Project work / Master / Diploma topics in the TEM Gemini Centre, 2023/24

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 2023, we have at IFY 3.4 (assoc.) professors, 2 engineers, 6 SITEEF researchers, ~10 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, nanomaterials 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 and materials science 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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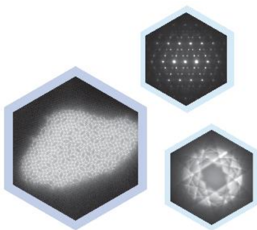

We offer

- 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.

We offer several projects connected to industry where we also offer summer jobs! See the different proposals - 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

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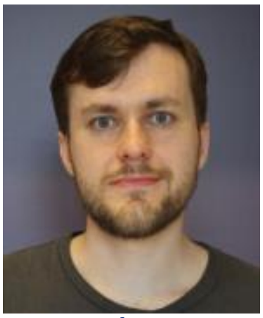

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References: (master students in bold)

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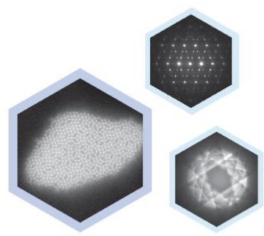

Joining for a Multi-Material Future

Motivation

The development of lightweight multi-materials in vehicles is inevitable to reduce the environmental impact and to increase fuel efficiency. This is especially important in battery electrical vehicles, where the battery pack alone can comprise more than 25% of the total vehicle weight. Here, replacement of Cu with Al in busbars and 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. Another, more established technique is called friction stir welding (FSW). Structural characterization on the nanoscale of multi-material joints and of the filler wire before and after joining is important to understand both the joining technique and the mechanical properties of the resulting joints. In the In-Sane project we have studied HYB joints and also done nano-joining in a FIB.

An optical image of a FSW copper- Aluminium Joint.

Your project

The student will characterize joints with transmission electron microscopy (TEM), focusing on FSW joints made by SINTEF for Hydro. 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

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 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), Professor Randi Holmestad (randi.holmestad@ntnu.no) and PhD student Jørgen A. Sørhaug, (jorgen.a.sorhaug@ntnu.no), Department of Physics, NTNU.

The project is a collaboration with SINTEF Manufacturing (Siri Marthe Arbo, siri.marthe.arbo@sintef.no) and
Hydro Extrusions (Jonas K. Sunde, jonas.sunde@hydro.com)

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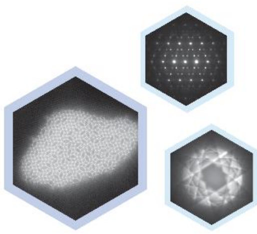
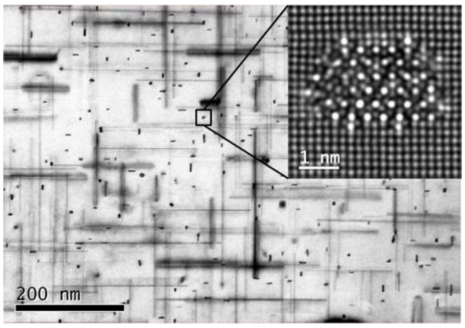


TEM investigations of an aluminium alloy from Hydro

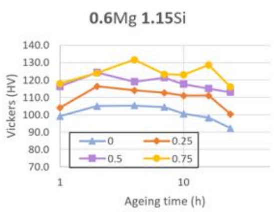
The Origin of Double-Hardness-Peaks in Aluminium Alloys with Cu

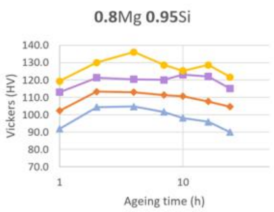
Motivation



Pure Aluminium is a relatively soft metal, but with small additions of other elements it is possible to create alloys with significantly increased strength. Al-Mg-SI-alloys are usually extruded into their final shapes and are subsequently heat treated to gain their high strength. The strength increase is achieved by small additions of Si and Mg which form nanosized particles called precipitates. These strengthening phases are so small that a transmission electron microscope (TEM) is required to study them. When documenting the hardness evolution during heat treatment, one usually finds a maximum hardness after a certain ageing time (peak-aged condition). However, a double-peak has appeared in literature and little is known about its origin. Hydro has measured several double-peaks in 6082 alloys containing Cu, and would like to gain a better understanding of the precipitates that are present in each peak. This work is connected to the SumAl project The student will be invited to internal aluminium meetings as well as to project meetings in Trondheim or/and at industry sites.

Your project





The main goal is to contribute to research looking into the origin of the double-hardness-peak when heat treating 6xxx alloys. The main task will be documenting precipitate types present in the peaks by TEM. Precipitate quantification should be used as input to a strength model to determine the cause of the double peak.

The student will do experimental testing of a few selected 6082 alloys with different Cu levels, produced by Hydro Aluminium AS. This includes Heat treatments, Mechanical testing, Hardness (and electrical conductivity) measurements, TEM sample preparation and TEM imaging. If time, or for continuation into a master project: Scanning Precession Electron Diffraction (SPED) for phase identification.

Requirements

Background in materials physics, nanotechnology or chemistry is an advantage. We seek students motivated to do experiments and interested in connecting large scale material properties to materials micro- and nanostructure.

Contact persons

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Christoph Hell (PhD student, Physics, NTNU, christoph.hell@ntnu.no)
People involved from Hydro (R&D centre at Sunndalsøra) : Ulf Tundal, Martha Indriyati, Jostein Røyset, Elisabeth S. Thrane

*Pictures adapted from hydro.com

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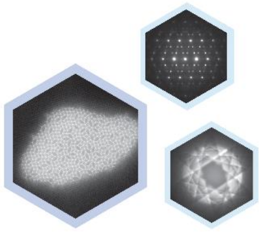
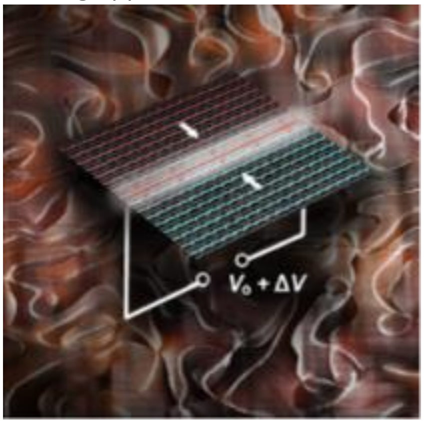


Domain imaging in ferroelectric oxides

Motivation

Ferroelectric materials exhibit a spontaneous electric polarization 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 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 science, where the ferroelectrics are studied in order to enable next-generation nanotechnology. Central in this sub-project are novel and exotic ferroelectric crystals. 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

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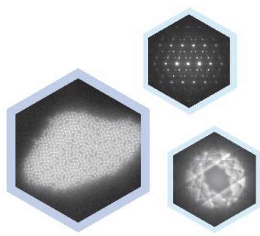

Extracting meaningful data from BIG electron diffraction data sets

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 or addressing fundamental challenges in this type of data. 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) and Tina Bergh (Tina.bergh@ntnu.no)

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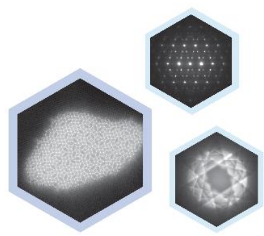

Orientation mapping of silver nanocrystals by vector analysis
- *use programming skills to see crystals in three dimensions*

Motivation

The TEM community has recently started to take more and more advantage of computational power and fast new detector technology to record bigger datasets which holds more information. By scanning a fine electron probe (nanometre- to sub-Ångström-sized) and recording a diffraction pattern for each probe position (4D-STEM), a 4D dataset is obtained. Each diffraction pattern can be analysed to get maps giving information on the local crystal structure in the material. At NTNU we have a state-of-the-art setup for one such method which is called scanning precession electron diffraction (SPED). The conventional way of analysing SPED data is based on comparing experiment and simulated patterns and has its limitations. We have worked on a novel alternative method which is based on the underlying physics, referred to as vector analysis. We now aim to generalize the method to handle orientation mapping, starting with a case study on polycrystalline silver. Examples of orientation maps from silver are shown in the figure below. Silver is used as a catalyst in industrial production of formaldehyde from methanol, which is one of the focus areas of the centre iCSI – industrial Catalysis Science and Innovation at IKP.

Your project

We will give you a python code and a relevant dataset from silver to start playing with. You will expand the vector analysis code to handle a range of crystal orientations, and we will compare your results to the conventional method of template matching. There are many ways that the vector analysis routine can be made more sophisticated. In the project you will work towards finding the best solution to a hot topic, challenging both your analytical skills and creativity. Your findings will be put into a bigger context and improvements will likely be part of a publication, presentation at an international conference and/or open-source packages. You can join sessions on the transmission electron microscope to better understand the sample and the data collection. We will organise weekly supervision meetings, and you will be invited and encouraged to join the weekly TEM lunch and the monthly SPED discussion meetings. The project can be adjusted to 15, 30, 45 or 60 ECTS.

Required from the student

We look for a student who enjoys programming and data analysis, at the same time as you happily collaborate and discuss scientific work with others. You should have some basic background with programming in python and value community-based open-source software developments. In this project we will aim to find new and better ways of solving the 3D analytical task, and we will encourage you to share your own thoughts and think outside of the box. While being strong in mathematics, you should also be able to add a touch of creativity. Some familiarity with crystallography and diffraction will be a great advantage. Relevant courses include Numerical Physics, Solid State Physics, and Materials Physics.

Contact persons

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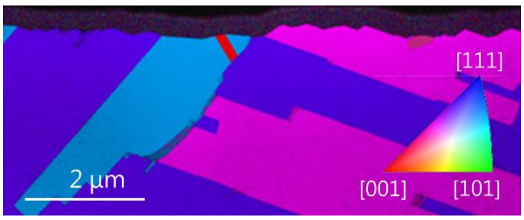

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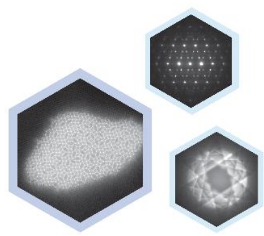

Method development for TEM studies of catalysts before and after reduction in an environmental cell TEM holder

Motivation

(Scanning) transmission electron microscopy (S)TEM is an invaluable tool in the characterisation of catalysts and allows us to study for instance the morphology and particle size, the chemical composition, and the oxidation state of a catalyst at the nanometre scale. A metal catalyst is typically active in its reduced state and may oxidise quickly if exposed to air. However, conventional (S)TEM specimen preparation and handling are done in air, which makes it very challenging to study reduced catalysts by (S)TEM. The TEM group at NTNU has an environmental cell TEM holder which allows exposing a TEM specimen to various reaction atmospheres while heating it to temperatures up to 700^{o}C. We are seeking to develop a methodology for using this holder to reduce catalysts, which will allow us to study the same TEM specimen before and after reduction, without any air exposure. We will start by studying a well-known system suitable for proof-of-concept studies, and we will also use a material which decomposes at a specific temperature to check the temperature calibration of the holder. The project will be a part of the centre iCSI – industrial Catalysis Science and Innovation and both the TEM and the KinCat Gemini Centres.

Your Project

In the beginning of your project, you will synthesise Pt catalysts on alumina supports by incipient wetness followed by calcination in air. The TEM engineers will give you TEM training so that you become an independent TEM user. After that, you will learn to operate the environmental cell TEM holder and create a setup in Chemistry Hall D that allows sending a controlled hydrogen gas flow through the holder. You will study your catalysts in terms of Pt particle size and oxidation state before and after reduction within the environmental cell holder and compare it to conventional bulk reduction. In addition to TEM characterisation, you can characterise your catalysts using several complimentary characterisation techniques, such as chemisorption and XRD, depending on your preferences. We will discuss your work during our weekly supervisor meetings, and we will invite you to the weekly TEM lunch meetings and the bi-weekly KinCat group meetings. The project can be adjusted to 15, 30, 45 or 60 ECTS, and it can be expanded to a Master thesis where Fe-based catalysts used in the Fischer Tropsch synthesis will be studied using the setup that you developed. These studies would then be done in collaboration with a larger research group that involves industry partners, and your work is likely to be a part of a publication.

Required from the student

We look for a student who enjoys lab work and would like to carefully design and calibrate a new setup. You should be happy to collaborate and discuss scientific work with others. Background within nanomaterials, catalysis and/or electron microscopy is an advantage. Relevant courses include Nanomaterials, Fabrication and Application of Nanomaterials, Solid State Physics, Nanotools, and Materials Physics.

Contact persons

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Hilde J. Venvik, IKP, Hilde.Venvik@chemeng.ntnu.no


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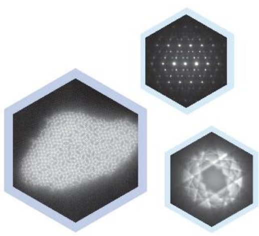


TEM studies of catalysts and membranes

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

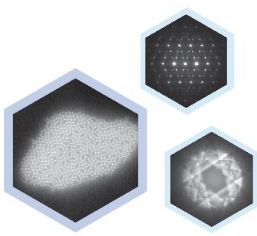
You will get TEM training to become an independent user, and you will employ a combination of imaging, spectroscopy, and diffraction techniques to characterise your material system. S*tate-of-the-art* instruments at the Norwegian national infrastructures NORTEM (TEM) and NorFab (SEM and FIB) will be 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 projects 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_2O. 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_2. Investigating the structural properties and changes occurring during separation could yield information critical to performance and stability improvements.

Contact persons

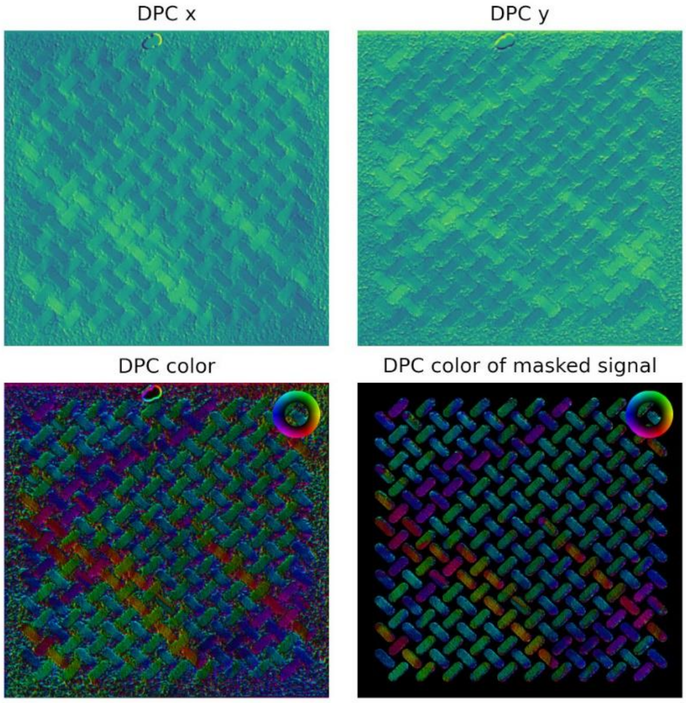
Supervisors: Adjunct Professor (Prof. II) Per Erik Vullum (pererik.vullum@sintef.no) and Postdoc Tina Bergh (tina.bergh@ntnu.no)

Co-advisors: Prof. Hilde J. Venvik (Hilde.Venvik@chemeng.ntnu.no), Dept. of Chemical Engineering (IKP), Dr. Ingeborg-Helene Svenum, Research Scientist at SINTEF Materials and Chemistry and Adjunct Associate Professor, IKP-NTNU.



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

Motivation



With the increasing demand for more powerful and energy efficient computing devices, there is a need to move away from silicon based semiconductors. One alternative is the nanostructure artificial spin ice (ASI), where a large number of nanometer scale magnets is arranged in a lattice sufficiently close to interact with each other as shown in the figure. By tuning the size, shape and distance between the magnets the large scale behavior changes, possibly allowing them to be used as in-materio computational devices by applying external magnetic fields. However, to properly study magnetic properties of these systems, both the full lattice and individual nanomagnets, there is a need for techniques which can study the magnetic properties at nanometer length scales.

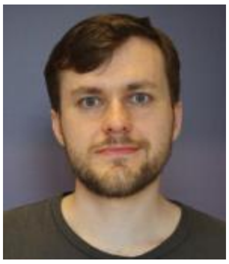
Transmission electron microscopy (TEM) is such a technique, which can image both the crystal structure, chemical composition and magnetic fields in materials at nanometer length scales. In addition, external magnetic fields can easily be applied to the studied materials, allowing for the “switching” behavior of the magnetic domains to be imaged.

Your project

You will study the ferromagnetic domain structure of ASI systems using the TEM. This will involve using the Scanning Transmission Electron Microscopy – Differential Phase Contrast (STEM-DPC) technique, which gives magnitude and direction of the magnetic field in the materials (see the color maps in the figure). The aim will be to examine how the magnetic domains in the ASIs responds to the application of external magnetic fields, as a function of the ASI’s lattice structure. 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 will also include micromagnetic simulations, and possibly using the Nanolab’s Focused Ion Beam (FIB) to create the ASI structures. 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.



Contact person

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

The TEM Gemini Centre is a strategic collaboration between NTNU and SINTEF. We work within the fields of solid state physics and materials science 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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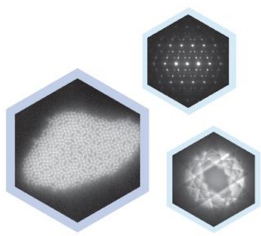
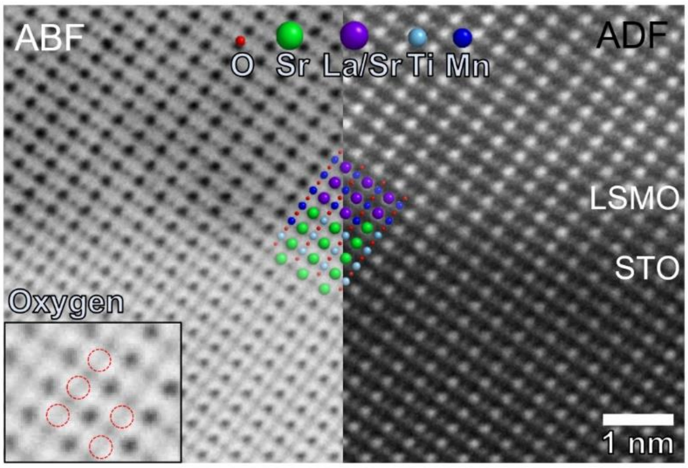


Nanoscale structural and composition studies of perovskite oxide superlattice thin films using TEM

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 is11ecessaryy to study them at the nanoscale: both the chemical composition, crystal structure, and functional properties. An example of this is seen in the figure, which shows the atomic ordering across a substrate and thin film interface.

(S)TEM-ADF and ABF of LSMO/STO interface



Your project

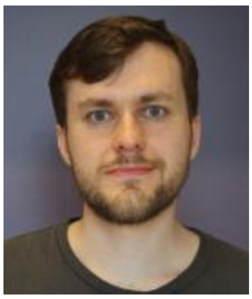
You will use the Transmission Electron Microscope (TEM) to study magnetic perovskite oxide thin film materials. The aim will be to characterize both the crystal structure and chemical composition of the films, to better understand the coupling between the structure and functional properties. This will 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 La0.7Sr0.3MnO3, LaFeO3 or La2NiMnO6. The project can be adjusted to 15, 30, 45 or 60 ECTS.

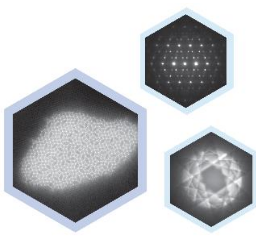
Requirements

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.

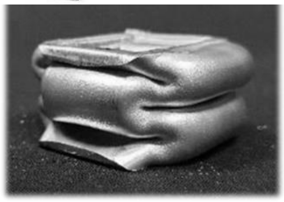
Contact person

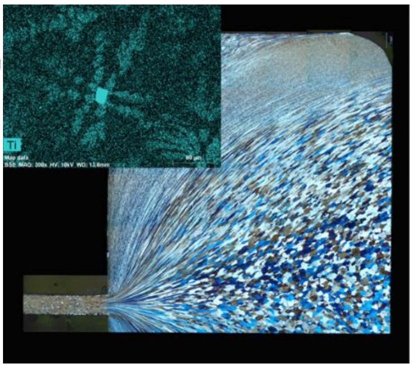
Magnus Nord, Associate Professor, Department of Physics, NTNU, magnus.nord@ntnu.no

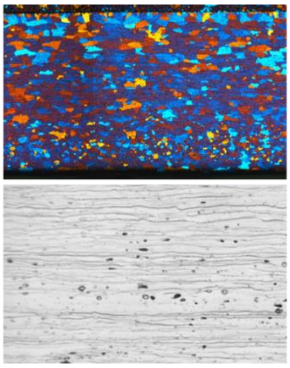


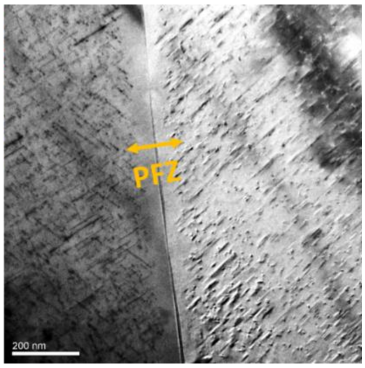


TEM study of Ti and V Microbands in 6008 Aluminium Alloys









Motivation

Pure Aluminium is a relatively soft metal, but with small additions of other elements it is possible to create alloys with significantly increased strength. Al-Mg-Si-alloys are usually extruded into their final shapes and are subsequently heat treated to gain their high strength. The strength increase is achieved by small additions of Si and Mg which form nanosized particles called precipitates. These strengthening phases are so small that a transmission electron microscope (TEM) is required to study them. Also adding Ti and V to these alloys can significantly improve the energy absorption in crash components for cars and improve corrosion resistance. This effect is attributed to nanosized Ti/V-bands formed during extrusion of these components. Experiments have shown that Ti and V counteract the bad effect of slow cooling after extruding in production. **This project includes a 4 week summer job (**at Sunndal and Trondheim)!

Your project

Hydro would like this project to focus on the reason behind the beneficial effect from Ti and V. One of the main questions is whether the Ti/V-bands help slow down diffusion of solutes (Si and Mg) to the grain boundaries in Aluminium. By investigating the precipitation free zones (PFZ) at the grain boundaries by TEM, we can get an indication of the effect from Ti and V on diffusion. The goal is to determine and explain the effect of Ti and V microbands on PFZ-width and properties. The work will include scanning electron microscopy (SEM) of primary particles (@Hydro Sunndal), grain orientation measurements of the different alloys (Hydro Sunndal), TEM (imaging and chemical analysis) focussing on PFZs, grain boundaries and precipitates.

Requirements

Background in materials physics, nanotechnology or chemistry is an advantage. We seek students motivated to do experiments and are interested in connecting large scale material properties to materials micro- and nanostructure.

Contact persons

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Ruben Bjørge (ruben.bjorge@sintef.no),
Sigurd Wenner (Sigurd.wenner@sintef.no)

People involved from Hydro (R&D centre at Sunndalsøra): Jostein Røyset, Elisabeth S. Thrane (also Eva Mørtsell from January 2024)

*Pictures adapted from hydro.com

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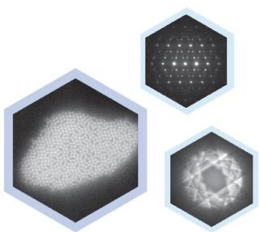


Mineralogy and TEM: nm-scale characterization of beautiful systems

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

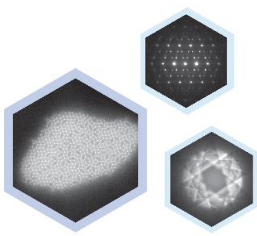
The student will learn how to operate a TEM to characterize mineral crystallographic and compositional properties. The project aims to link observations at different size scales (eg. optical microscopy/petrography – SEM – TEM) and different techniques (eg. microscopy, EDS, XRD). Consequently, sample 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. Alternatively, the project can focus on finding crystal structure of debated minerals using (3D) electron diffraction. Such a project will be a combination of computational and practical work. Both project suggestions 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)



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.

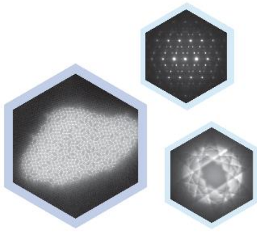
Requirements

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

Professor Ragnvald Mathisen, IFY, ragnvald.mathisen@ntnu.no
Senior engineer Emil Frang Christiansen,
emil.christiansen@ntnu.no
Professor Randi Holmestad, IFY, randi.holmestad@ntnu.no

Materials will be provided by
Hydro Precision Tubing through
Dr. Jonas K. Sunde, jonas.sunde@hydro.com



Strain and orientation mapping of next-generation Li-ion battery cathode material

Motivation

The Li-ion battery technology has enabled wide-spread use of consumer electronics and it is currently playing a crucial role in the transition to a greener economy via wide-scale deployment of electric vehicles and ships. But there is still a need for improvement of these batteries. The energy density of current Li-ion batteries is limited by the cathode. A potential new cathode material for next generation batteries is $LiNi_{0.5}Mn_{1.5}O_4$ **(LNMO), a cobalt-free alternative. It is also a material resistant to moisture, thereby reducing the energy needed during production. However, its commercialization has been hampered by severe capacity fade. To understand why LNMO suffers from this capacity fade, it is important to understand the structure on the nm scale at different stages of the charge cycle, for example when it is fully lithiated, when it is delithiated, and after extensive cycling.**

The scanning precession electron diffraction (SPED) technique in TEM has proven to be very powerful to detect changes in crystal structure. Here we are interested in changes in lattice parameters (strain), change in grain size and loss of crystallinity. These characteristics can be deduced from changes in the SPED patterns. The TEM Gemini Centre hosts a state-of-the-art system for SPED, using a sensitive direct electron detector. This has been used to acquire SPED datasets from LNMO at different charge states.

Your project

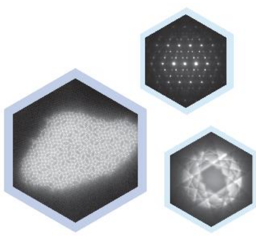
The project concerns analysis of large SPED datasets, with an emphasis on extracting accurate strain quantification and orientation maps to understand the capacity fade of LNMO cathodes better. You will link your results to how the cathode material is affected structurally when it is delithiated, and how extensive cycling affects the strain state of the material. Initial SPED datasets will be available at semester start. There are demo python notebooks with example data to become familiar with the analysis of SPED. There are weekly meetings with supervisors, you can join data collection and code & SPED data analysis meetings where all SPED users meet. The project can be adjusted to 15, 30, 45 or 60 ECTS.

Required from the student

We search for a student with background in materials physics/solid state physics, interested in doing python-based data analysis. Interest in applying skill in python and basic solid state physics to a practical task and potentially contribute to open-source software. Good communication and interaction with collaborating scientific and academic staff is essential.

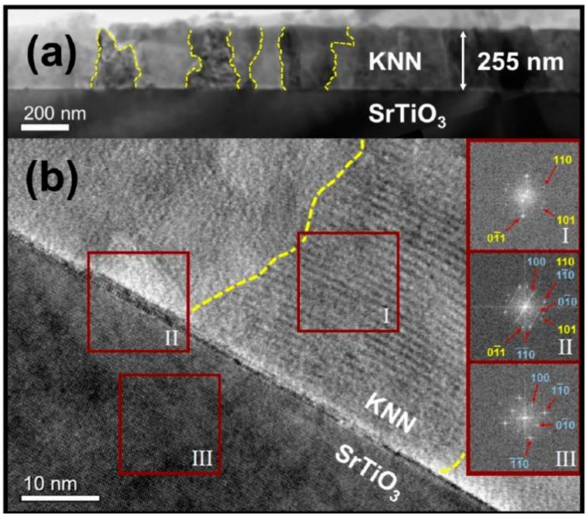
Contact persons

Ton van Helvoort (a.helvoort@ntnu.no),
Inger-Emma Nylund (inger-emma.nylund@ntnu.no),
Ruben Bjørge, SINTEF Industry (ruben.bjorge@sintef.no).



TEM characterization of oxide thin films made by chemical methods

Motivation



TEM figure made by Andreas Toresen, MSc student in TEM group in 2018 [1].

Ferroic materials constitute a unique class of materials possessing either ferromagnetism, ferroelectricity or ferroelasticity. Two or more of these properties are found in so-called multiferroics. These materials have many applications in information and communication technology as well as in energy and in medical technology. Applications include sensors, transducers, actuators, etc. Lead-free materials such as $K_{0.5}Na_{0.5}NbO_3$ (KNN) and $Bi_{0.5}Na_{0.5}TiO_3$ (BNT), ferroelectric tungsten bronzes such as $Sr_{1-x}Ba_xNb_2O_6$ and multiferroic materials such as $BiFeO_3$ and $YMnO_3$ have been central to the research in the last decade. At Department of Materials Science and Engineering, NTNU they have many years of experience in developing these materials and the characterization of their structural and functional properties. TEM investigation allows determination of the detailed structure which can be related and compared to first principles calculations and functional properties.

Your project

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

Requirements

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

Contact persons

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

This project is in collaboration with Mari-Ann Einarsrud from Department of Materials Science and Engineering.

[1] 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.

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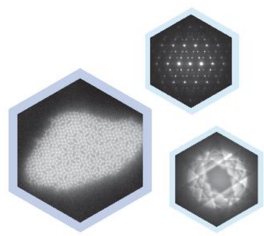


Characterization of Ce-phases in austenitic steels

Motivation

Grain refinement is a critical process in the production of metals, particularly cast iron and steel. In these alloys, reducing the grain size of austenite can significantly improve their mechanical properties. For that purpose, alloys containing Ce were developed and studied to refine the grains in austenitic stainless and manganese steels [1-3]. However, the role of Ce in these alloys remains unclear, as Ce can form several oxysulphides and aluminates compounds with different crystal structures.

As a highly reactive rare-earth element, cerium forms stable inclusions when added to the steel melt. These inclusions, including cerium oxides, sulfides, aluminates and oxysulphides are supposed to act as nucleation sites for melted steel to solidify into steel grains. The nature of these microparticles is still debated and not yet understood. A potential Ce-oxide phase is shown in Figure 2

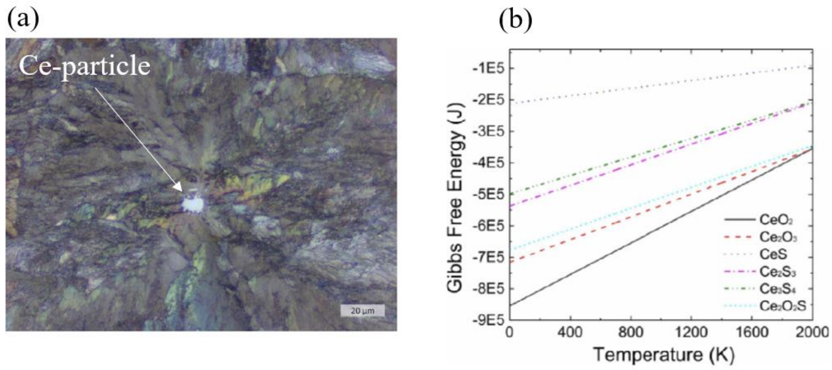


Figure 1: (a) Ce-particles in the middle of an iron crystal. (b) Types of different Ce phases and their free energy of formation as a function of temperature [4].

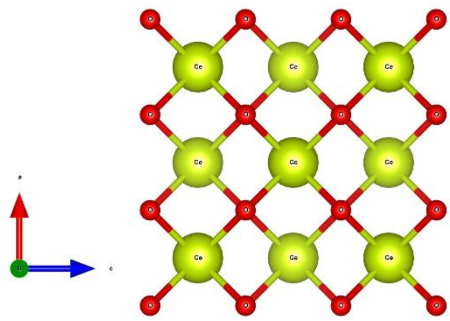


Figure 2: CeO2 unit cell

Your project

The student will characterize Ce-containing microparticles in austenitic steels made by Elkem Silicon Products. The student will learn to use transmission electron microscopy (TEM) and to determine the chemical composition and crystal structure of the Ce-containing phases and their orientation relationships to the austenite grains. **For this project there is a possibility for a summer job, and travel to Kristiansand to prepare materials.**

Requirements

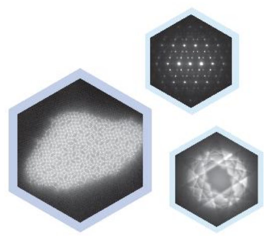
Background in materials physics, nanotechnology or chemistry is an advantage. We seek students motivated to do experiments and interested in connecting large scale material properties to materials micro- and nanostructure.

Contact persons

This topic is a collaboration with Elkem Silicon Products and is a part of SFI PhysMet.
Randi Holmestad (NTNU) randi.holmestad@ntnu.no , Yanjun Li (NTNU) yanjun.li@ntnu.no
Co-supervisors from Elkem: Leander Michels leander.michels@elkem.com , Håkon Mauset hakon.mauset@elkem.com

References

[1] C. Van der Eijk, F. Haakonsen, S. Ole, and G. Øystein, AISTech 2011 Proc 2, 559 (2011).
[2] F. Haakonsen, J. K. Solberg, O. S. Klevan, and C. van der Eijk, AISTech 2011 Proceedings 2, 763 (2011).
[3] C. Van Der Eijk, J. Walmsley, O. Grong, O. S. Klevan, and A. Elkem, in ELECTRIC FURNACE CONFERENCE (Citeseer, 2001), pp. 51.
[4] Fei Pan et al. Scientific Reports 6 (Oct. 2016), pp. 1–6. doi: 10.1038/srep35843.



Calculation of energy barriers for atomic motion

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 machine learning (ML) algorithm. These methods can be used to efficiently calculate the energy barriers of a configuration based on parametrisation. Accurate NEB calculations are used in the training set.

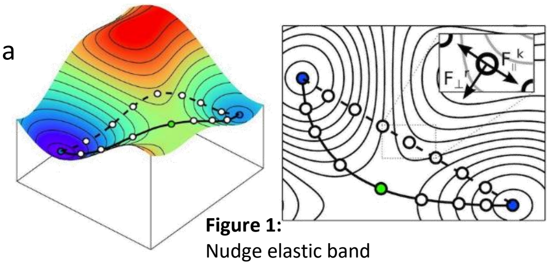
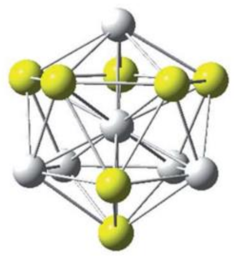


Figure 1:
Nudge elastic band

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 ML techniques. 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.

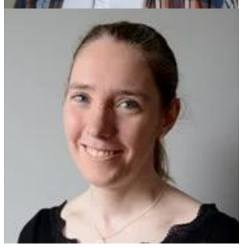
Figure 2:
Al6Sc7 (ref. *doi.org/10.1039/D1RA06994B)*

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.

Other aspects:

The use of ML algorithm 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. This topic is also coupled with 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), Inga Ringdalen (inga.g.ringdalen@sintef.no)
Others involved in the project: Jaakko Akola and Jesper Friis

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