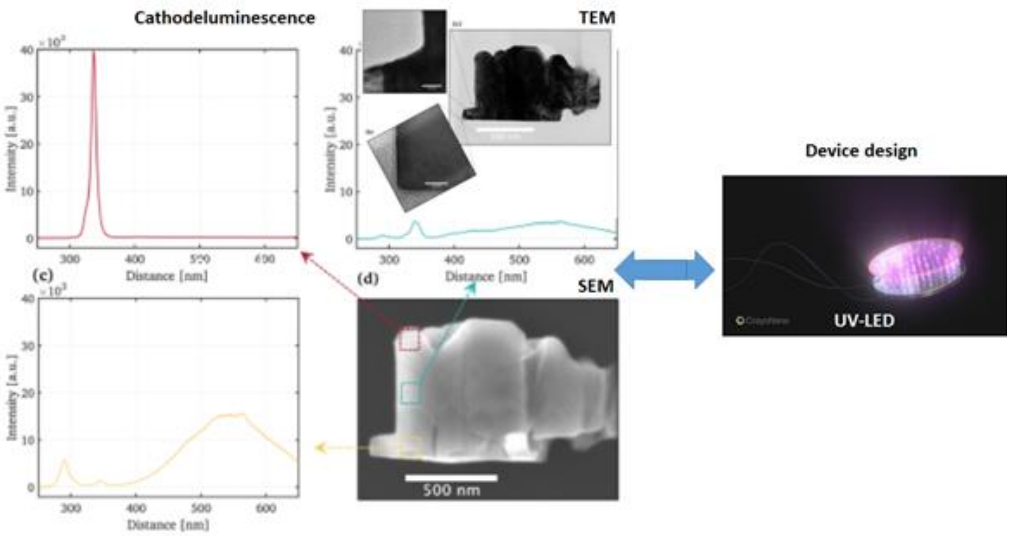




# Nanowire-based devices

## Motivation

CrayoNano has developed a method where heterostructured III-nitride semiconductor nanowires with high quality are grown on graphene. From them light emitting diodes (LEDs) emitting light in the UV-range are constructed. At Sluppen-Trondheim CrayoNano has a brand new Metal-Organic Chemical Vapor Deposition (MOCVD) lab. They are now continuously producing nanowire samples which need further processing and characterization. Because of their small size, the heterostructured nanowires and device elements have to be studied by characterization techniques with a high spatial resolution as for example Transmission Electron Microscopy (TEM).




## Your project

You will study a specific batch of nanowires with interesting optoelectronic properties. Your feedback helps to further optimize the growth conditions of the semiconductors (to be specific GaN and AlGaN segments grown with the new MOCVD). It is important to understand the relation between the optical properties as measured by cathodoluminescence (CL) and the crystal structure/lattice defects/composition as determined by you using TEM. You will learn to use basic TEM techniques as well as scanning electron microscopy (SEM) and CL.

## Requirements

- Interest in experimental work using SEM/CL and TEM.
- Have regular meetings with researchers at CrayoNano. You should be able to clearly communicate and relate your results to others in the project and understand what feedback they expect from your work.
- An interest in programming (Python/Hyperspy) is an advantage as these are valuable tools in the processing of the acquired data.

This is a unique opportunity to be part of applied nanotechnology and the dynamic practice in a high-tech start-up company. The obtained skills can be applied to study other nanostructures in academia and industry.

## Contact persons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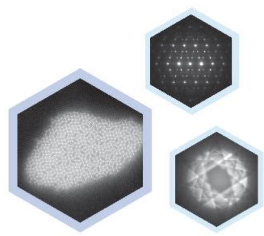
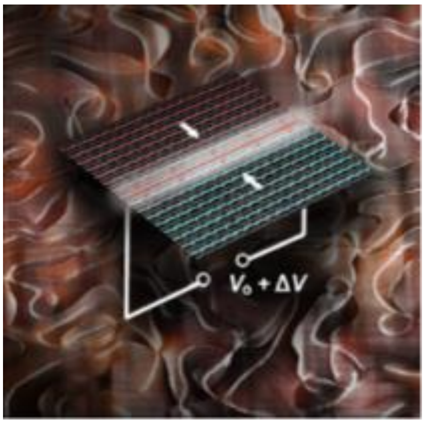




# Domain imaging in ferroelectric oxides

## 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.

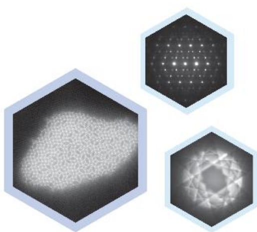
## Requirements

- 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.

## Contact persons

Ton van Helvoort (IFY, a.helvoort@ntnu.no) and Dennis Meier (IMA, dennis.meier@ntnu.no).







# 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.

## Contact person:

Ton van Helvoort (a.helvoort@ntnu.no) Others involved: Magnus Nord (Magnus.nord@ntnu.no), Phillip Crout (University of Cambridge) and Randi Holmestad (randi.holmestad@ntnu.no)

TEM Gemini Centre

NTNU SINTEF

# Transmission electron microscopy investigations of catalysts, membranes and process materials

## Motivation

Specialization projects are available within a collaboration between the TEM and KinCat NTNU Gemini Centres with link to iCSI – industrial Catalysis Science and Innovation – a Centre for research based innovation appointed by the Research Council of Norway and hosted by Department of Chemical Engineering, NTNU. Development of state-of-the-art research methodology is at the core of iCSI's generic activities and includes investigating catalysts and process materials at the nanoscale. The projects involve collaboration with ongoing research. Additional investigations by spectroscopy (e.g. Raman, IR, XPS, Auger) or theoretical modelling (DFT) can be included to the projects depending on the relevance and interests of the candidate.

## Your Project

The project concerns TEM-based investigations on one of the two following systems of high industrial and environmental relevance, dependent on the candidate's interests:

1. Silver (Ag) catalysts for partial oxidation of methanol to formaldehyde (MTF) - characterization of Ag restructuring and O 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, $CH_2O$. Better understanding of the crystalline structure and chemical interactions before, during and after 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 $CO_2$. Investigating the structural properties and changes occurring during separation could yield information critical to performance and stability improvements.

Both projects involve use of *state-of-the-art* instruments at the Norwegian national infrastructures NORTEM (TEM) and NorFab (SEM and FIB). The project can be adjusted to 15, 30, 45 or 60 ECTS.

## Contact person


Supervisors: Adjunct Professor (Prof. II) Per Erik Vullum (pererik.vullum@sintef.no) and Prof. Randi Holmestad (randi.holmestad@ntnu.no)

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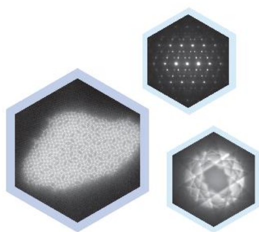
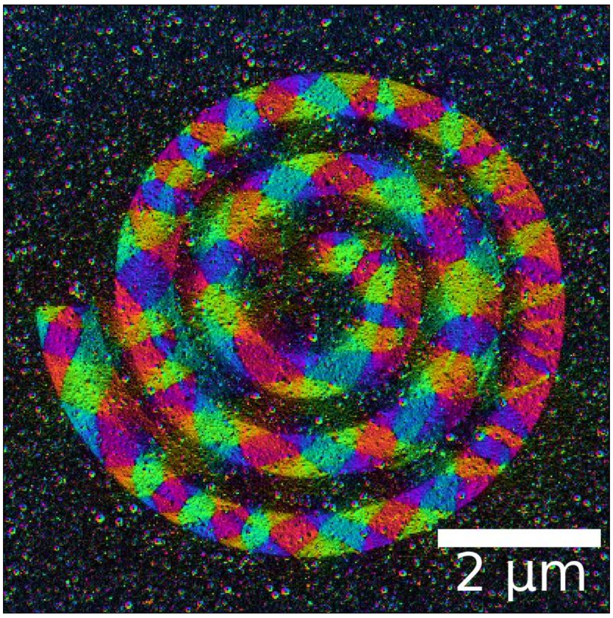


# Nanoscale imaging of magnetic structures using Transmission Electron Microscopy

## 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, such as the spiral structure seen in the figure. These magnetic nanostructures not only allow for new types of device concepts, but they are also ideal as nanoscale physics “model systems” as potentially any shape can be made, essentially acting as an experimental “nano lab” for studying magnetic theory.

To properly understand the magnetic properties of these materials, it is of vital importance to not only be able to image magnetic fields at nanometre length scales, but also to visualize the crystal structure in the same area simultaneously. Thanks to advances in fast cameras used in transmission electron microscopes (TEM), this is now possible. However, as this is a very recent development, much work is need in both developing better experimental techniques and data processing routines. The latter requires the implementation of “big data” data analysis, as the datasets can range from 8 gigabytes for small sets, up to hundreds of gigabytes for larger ones.




*TEM image of ferromagnetic domains in a spiral shaped nanostructured thin film. The colours showing the magnitude and direction of the magnetic domains.*

## Your project

You will study both the crystal and ferromagnetic domain structure in permalloy thin films using the TEM. Here, you will learn how to do basic TEM, followed by state of the art magnetic imaging. Initially this will be done with the Fresnel imaging technique, which is faster, easier to use and well-suited for studying how the ferromagnetic domain structures respond to external magnetic fields. This will be followed by the more advanced differential phase contrast technique, which yields much more information, but is more difficult from an experimental and data processing point of view. The latter will involve learning “big data” processing using the Python library HyperSpy, pyXem and dask, and best practices within software development. You will also learn how to use the state of the art Merlin fast electron detector. 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 and Material Physics.

## Contact persons

Magnus Nord, Associate Professor, Department of Physics, NTNU, magnus.nord@ntnu.no

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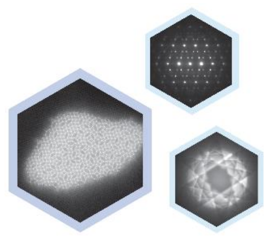


# Electron microscopy of thin films for spintronics applications

## 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 $CuFeS_2$. 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

Sigurd Wenner, Associate Professor II, Department of Physics, NTNU. Office: Realfagbygget D4-118. E-mail: sigurd.wenner@sintef.no.

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



# 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

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.

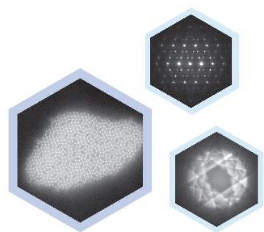
## Required from the student

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.

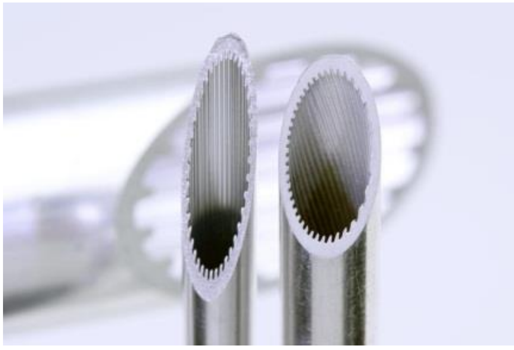
## Contact persons

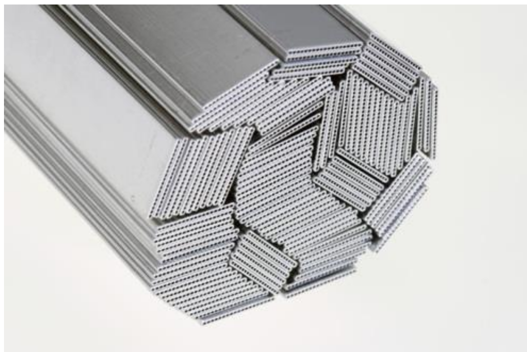
Ton van Helvoort (a.helvoort@ntnu.no) and Maarten Broekmans (maarten.broekmans@ngu.no)

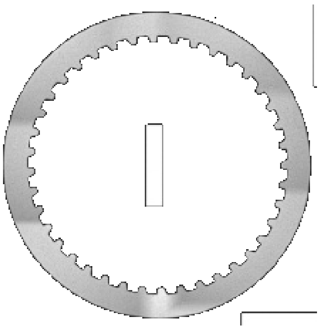




# Characterisation of Aluminium Round Tubes







Hydro Extrusions is the leading producer of extruded aluminium products in the world and the products are used in diversified areas such as automotive industry, buildings, ship and offshore, trains, electronics and even design furniture. This leading position is maintained through a combination of local expertise, a global network, and strong R&D capabilities.

Precision Tubing which is a business unit within extruded solutions manufacture extruded and drawn round and flat multi-port extruded (MPE) tubes for heat transfer applications. Most of the production is within the 1xxx and 3xxx series (Al-Mn) but also 5xxx (round tubes) and 6xxx (round tubes, cables, forging stock, shapes) is used for some applications due to the combination of strength and corrosion resistance.

Currently round tube alloys in the 5xxx series are 5049 alloy only with a high Mg content. This reduces the productivity of the alloy significantly. In an attempt to improve the productivity while still obtaining reasonably good mechanical properties and corrosion resistance, an intermediate Mg containing 5xxx alloy is being evaluated.

The aim of the current project, therefore, is to characterize the microstructure of the alloy in question as a function of processing (extrusion and drawing). Microstructural techniques such as SEM, EBSD, TEM will be used.

## Contact persons

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Randi Holmestad (NTNU, randi.holmestad@ntnu.no)

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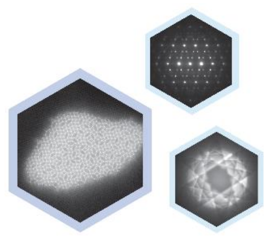

# Characterisation of Microstructure and Corrosion Susceptibility in Extruded Multi Port Tubes

Hydro Extrusions is the leading producer of extruded aluminium products in the world and the products are used in diversified areas such as automotive industry, buildings, ship and offshore, trains, electronics and even design furniture. This leading position is maintained through a combination of local expertise, a global network, and strong R&D capabilities.

Precision Tubing which is a business unit within extruded solutions manufacture extruded and drawn round and flat multi-port extruded (MPE) tubes for heat transfer applications. Most of the production is within the 1xxx and 3xxx series (Al-Mn), but also 5xxx (round tubes) and 6xxx (round tubes, cables, forging stock, shapes) are used for some applications due to the combination of strength and corrosion resistance. Figure 1 shows an example of a brazed and corrosion tested heat exchanger sample used for the ongoing tube alloy development.

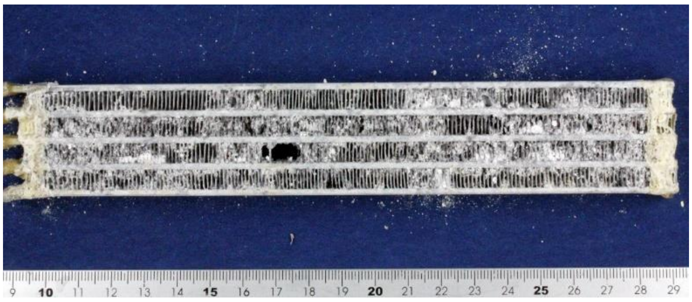


*Figure 1: An example of a brazed mini heat exchanger sample after corrosion testing. The fins have become detached from the tube due to the corrosive environment.*

During corrosion testing we see that there is a tendency to preferential corrosion along grain boundaries (intergranular corrosion (IGC)) as a function of alloy chemistry, braze coating applied and brazing exposure. Figure 2 shows in a closer view of a cross-section of the multi-port extruded (MPE)

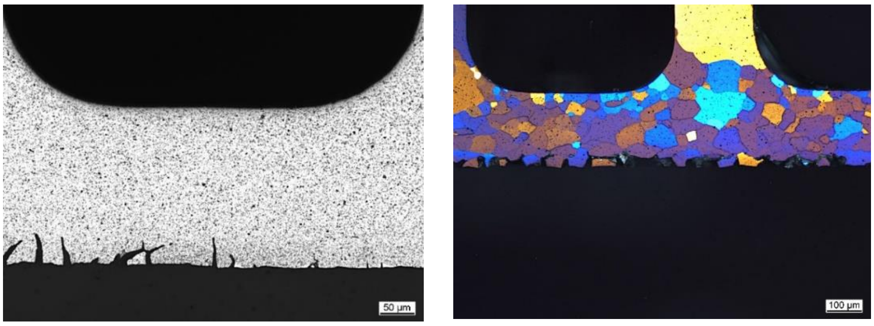


*Figure 2: Cross sectional characterisation of a brazed heat exchanger MPE after corrosion testing. Initiation of IGC and smaller grains falling out can be seen.*

One goal with the alloy development is of course to make the alloys as corrosion resistant as possible. The aim of the current project therefore is to characterize the microstructure of different MPE alloys both in the as extruded and as brazed condition in order to understand possible drivers for the IGC susceptibility better. The importance of grain misorientation, Mn depletion along the grain boundaries and Si content (from braze coatings) will be investigated using microstructural techniques such as SEM, EBSD, TEM.

## Contact persons

Jan Halvor Nordlien, Hydro, phone; 95295899, jan.h.nordlien@ntnu.no, jan.halvor.nordlien@hydro.com

Randi Holmestad (NTNU, randi.holmestad@ntnu.no)

# Effect of Al, Mg and Si in the Nitride Microparticles in a Spheroidal Graphite Irons

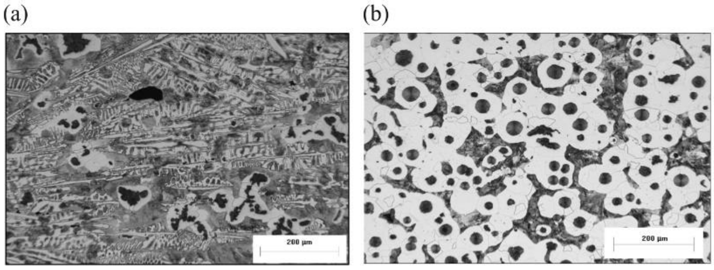


*Figure 2: (a) SGI without inoculation, (b) after inoculation.*

## Motivation

Iron-Silicon-Carbon nanocomposites (cast iron) have a carbon-rich phase, manifested as either graphitic layers or carbides. They have applications in several sectors of society that range from automotive to wind turbines. In spherical graphite irons (SGI), graphite particles take a spherical shape(see **Error! Reference source not found.**).

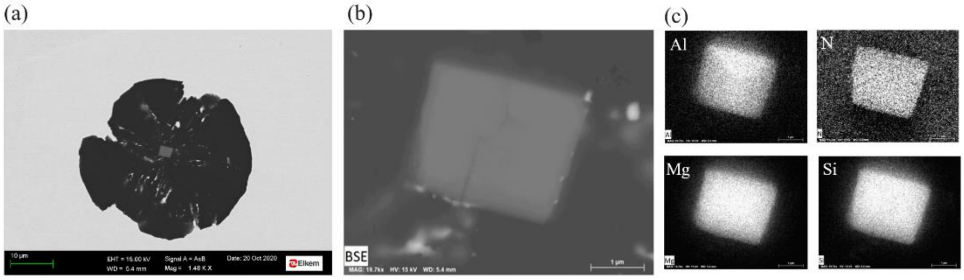


*Figure 3: (a) A graphite nodule with its nitride nuclei. (b) nitride in a higher magnification. (c) elemental composition of the nitride microparticle.*

These graphite particles need a substrate to nucleate with lower undercooling, otherwise C will precipitate as iron carbides-$Fe_3C$ (Figure 1a), and the material will lose its main properties. Therefore, inoculants are added to prevent carbides and ensure that C precipitate as graphite. These inoculants are ferrosilicon alloys that typically contain Al and Ca. They modify the existing substrates in the melt, which cause them to be more suitable for graphite nucleation [1]. One of the substrates found in the center of graphite nodules are the nitrides [2], which are reported to be $AlMg_{2.5}Si_{2.5}N_6$ [3], but others have proposed different compositions [4, 5]. These nitrides, having a similar structure as AlN, contribute to up to 30% of all microparticles in SGI. See as an example. Currently, a trend in alloy production is to use raw materials from recycling. Partly, this means that Elkem's ferrosilicon products would contain less Al, which could significantly reduce the final casting properties.

## What the student will do in the project

SGI samples with low and high Al will be produced in Elkem facilities using ferrosilicon alloys. The student will learn to use TEM and evaluate the actual composition and crystal structure of the nitrides, especially the role of Al, Si and Mg in these microparticles.

This topic is a collaboration with Elkem Silicon Products and is a part of SFI PhysMet. **There will be possibilities for a summer job at Elkem in this project! Contact us for details!**


## Contact persons: Leander Michels (Elkem), leander.michels@elkem.no, Sigurd Wenner (SINTEF) sigurd.wenner@sintef.no and Randi Holmestad (NTNU) randi.holmestad@ntnu.no


### References


1. Skaland, T., Ø. Grong, and T. Grong, A model for the graphite formation in Ductile Cast Iron: Part I. Inoculation Mechanisms. Met.Trans. A, 1993. 24, 2321.
2. Igarashi, Y. and S. Okada, Observation and analysis of the nucleus of spheroidal graphite in magnesium-treated ductile iron. Int. Journ. of Cast Metals Res., 1998. 11, p. 83.
3. Solberg, J. and M. Onsøien, Nuclei for heterogeneous formation of graphite spheroids in ductile cast iron. Materials Sci. and Tech., 2001. 17, 1238.
4. Stefanescu, D., et al., Growth of spheroidal graphite on nitride nuclei: Disregistry and crystallinity during early growth. Met. and Mat.Trans. A, 2019. 50, 1763.


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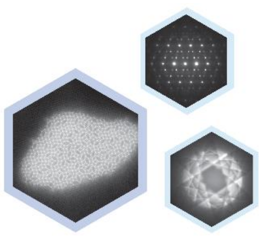
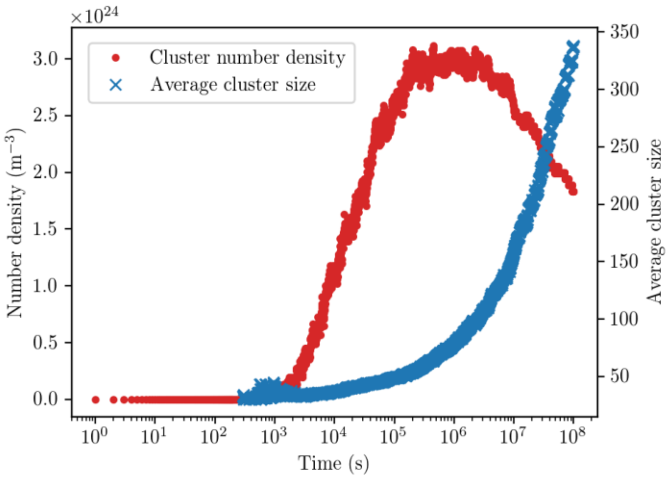


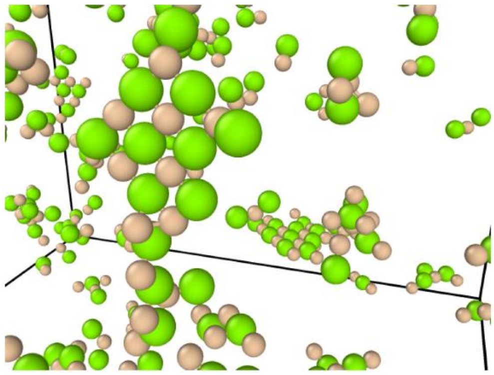
5. Laffont, L., et al., STEM observation of a multiphase nucleus of spheroidal graphite. Jour. of Mat. Res. and Tech., 2020. 9, 4665.

# 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.



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

## 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 and extending an existing code. 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.

## 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. Experience with C or Python is essential.

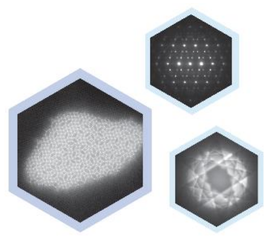
## Other aspects

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 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.

## Contact persons

Jesper Friis (jesper.friis@sintef.no), Jonas Frafjord (jonas.frafjord@ntnu.no)
and Jaakko Akola (jaakko.akola@ntnu.no). Others involved in the project are Randi Holmestad, Inga Ringdalen and David Kleiven.







# Modelling of early stage precipitation in aluminium alloys by cluster dynamics

## Motivation:

The global demand for aluminium alloys is increasing along with the focus on more environmentally friendly materials in industrial applications. Hardening precipitates are one of the most important features for optimising the properties of the alloy. These precipitates form after an initial clustering of atoms, such as in **Figure 1**. The structures of precipitates are well understood, but the early stage formation is still challenging to model. Fundamental understanding of the nucleation and growth of nanoscale clusters is a key ingredient to accurately model the full precipitation sequence.

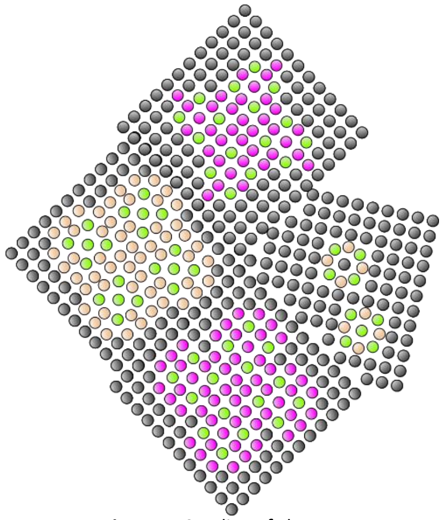


**Figure 1:** 2D slice of clusters

## What the student will do in the project:

The student will study nucleation and growth of nanoscale clusters by using cluster dynamics (CD). An existing code can be used as a reference and will give basic understanding of the method. The study will involve improving and extending this code.
The student will also be part of a group of other researchers and students that are investigating aluminium with density functional theory, Monte Carlo techniques and transmission electron microscopy. The project can be adjusted to 15, 30, 45 or 60 ECTS.

## 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.

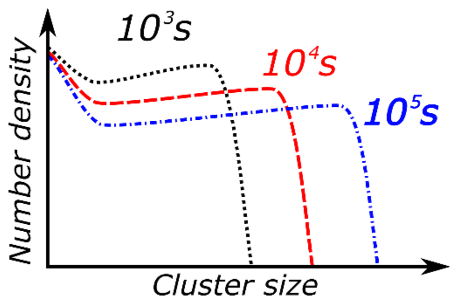



**Figure 2:** Custer size distribution at different times

## Other aspects:

There are many people 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 meeting 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.

## Contact persons:

Jonas Frafjord (jonas.frafjord@ntnu.no), Jaakko Akola (jaakko.akola@ntnu.no), Jesper Friis (jesper.friis@sintef.no).