Norwegian X-ray Centre

Master Projects in Materials Physics, 2013 / 2014

X-ray based characterization of functional materials

Are you interested in experimental physics and/or advanced data analysis?
- Then we have the right project for you!

The group headed by Breiby and Mathiesen is the leading national competence centre in X-ray science in general, and X-ray based materials characterization in particular. The group was founded in 2007, and has gained sizable momentum both in terms of laboratory facilities, external funding and group activities. Presently, the group has four PhD students, two post-docs, several project and master students and an engineer (part time), all working on activities related to the projects described here. The group has an excellent international network, and is regularly assisting MSc students in finding appropriate locations for a semester or two abroad. Through the network the group also frequently hosts visiting students and scientists.

Through the Norwegian Resource Centre for X-ray Scattering and Imaging (RECX), we are presently (spring 2013) in the process of installing a brand new X-ray tomography instrument that will be a work horse for our home laboratory activities, enabling 3D imaging of materials and components. Note that this is the same technology as used in CT (computed tomography) at hospitals, with a key difference being that our instrument is optimized for higher resolution (better than 10 μm). We offer challenging and relevant projects for students interested in materials physics, nanotechnology, biophysics and medical imaging.

SOLIDIFICATION MICROSTRUCTURES IN METAL ALLOYS

Our group has extensive international collaborations within the field of solidification fundamentals of metals and alloys. The NTNU group is well recognized internationally for its leading contribution to X-ray imaging-based *in situ* diagnostics which have proven decisive for guidance and validation of numerical modelling codes, and opened for new phenomenological insights.

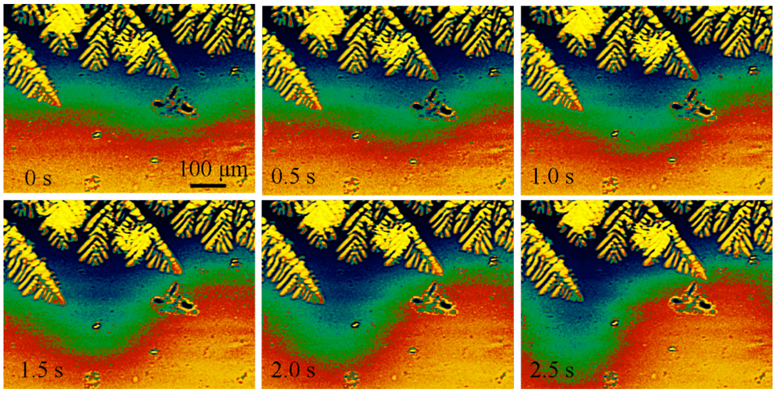
Columnar-to-equiaxed transitions in dendritic growth.

With Prof. Henri Nguyen-Thi and Prof. Bernard Billia, Univ. Marseille, France

The micro- and nanostructures that form during solidification of metal alloys are archetypes of selforganised structures realised under non-linear transport dynamics in systems far from equilibirum. The most prominent growth process is in alloy solidification is so-called dendritic growth. Generally, dendritic growth processes invovle a complex interplay between mass- and heat diffusion, convection, capillarity and attachment kinetics. The microstructure evolution is characterized by tracking the solid-liquid interface under the influence of local heat- and mass gradients. Due to the anisotropy of the interface there is no analytical solution to the problem even for the simplest case, and with its evolution influenced by local gradients, the problem constitutes a so-called classical free-boundary value problem.

Due to the low viscosity of liquid metals, diffusion and convection most often co-exists and interact with one another as their characteristic time- and length scales partly overlaps. It is therefore a strong motivation to do critical experiments in low-gravity environments in order to provide validation data for purely diffusive models. So-called columnar-to-equiaxed (CET) dendritic transitions occur frequently in many castings, but the governing physics of the transitions is complicated and yet far from understood. In the spring of 2012 the X-ray physics group participated in an experiment by the European Space Agency (ESA) to study CET in situ for the first time by X-ray diagnostics in micro gravity environment. The project is a collaboration between ESA, Univ. Marseille, ACCESS eV Aachen and NTNU. The student will participate in all stages of preparatory work for the experiment, including possible parabolic flight test campaigns. A natural extension to the work will be to participate in the actual micro gravity experiment, with a period during spring 2012 at the S-range sounding rocket launch site in Sweden, as well as taking part in the post experiment data processing and analysis.

Analysis of transient columnar dendritic growth under diffusive-convective mass transport.



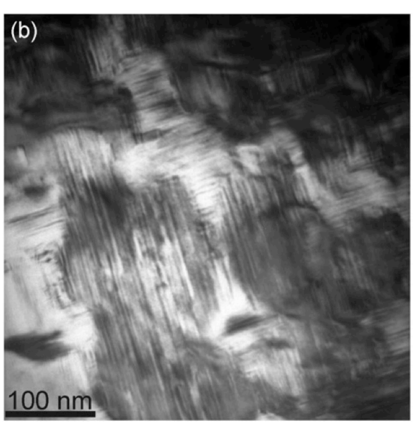
Images from a video sequence on columnar dendritic growth under convective-diffusive mass transport

This project will be focused at image processing/analysis of time-resolved high-resolution video sequences measured by in-situ X-ray imaging during solidification experiments. By image processing we aim to extract quantitative time-resolved data of physical quantities that are fundamentally linked to the self assembling pattern selection and growth process, such as solid-liquid interfaces, local propagation velocities, diffusion fields and liquid flow velocities for comparison with existing theories and simulation models.

Recrystallisation and thermomechanical stability in ultra-fine grained Aluminium alloys.
With Dr. Yanjun Li, SINTEF Materials Technology

Metals can be processed by so-called severe plastic deformation techniques to form ultra-fine grained structures (sizes ~ 10^{-8}-10^{-6} m). By further thermomechanical processing such materials can be converted to exhibit bimodal grain size distributions, which result in unique mechanical properties such as ultra-high strength *and* high ductility/formability. In this project work will be focused on studying grain growth and grain-growth control mechanisms *in situ* during thermomechanical processing of ultra-fine grained Aluminium alloys by X-ray diffraction. The work will involve experiments, data analysis and programming.

Phase transitions and domain structures in polycrystalline ferroelastics
With Prof. Tor Grande, IMT



Sr substituted LaMnO3 or LaCoO3 show ferroelastic properties, with ferro→paraelastic curie temperatures that can be tailored by the amount of Sr. The project will involve characterisiation of the ferroelastic domain structures by diffuse X-ray scattering, particularly addressing the effects T_c/Sr-level variation and/or grain size have to the domain distributions.

MECHANICS OF CONDUCTING MICROBEADS

In collaboration with Prof. Zhiliang Zhang and Assoc. Prof. Jianying He of the NTNU Nanomechanics Laboratory, and Conpart AS.

Based on metal-coated monodisperse microspheres, originally invented by Prof. Ugelstad, the Norwegian company Conpart is developing new interconnect technologies for the electronics industry. The mechanical behaviour of these spheres under thermal and mechanical stress is of high importance to their reliable functioning in electronics. We are using optical and X-ray imaging techniques to follow their deformation behaviour in situ.

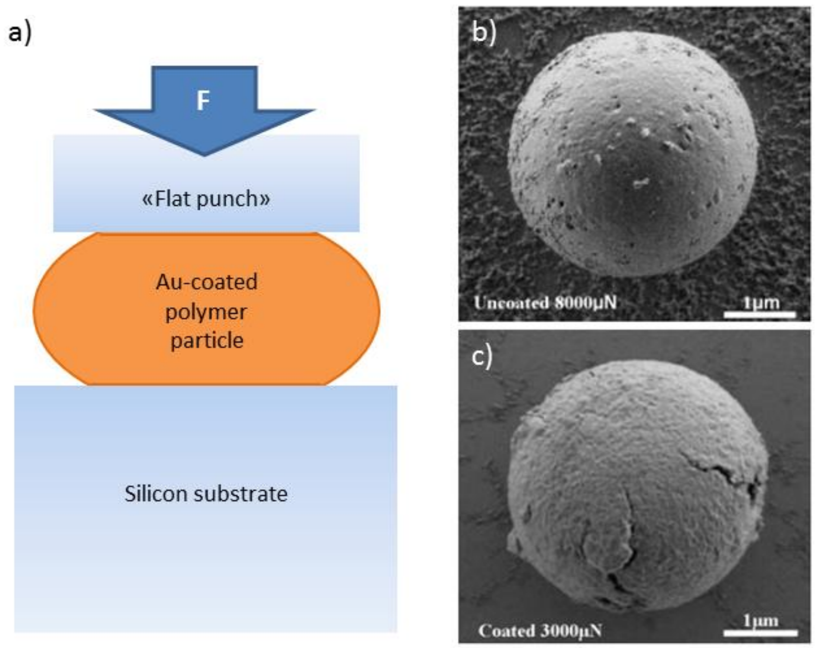


Figure. a) Sketch showing of mechanical testing of polymer beads under applied pressure. b) SEM image of a polymer particle, not exposed to mechanical stress. c) Metal-coated particle imaged after having been exposed to compressive stress.

Tomography studies of metal-coated microbeads (1 or 2 students)
Combining the tomography setup with our on-going studies of metal-coated microbeads, we offer student projects in the cross section between materials physics, numerical modelling and nano-/micro-electronics. Of particular interest for this project is the in situ study of fusion of small clusters of microbeads as a function of temperature, which is clearly a key experiment for validating this technology for use in industry.

Plan for the project:
- Carry out temperature-controlled tomography measurements in the laboratory
- Analysis of the 3D structural data by fitting of finite-element numerical models
- *Optional*: include electrodes to measure the electrical conductivity through the multi-bead assemblies, and to correlate the data via percolation models to the obtained 3D structures.

FIBRES, POLYMERS and BIONANO

In collaboration with SINTEF Materials and Chemistry.

X-ray fibre diffraction is a powerful method for determining organic structures, the most famous example being the DNA double helix. Our group receives considerable attention internationally for the work we do on organic materials, notably polymers, small-molecule organic films, liquid crystals and biomaterials.

In situ X-ray raster scanning imaging – diffraction (1 student) New equipment developments facilitate raster scanning scattering experiments. By scanning the material sample with a narrow X-ray beam (~µm), systematic variations in the measured signal can be related to macroscopic features of the sample. The samples to be studied in this project will be received from SINTEF, and are injection-moulded structural polymers for use in the automotive industry. We have recently demonstrated how important this raster-scanning is to get a true impression of the processes taking place during injection moulding, cf. Granlund *et al* (*Polymer* 2013, in press). In the project proposed here, we plan to take this technology one step further by doing *in situ* stretching experiments, for which we already have developed the necessary hardware.
Plan for the project:

- Carry out raster-scanning measurements in the laboratory
- Analyse the data by fitting to finite-element models
- Challenging option: Develop new algorithms for synthesizing 3D real-space images.

GPU-IMPLEMENTATION OF MULTILAYER THIN-FILM SCATTERING

In collaboration with Assoc. Prof. Anne C. Elster

Simulations of multilayer scattering (1 student). The specular reflectivity from thin film multilayer structures can be calculated analytically using well-established methods. Also the diffuse non-specular scattering can be modelled, using for example the *Distorted Wave Born Approximation* (DWBA). However, there are many issues that are difficult to formulate in this framework, including a polychromatic and non-parallel incoming beam, surface terraces, and structural defects. Starting out with the simplest possible geometries (point scatterers in a thin single-layer film), we will explore the possibilities of modelling the scattering using Monte-Carlo methods, accelerated using graphical processing units (GPUs). The project is suitable for students having a good understanding of physics and excellent programming skills.

COHERENT DIFFRACTION IMAGING

The project described here is particularly suitable for a strong physics candidate with a good understanding of Fourier optics and interest in experimental work.

Phase contrast X-ray microscopy is a hot topic in the field of X-ray science. It requires a (partially) coherent beam, and is thus done at synchrotrons. *Ptychography* is a specialized technique for evading the "phase problem" (the fact that since the *phase* of the scattered beam cannot be measured, thus complicating the analysis of diffraction data) by combining partly overlapping exposures with iterative algorithms for phase retrieval.

Ptychography using light in the visible range. The aim is to develop a laboratory setup using a laser that can perform ptychography measurements with light in the visible range. Such a setup is ideal for testing ptychography algorithms, as it allows exploring the interplay between the choice of experimental parameters and the reconstruction strategy.

Proposed plan for the project:

- Plan and design a setup for performing ptychography using visible light
- Build the setup in close collaboration with our engineer
- Find suitable experimental parameters for image acquisition, confirm the functionality of the setup using test samples and characterize the setup in terms of resolution and image quality

Options for further work:

- Perform computer simulations of ptychography experiments
- Perform ptychography reconstructions using existing reconstruction algorithms for experimental and simulated data to assess the consequences of shifts in the sample position during data acquisition
- Develop methods to determine the shift of the sample during a ptychography scan by modifying the reconstruction algorithm

More reasons for choosing our group for your project or master:

- *Dynamic group with two dedicated scientists as leaders, excellent social environment*
- *You study physics, nanotechnology, materials technology or physical electronics*
- *Excellent access to high quality experimental equipment*
- *X-ray physics is a rapidly moving field of tremendous scientific impact*
- *Possibilities for research stays in leading research groups **abroad!***
- *You enjoy **experimental work**,* and/or
- *You enjoy **computer programming**, and wish to work with real physical data*
- *You may get the chance to participate in **experiments at synchrotron facilities!***
- *Excellent possibilities for collaboration with SINTEF, other leading groups at NTNU, and Norwegian industry including Statoil and Hydro.*
- *"Real" nano-science problems relevant for future careers both in academia and industry*
- *Possibility of continuing with a PhD*
- *High-quality student work will be incorporated in academic publications*

The suggested topics are suitable for students interested in physics, nanotechnology or material science, who enjoy experimental work and computer programming. In particular with the new tomography setup, we can also offer projects for students interested in biophysics and medical imaging. The projects can be modified according to the particular wishes of the students, and can be adapted for 9th semester project and final Master projects.

TEAM LEADERS

Dag W. Breiby started working as associate professor at the Department of Physics in July 2007. Breiby holds a PhD in materials physics from NTNU (2003), and has later on been working at Risø DTU, the University of Copenhagen and Vestfold University College. Breiby has supervised more than ten Danish and Norwegian MSc students. Focus has been on X-ray characterization of functional materials, with material systems ranging from nano-particles and polymers to small organic molecules and liquid crystals. Office D4-145, Dag.Breiby@ntnu.no, (735) 93594.

Ragnvald Mathiesen is employed as associate professor at the Department of Physics since September 2007. Mathiesen has MSc and PhD (1997) academic degrees in materials physics from NTNU. After obtaining his PhD, Mathiesen worked as post doc at NTNU and at the ESRF in Grenoble, later as scientist at the Department of Inorganic Chemistry, UiO. From 2001 to 2007 Mathiesen was a senior scientist and group leader within SINTEF Materials. Mathiesen has worked both on diffraction physics and with the use of synchrotron X-ray radiation for studying a long range of different materials and areas within solid state physics.
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