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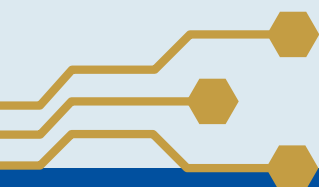


Quality Panorama Hotel, Trondheim

16 – 17 October 2019



PROGRAMME



Synthesis, Phase Transfer and Study of Growth Kinetics of Iron Oxide Nanoparticles Using Thermal Decomposition Method

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Iron oxide nanoparticles (IONPS) have attracted interest due to high monodispersity and superparamagnetic nature.¹ Synthesis of IONPS using iron oleate as precursor has been studied to control size and distribution.² Nucleation and growth mechanisms have been studied but a definitive mechanism connecting classical crystallization theories and reaction energy landscapes is missing.³ Our work involved study at nucleation onset temperatures of 220°C, 250°C and growth onset temperature of 310°C using high resolution transmission electron microscopy (HRTEM), scanning transmission electron microscopy (STEM) and Fourier transform infrared spectroscopy (FTIR). Apart from premature growth of some particles stochastically, experimental data supports existing mechanisms. The later part of the work involved phase transfer of IONPS from organic to aqueous medium using trimethoxy[3-(methylamino)propyl]silane (TMAPS), hexadecyltrimethylammonium bromide (CTAB) or sodium citrate. The following zeta-potentials were recorded; IONPS with TMAPS (28.1 ± 0.78 mV), CTAB (31.2 ± 2.8 mV) and sodium citrate (-40.2 ± 0.96 mV) showing stable phase transfer, whereby opening up for future biomedical applications among others.

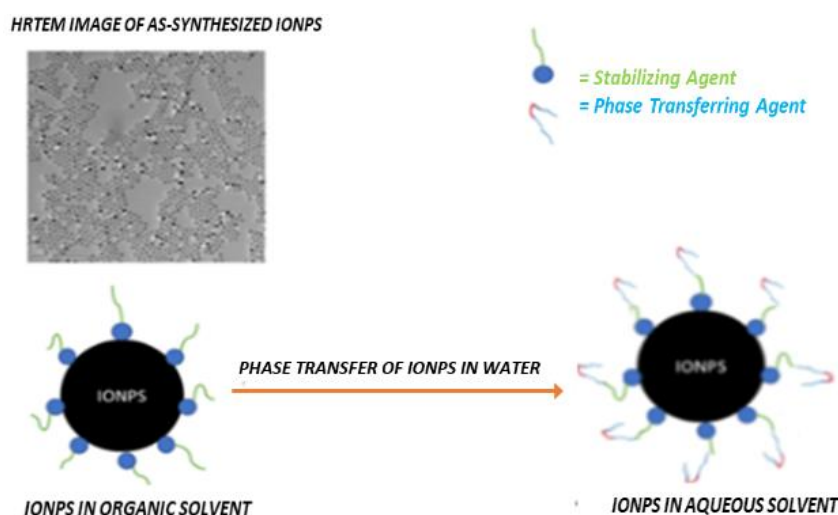


Fig-1 Synthesis of IONPS and Phase Transfer in Aqueous Medium Using Phase Transfer Agents

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Orientation dependent interfaces between SrTiO₃ substrates and BaTiO₃ thin films

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BaTiO₃ is a widely used material, e.g. in capacitors, due to its high dielectric constant, but it is also of interest for other applications due to the ferroelectric properties inherent to the material. Chemical solution deposition (CSD) of thin films is attractive because it can produce high quality thin films at low cost and scalability. Recently, BaTiO₃ thin films were prepared by aqueous CSD on (001), (011), and (111) oriented SrTiO₃ substrates, by heating to 1000°C. Due to the high processing temperature and the difference in thermal expansion coefficient between the thin film and the substrate, a tensile strain is present in the films [1]. In order to study the interface between the thin film and the substrate, transmission electron microscopy specimens were prepared using focused ion beam to create cross sectional lamellae. Different types of edge dislocations were observed for the differently oriented substrates. Further, they are periodically spaced with 14 nm and 19 nm between them, in the case of the (001) and (011) substrate, respectively. The periodicity is discussed with respect to the lattice mismatch between BaTiO₃ and SrTiO₃.

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Preparation of LaAlO_3 substrates for thin film deposition

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At NTNU there is an activity on making so-called intermediate band materials based on TiO_2 . The TiO_2 films will be deposited in LaAlO_3 substrates, and it is known that the substrate preparation prior to deposition affects the film properties. In this work, we have therefore studied of how the annealing parameters (temperature and duration) and the subsequent water leaching (etching) affects the substrates. We observe that the as-received substrates have a rather rough and non-uniform surface, and that the surface gets smoother and more uniform after the treatment, as expected. We have imaged the $10 \times 10 \text{ mm}^2$ substrates using AFM, Micro- Raman spectroscopy and 3D-optical Profiler in NTNU NanoLab. Large areas of the substrates are imaged to get data on the homogeneity prior to and after the substrate preparation.

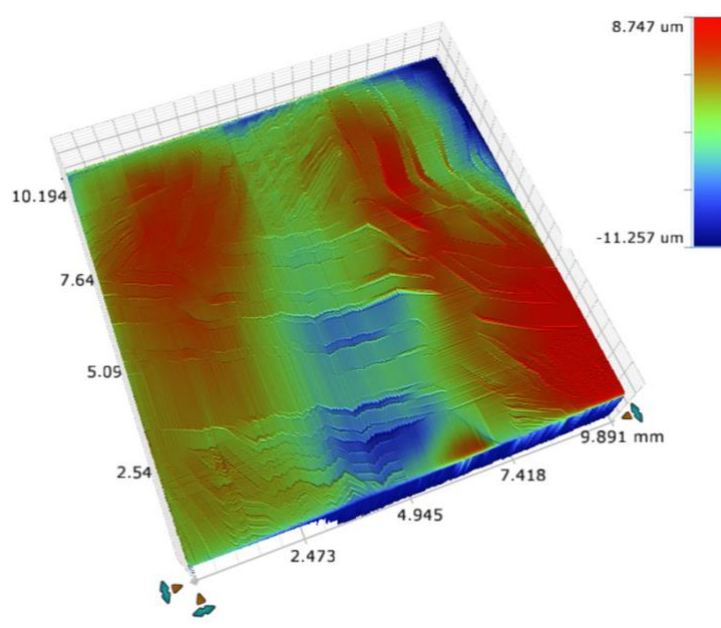


Figure 1: 3D representation of an image of an as-received $10 \times 10 \text{ mm}^2$ LaAlO_3 substrate imaged using the 3D optical profiler.

Nanoscale chemical mapping in 3D by atom probe tomography: Needle preparation

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The functional properties of materials are intimately related to the atomic-scale structure and chemistry in all three dimensions. While high-resolution electron microscopy (HREM) techniques enable imaging with great structural detail, they lack depth resolution of the chemical composition. Atom Probe Tomography (APT) is an advanced analytical method that allows 3D quantitative mapping of the chemical composition with better than 100 ppm sensitivity and sub-nanometer spatial resolution. In order to enable high-resolution APT studies, careful preparation of nanoscale needle-shaped specimens from areas of interest is an essential first step.

As an instructive example and to demonstrate associated possibilities for the study of functional materials, the controlled extraction of a needle containing a single ferroelectric domain wall (DW) from a hexagonal manganite (ErMnO_3) single crystal is presented using a Focused Ion Beam (FIB) system (Figure 1). Based on first APT test measurement a 3D chemical map of around $80 \times 60 \times 30 \text{ nm}^3$ is gained, providing insight into the material's composition with atomic-scale spatial resolution and high chemical sensitivity. Our goal is to resolve the local chemical structure at ferroelectric DWs with unprecedented precision to clarify the origin of their intriguing physical properties.

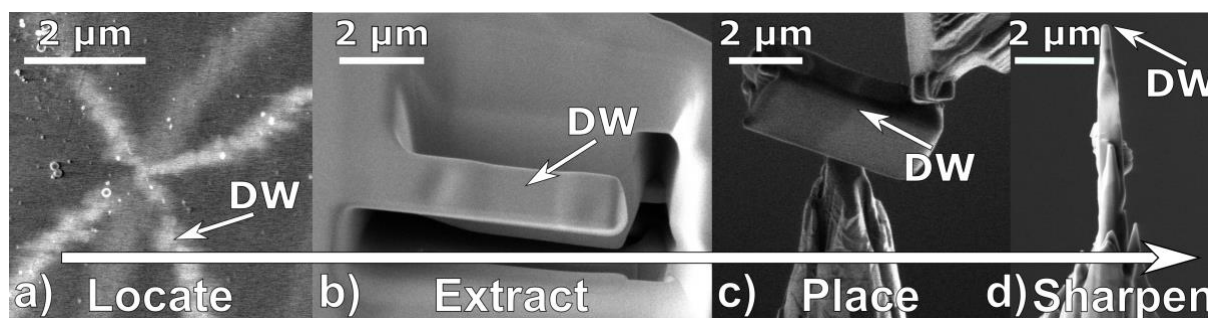


Figure 1. The needle preparation process for APT of a DW. a) Locating the DW with scanning electron microscopy, b) the selected DW is extracted using a FIB, c) the lift-out lamella is placed on a needle support and d) the APT needle including the DW is sharpened.

Near-vertical Subwavelength Nanostructure Grating Coupler for Silicon Nanophotonic Devices

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A compact planar lightwave circuit has been developed on silicon-on-insulator platform. Due to high index contrast and CMOS fabrication compatibility, high density of optoelectronic components is possible. However, it encounters high coupling losses caused by mode mismatch between the optical fiber and submicron silicon waveguide. To improve coupling efficiency, various fiber-to-waveguide coupling techniques have been reported, e.g., inverse taper edge-coupler, prism coupling, end-fire coupling and grating coupling. Among them, grating coupling is promising for vertical coupling schemes.

We present fabrication and characterization of near-vertical subwavelength nanostructure grating couplers for telecommunication wavelength bands. All photonic components are fabricated on amorphous silicon-on-insulator using electron-beam lithography and one-step silicon etching. Optimizing the grating coupler parameters yields the desired central wavelength with enhanced coupling efficiency and alignment.



The influence of AlN buffer layer on the growth of self-assembled GaN nanocolumns on graphene

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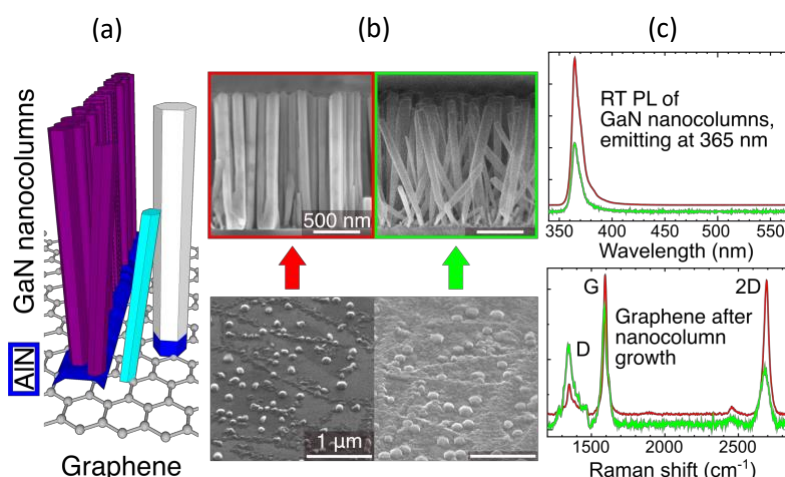
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In this work, GaN nanocolumns were synthesized on graphene via radio-frequency plasma-assisted molecular beam epitaxy. By varying the number of migration-enhanced epitaxy (MEE) cycles of the AlN buffer layer, distinct growth behaviors of the GaN nanocolumns on graphene were identified. Due to the weak nucleation on graphene, instead of an AlN thin-film we observe two distinguished AlN formations which affect the subsequent GaN nanocolumn growth: (i) AlN islands and (ii) AlN nanostructures grown along line defects (grain boundaries or wrinkles) of graphene. Structure (i) leads to the formation of vertical GaN nanocolumns regardless of the number of AlN MEE cycles, whereas (ii) can result in random orientation of the nanocolumns depending on the AlN morphology. Additionally, there is a limited amount of direct GaN nucleation on graphene, which induces non-vertical GaN nanocolumn growth. The GaN nanocolumn samples were characterized by means of scanning electron microscopy, transmission electron microscopy, high-resolution X-ray diffraction, room temperature micro-photoluminescence (RT PL), and micro-Raman measurements. Surprisingly, the graphene with AlN buffer layer formed using the less MEE cycles, thus resulting in lower AlN coverage, has lower level of nitrogen plasma damage. Additionally, this AlN buffer layer leads to the growth of high-quality and vertically-aligned GaN nanocolumns.



(a) Schematic of the AlN buffer structures (blue) and three possible GaN nanocolumn formations (purple, white and cyan) on graphene substrate.

(b) SEM images of bottom: AlN (bird's eye-view) at two different extreme MEE cycles, resulting top: two distinct structures of GaN nanocolumns (cross-sectional) on graphene.

(c) Optical (top, using RT PL) and structural (bottom, using micro-Raman) characterizations of GaN nanocolumns and graphene, respectively.

Deconvoluting conductance contributions at charged ferroelectric domain walls using machine learning

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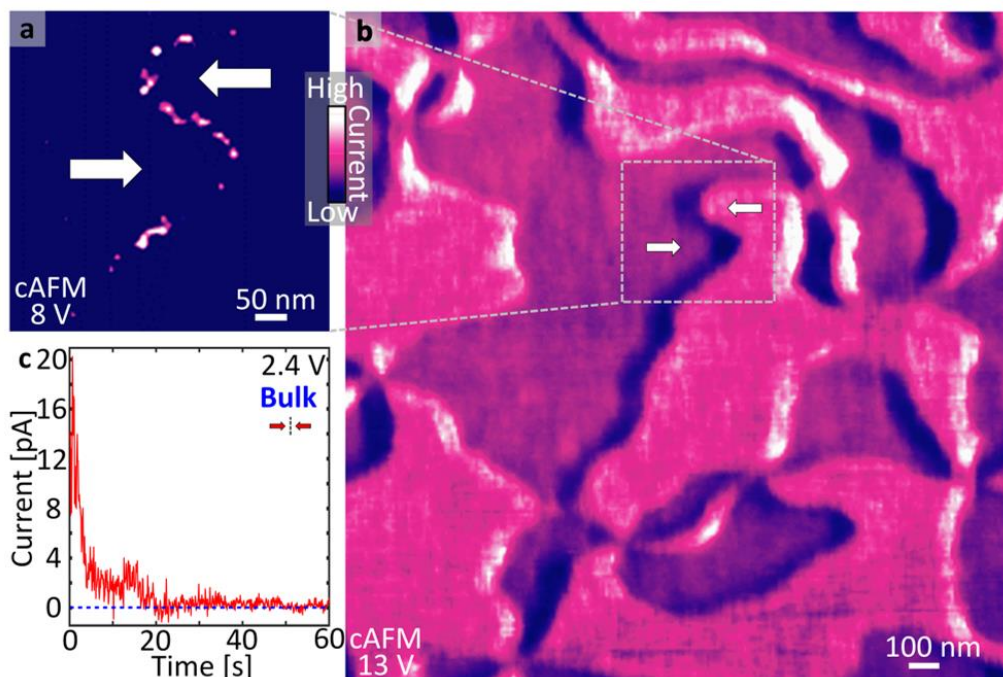
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Ferroelectric domain walls are spatially mobile interfaces that occur in materials that develop a spontaneous electric polarization. Some ferroelectric domain walls have non-linear electronic properties, and therefore hold promise as functional components for nanoelectronic devices. Despite this potential, however, it remains a challenge to probe their intrinsic properties.

This poster presents a comprehensive characterization of the domain walls in the hexagonal manganite $(\text{Er}_{0.99}\text{Zr}_{0.01})\text{MnO}_{3+\delta}$ using density functional theory calculations, dielectric spectroscopy, and scanning probe microscopy. The investigation unveils previously unobserved electronic responses at charged head-to-head domain walls: *n*-type-like or *p*-type-like transport, depending on voltage and time. We disentangle and analyze these responses using a neural network autoencoder. Thus, as well as observing new domain wall phenomena, we show how machine learning can be used to extract intrinsic domain wall properties.



Simulated Mueller matrices of diffractive polarization beam splitters

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Optical metasurfaces have in recent years gained widespread attention for enabling full optical wavefront manipulation using surfaces structured at the nanoscale [1]. By careful design and material selection, it is possible to create ultra-thin optical components with functionality comparable to complicated conventional optical systems [2]. Here we simulate and analyse surfaces that selectively scatters light based on the incoming polarization state.

We first simulate the optical response of lattices of phase shifting structures composed of either dielectric or plasmonic patch particles (metal-oxide-metal structures), before arranging the structures into both linear and Pancharatnam Berry-type gradient surfaces supporting several diffracted orders. The simulated spectroscopic Mueller matrices of the diffracted orders are then analysed using Mueller matrix decomposition techniques [3]. Finally, we discuss ongoing efforts for fabrication of the designed surfaces, as well as the development of custom instrumentation for rigorous optical characterization.

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Determining passive mixer efficiency for biomarker delivery in microfluidic channels.

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Microfluidic flow channels are combined with biosensors to enhance performance with respect to detection limit and reduced readout time. Despite the potential performance enhancement, the laminar flow regime in microfluidics reduces the full potential due to diffusive transport limitations of the biomarkers. Therefore, the fraction of biomarkers in the sample reaching the sensing area during the passage time is limited.

The mass transfer of the biomarker, and hence the probability of contact between the biomarker and the immobilized capture molecules can be increased by integration of passive mixing structures in the microfluidic channels.

In the present contribution, we address the efficiency of different passive mixers for microfluidic devices to enhance biomarker delivery and mixing within the channels.

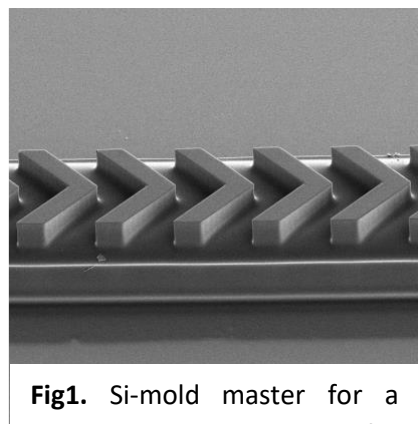


Fig1. Si-mold master for a passive mixing structure for integration in microfluidic channels.

Topological Domain Walls in Helimagnetic FeGe

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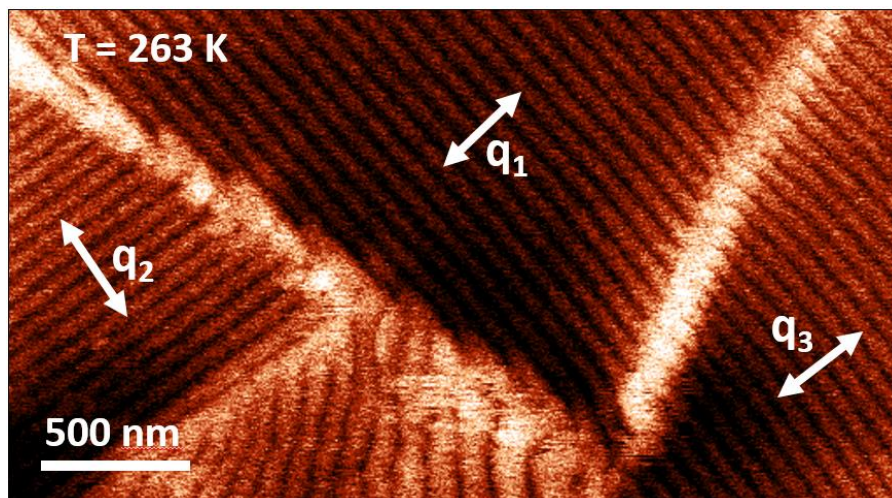
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In non-centrosymmetric ferromagnets, the so-called Dzyaloshinskii-Moriya interaction is symmetry-allowed and can lead to a canting of the spins, introducing complex spin spiral structures. Examples are transition-metal silicides and germanides, which crystalize in the non-centrosymmetric B20 structure and which display a helimagnetic ground state. Such helimagnetic order is at the center of our microscopy studies, motivated by both the unusual physical properties and the potential for novel device applications.



We use magnetic force microscopy (MFM) to investigate magnetic long-range order in the near room-temperature helimagnet FeGe. Completely new types of helimagnetic domain walls are observed, connecting regions with different orientation of the helical structure. Analogous to the much-studied Skyrmions, the walls can exhibit a nonzero topological winding number and, hence, possibly give rise to emergent electrodynamics. Our goal is to control the domain wall formation and positioning, demonstrating new opportunities for future applications in spintronics.

Functionalization of Magnetic Nanoparticles with DNA for Water Management.

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The field of hydrological tracers is plagued by the availability of different unique tracers (8 – 10) which are usually fluorescent dyes and salts, whereby, restricting multiple tracer experiments. We aim to develop a range of environmentally friendly, easily recoverable hydrological tracers using DNA as a fingerprint for the uniqueness of the tracers.

Here, we present fabrication of DNA-based hydrological tracers where the magnetic core is synthesized using co-precipitation or thermal decomposition.¹ The NPs are characterized using dynamic light scattering (DLS), zeta potential measurements, transmission electron microscopy (TEM) and DNA quantification done using qPCR. Our results show successful encapsulation of dsDNA bound to magnetite NPs inside monodisperse silica particles with high colloidal stability (zeta potential = -36 ± 0.3 mV) or within poly lactic-co-glycolic acid (PLGA) shells. These DNA-based magnetic tracers are expected to impact tracking of water flow paths using multiple tracers for both ground and surface water applications.

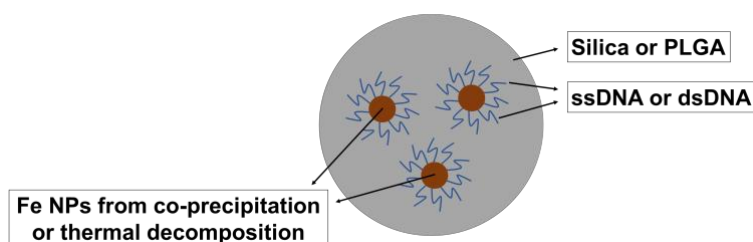


Figure 1. Schematic showing composition of DNA-based hydrological tracer.

References

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Silicon photonic waveguide sensor

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In recent years, there has been growing interest in development of optical waveguide-based sensors for chemical, biological and physical sensing. Sensor designs such as ring resonator, Mach-Zehnder interferometer, and spectroscopy-based waveguide sensors have shown applicability in detection of specific enzymes, proteins, etc. We present the fabrication and characterization of an integrated micro-ring resonator (RR)-based waveguide sensor. The RR sensor was fabricated on an amorphous silicon-on-insulator (SOI) platform by using electron beam lithography. To realize lab-on-a-chip (LOC), polydimethylsiloxane (PDMS) microfluidics was fabricated using soft lithography and integrated with the photonic chip. For characterization, a tunable external cavity laser with 1550 nm center wavelength was coupled to the RR sensor using tapered fiber. A single mode fiber was used to couple output power from the RR sensor to a photodetector. The RR sensor responsivity was analyzed by measuring the relative resonance shift with different concentrations of saline solution.

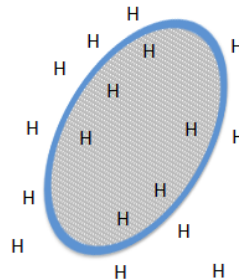
Dislocation Evolution Model of Nano Indentation in connection with Hydrogen Embrittlement

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The effect of hydrogen on mobility and nucleation of dislocations in Nano Indentation is investigated using a dislocation evolution model. The displacement from a load controlled indentation at the nanoscale is estimated using ordinary differential equation for the dislocation density and plastic strain. The Orowan equation is used to couple the movement of the mobile dislocation density and plastic strain. Features such as dislocation nucleation, annihilation, junction formation, and mobility effects can be included. In this way, the experimental displacement achieved by the indenter can be estimated from the load and material-specific parameters. Different dislocation mobilities and nucleation criteria are tested; the model is validated using existing nanoscale indentation data.



$$E_{loop} = 2\pi r * \gamma$$

$$\Delta G = 2\pi r * \gamma - \tau b * \pi r^2$$

$$d\gamma = -\Gamma_H d\mu_H$$

$$\gamma = \gamma_0 + d\gamma_H$$

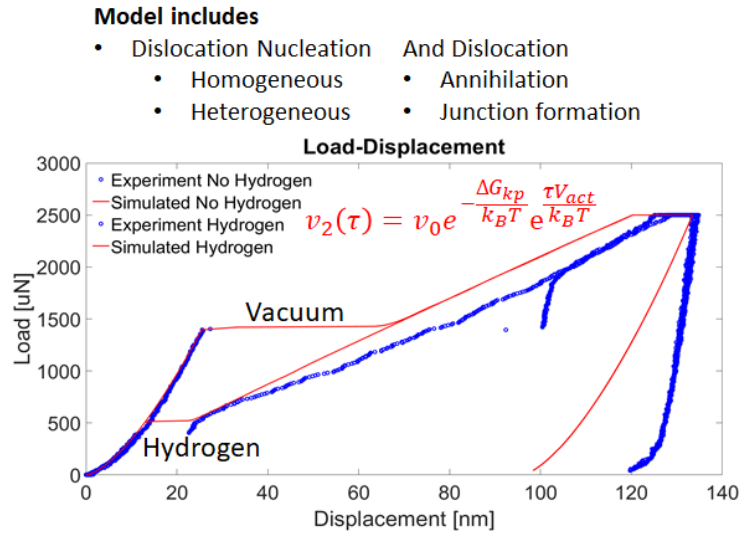


Figure 1. The defactant concept ascertains that hydrogen can decrease the energy of dislocations and other defects in the material. Using a homogeneous nucleation criterion for the formation of a dislocation loop in a solid, where the free energy term is based on the line energy of a dislocation balanced by the work for extending the dislocation loop per loop area. Using the defactant concept, and including hydrogen into consideration, we can show the hydrogen effect through lowering the line energy of the dislocation.

Ni-based electrodes for hydrogen evolution in anion exchange membrane electrolysis

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Renewable hydrogen generation is a crucial step to reach a sustainable society. Water electrolysis represents a cheap and effective method for hydrogen production. Anion-exchange membranes (AEM) water electrolysis utilizes cheap transition metal electrocatalysts, membranes, ionomers, and construction materials. AEM electrolysis is hampered by two main issues: stability and performance. Focusing on the latter, this work demonstrates a highly active NiMo nanosheets as cathode for hydrogen evolution in AEM electrolysis. We demonstrate an electrolyzer performance of 1 A cm⁻² at 1.9 V (total cell voltage) with a NiMo loading of 5 mg cm⁻² and an iridium black anode in 1 M KOH at 50 °C, that may be compared to 1.8 V for a similar cell with Pt at the cathode. The catalysts developed here will be significant in supporting the pursuit of cheap and environmentally friendly hydrogen fuel.

Chemical functionalisation of polymer nanostructures for cell studies

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Nanostructured surfaces with independently tuneable chemical structures and topographies can be used as synthetic cell interfaces with various applications such as the study and control of cellular processes. For such a system, the biocompatible and optically transparent epoxy-based polymer SU-8 can be used to fabricate high aspect ratio nanostructures on glass slides. The influence on cells from nanotopographies has been explored thoroughly, but less is known about the influence on cells from surface chemistry ^[1,2]. Therefore, the focus of this work is on the specific tuning of the surface chemistry. In order to functionalise the surface of the nanostructures without altering the substrate, a functional group in the SU-8 resist, namely the epoxy group, can be employed as anchor point for subsequent functionalisation. In this work different approaches to specifically tune the surface chemistry to attach biorelevant molecules will be analysed. One possible pathway is shown in the reaction scheme displayed in the figure below.

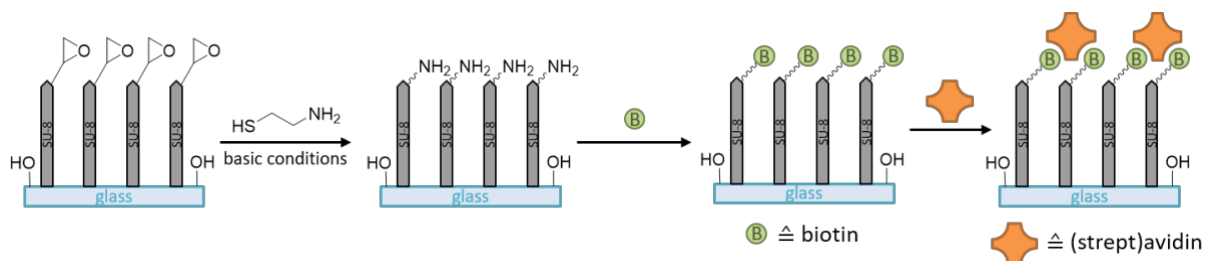


Figure 2: Reaction path to attach biologically relevant molecules onto SU-8 surface.

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Toward sustainable recovery of Rare Earth Elements: Separation of CeO₂, LaO₂, and Fe₂O₃ nanoparticles using biosurfactants

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Our project responds to the emerging need to develop a better fundamental knowledge and predictive model of the interactions of nanoparticles (NPs) with biomacromolecules (such as microbially-produced surfactants and proteins) and bacteria relevant to separation of valuable minerals from gangues in ore processing. In this preliminary study, we characterized commercial CeO₂ and LaO₂, as well as lab-synthesized hematite (α -Fe₂O₃) NPs using XRD, TEM, BET surface area, and zeta potential. We acquired a set of commercially available sugar-based biosurfactants and characterized them using FTIR.

Growth and characterization of topological magnetic systems

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Topology is a mathematical concept which is concerned with properties that are invariant under continuous deformation of space. A multitude of topological defects exist in magnetic materials, like domain walls, vortices or skyrmions. Especially, magnetic skyrmions have become very significant due to their non-trivial magnetic structures.

Molecular beam epitaxy (MBE) can be used to synthesize skyrmionic material systems with high crystalline quality and its properties can be investigated using magnetic probe microscopy. The goal is to realize high quality thin films of materials that were previously available only in form of bulk crystals and to create completely new skyrmion systems.

Among the different skyrmion systems, Fe_3Sn_2 is a very interesting material because of its high T_c (630K) and uniaxial easy axis magnetic anisotropy. Skyrmion bubble domains are observed in Fe_3Sn_2 lamella due to strong correlation between geometric and magnetic order.

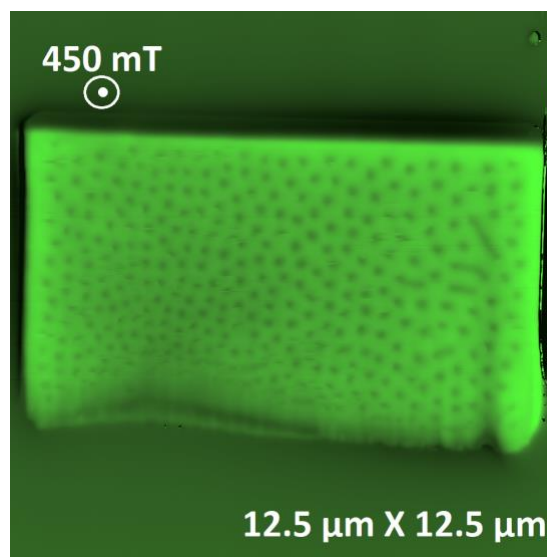


Fig: MFM image of Fe_3Sn_2 lamella

Enabling a novel in-situ reactor for high-resolution studies by HF vapor etching.

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A feasibility study for a novel in-situ reactor for high-resolution TEM imaging of thin film deposition processes was conducted at Stanford University. Using the Uetch HF vapor etch tool from SPTS it was shown, that a controlled and highly selective etch of a sacrificial SiO₂ tunnel surrounded by Al₂O₃ as etch stop layer is possible with a etch depth of several hundred μm. Freestanding Al₂O₃ tunnels with a thickness of 20-50nm were manufactured. An additional stabilization layer of poly-Si was used to enable better tunnel stability. For in-situ deposition processes, these tunnels can be used as reactors. Deposition happens inside the channel and can be imaged through the thin Al₂O₃ membranes on top and below the tunnel. Integrated tunnels in one chip serving as a reactor can significantly reduce space consumption and complexity of in-situ chips for high-resolution imaging.

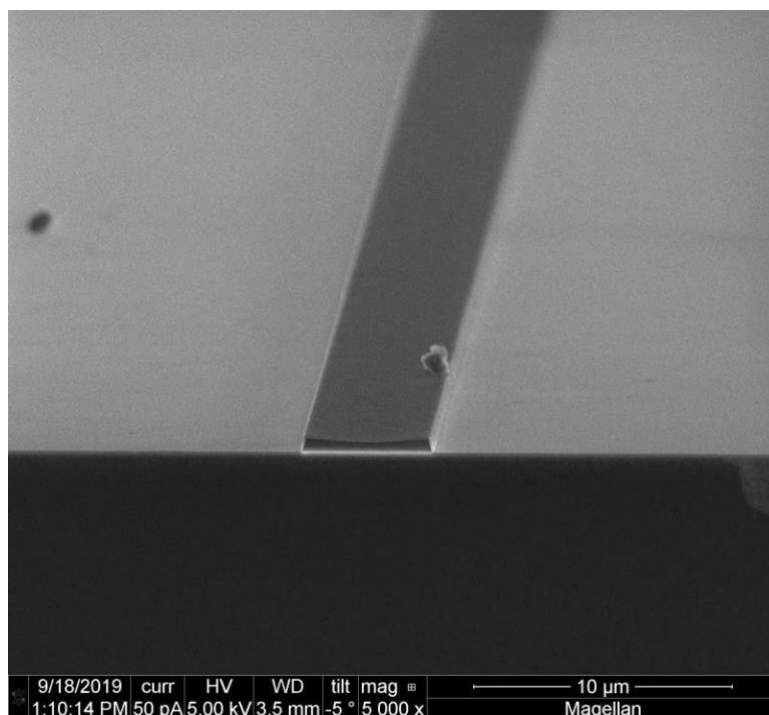


Figure 1 Freestanding Al₂O₃ tunnel with a wall thickness of 50nm and tunnel depth of 450μm

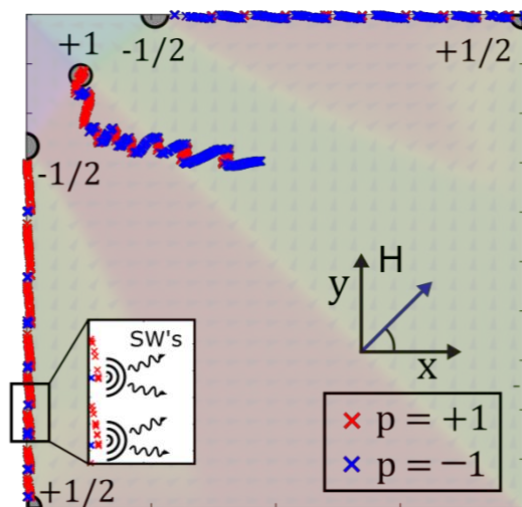
Exchange explosions of topological edge defects in a square micromagnet

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The magnetodynamic properties of a square thin film micromagnet ($2\ \mu\text{m} \times 2\ \mu\text{m} \times 16\ \text{nm}$) with a flux-closure magnetic ground state were investigated by micromagnetic simulations. The system was excited with an applied magnetic field, displacing the vortex core sufficiently far from its equilibrium position to result in a non-linear relaxation upon removal of the field. We find that creation of edge topological defects leads to exchange explosions and periodic emission of short wavelength spin waves emanating from these defects. The exchange explosions are investigated and explained in terms of creation of a vortex/antivortex pair with nucleation of a Bloch point. This finding could prove useful to the development of nanoscale devices for periodic generation of high-frequency microwave radiation.



Epitaxial growth of antiferromagnetic materials by Molecular Beam Epitaxy

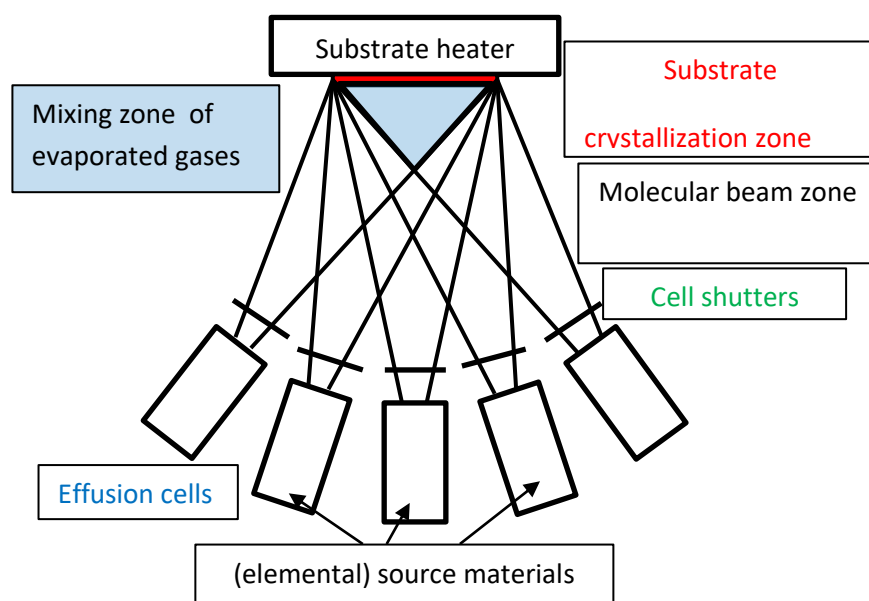
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The plan and prospect of new materials and high quality AFMs for antiferromagnetic spintronics are presented here. The focus will be placed on non-centrosymmetric materials for Dzyaloshinskii-Moriya interaction and complex magnetic textures (such as helical and skyrmionic structures). Molecular Beam Epitaxy offers a high amount of control in regard to crystal quality and purity, but also provides a control over material properties and interfaces. The chosen materials offer magnetic ordering well above room temperature, making them strong candidates for application purposes.



Growth of Anisotropic Gold Nanoparticles(AuNPs) – study on the effect of co-surfactants

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AuNPs have the potential to be used for biomedical applications like bio-sensing and imaging due to its excellent optical properties. Additional functionality like drug delivery can be added by functionalizing with polymeric NPs.¹ However, these functionalization methods can mask certain properties of the constituting NPs² and hence a fundamental understanding is required to make these NPs work synergistically. Here, we report a complementary approach to understand the effect of co-surfactants on the growth and optical properties of AuNPs synthesized by the seed-mediated³ method. Among other parameters, growth kinetics was studied using UV-Vis spectrometer and S(T)EM. In addition, Molecular Dynamics simulations were performed using GROMACS to study the effect of the co-surfactant and its interactions. The co-surfactant is found to interact with the surfactant micelles and also influence the kinetics which affects their shapes and properties. The experimental and simulation results will be used to setup Population Balance Equations to understand the evolution of these NPs.

Tailoring long-range order in arrays of magnetic nanodisks

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Magnetism since the inception of the digital age been the preferred method for mass data storage. However, intensive research to extend the use of magnetism to data processing and other applications is ongoing. Patterning of ferromagnetic thin-films at the nanoscale opens new opportunities for tailoring of magnetic properties and creating magnetic metamaterials with designed properties.

Here, we show how long-range magnetic order can be stabilized by dipolar interactions in two dimensional arrays of magnetic nanodisks. We use electron beam lithography and liftoff for patterning and the magnetization is imaged using XMCD-PEEM. We show that the individual nanodisks are in a monodomain configuration and that the long-range order depends on lattice geometry. For a square lattice of nanodisks the ordering is antiferromagnetic and for a hexagonal lattice the ordering is ferromagnetic.

Nano-enhanced Adsorptive Media for Nutrient Recovery from Wastewater

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The transition towards circular economy and recovery of nutrients from wastewater is a prominent action worldwide. Adsorption-based techniques are reliable and effective in removing nutrients. However, a viable adsorption-based nutrient removal requires a phosphate selective sorbent which is durable, cost effective and reusable. Commercially available anion exchangers are robust and durable but exhibit poor selectivity. In this study the application of a new class of adsorbents was investigated for nutrient recovery (phosphorus and nitrogen) from wastewater. The results showed that the tested media had high phosphate selectivity in the presence of other commonly encountered anions, namely, sulfate, chloride, and bicarbonate. The regeneration was effective to release the adsorbed phosphate with no noticeable loss in capacity. The customized regeneration resulted in N-P-K fertilizer as the final product.

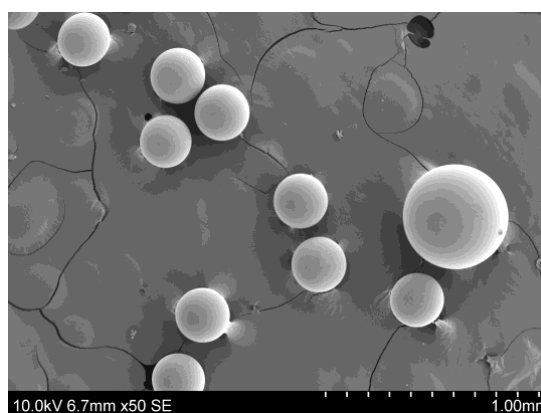


Figure: The SEM image of Nano-enhanced adsorptive media

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***In situ* synthesis of SiO₂ epoxy nanocomposites for high voltage insulation**

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Polymer nanocomposites are often produced using *in situ* approaches where an inorganic filler is synthesized directly in an organic matrix, resulting in improved dispersion of the filler. In this work, a sol-gel method has been adapted to synthesize surface functionalized SiO₂ *in situ* in epoxy, as epoxy-SiO₂ nanocomposites have demonstrated promising properties for application as high-voltage insulation materials. The synthesized SiO₂ moieties were dispersed in clusters of 10-80 nm. Raman and SAXS measurements indicated the formation of 4-membered D₁ rings, similar to that of POSS, and that the SiO₂ clusters consist of a hierarchical structure with an evolution from a mass fractal to a surface fractal structure. The nanocomposites displayed improved thermal stability, and the relative permittivity showed no significant changes from that of pure epoxy. The glass transition behavior and the onset of the dielectric relaxation varied with the structure and content of the SiO₂.

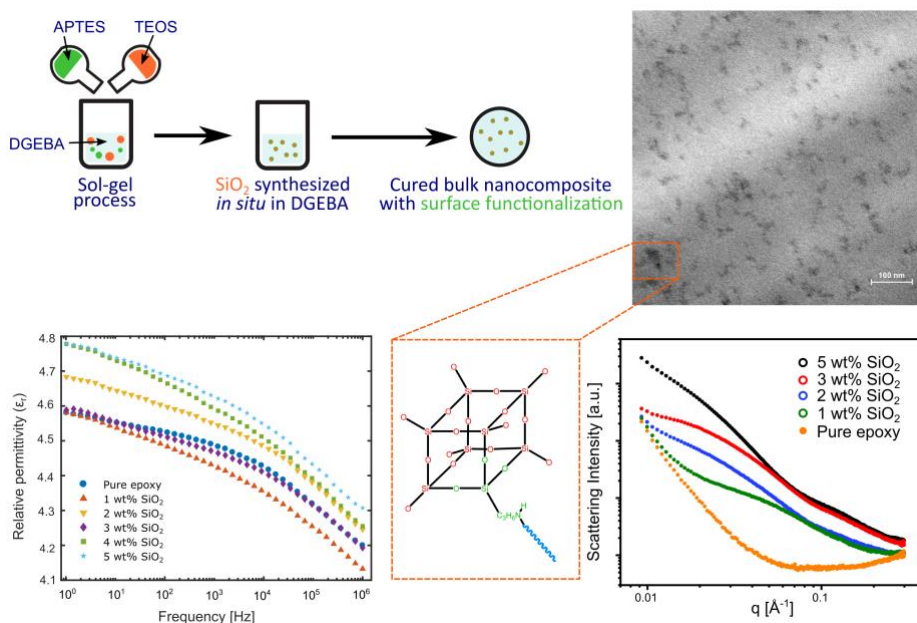


Figure 1. Graphical abstract for the synthesis and characterization of epoxy-SiO₂ nanocomposites

This work is funded by The Research Council of Norway through the project “Stipendiatstilling til SINTEF Energi AS” (Project No. 259866).

Microfluidically Augmented Dye-Sensitized Solar Cells: Integrating Nanoscale Materials with Microfluidics for Performance and Longevity Enhancement

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Integration of microfluidic capability into various architectures of dye-sensitized solar cells offers the benefit of overcoming the competitive electron diffusion bottleneck whilst simultaneously enabling dynamic replacement of degraded materials for constant uptime. We fabricated and characterized the performance of various iterations of microfluidically enabled devices that use TiO₂ and demonstrate the first instance of a ZnO based device with nanowires grown within microfluidic channels. Whilst circulating electrolyte, large-area microfluidic TiO₂ and ZnO nanowire devices showed increased conductivity where photocurrent was improved by 38% and 13%, respectively, compared to traditionally static electrolyte. Employing microfluidics in degraded devices allowed for the total replacement of the degraded layer with a fresh payload of dye resulting in greater than 100% and 83% photocurrent recover, post-degradation in TiO₂ and ZnO nanowire-based devices, respectively. Microfluidic capability is a unique platform to present alternative architectures modified by the flow of traditionally static components for enhanced performance longevity.

Inhibition of Metal Dusting corrosion on Fe-based superalloy

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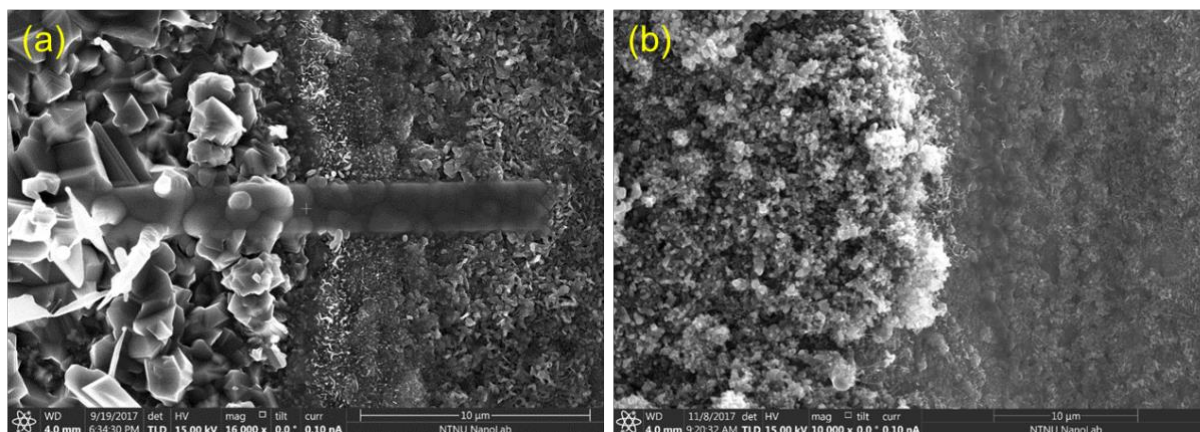
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Fe and Ni are excellent catalysts for producing carbon nanostructures due to their ability to activate gaseous carbon-containing molecules to form carbon-carbon bonds. However, when Ni- and Fe-based alloys are exposed to highly carburizing atmospheres, metal dusting corrosion - a costly and potentially catastrophic phenomenon - may occur. We have discovered a special thermo-mechanical surface pre-treatment method for Fe-based alloys that significantly inhibits carbon formation; see the comparison of treated and untreated regions below.

By use of facilities at NTNU Nanolab and NORTEM, we have identified some critical factors for the inhibition. The method promotes formation and stabilization of a thin, but uniform, Cr-rich oxide scale that prevents contact between the carburizing atmosphere and the Ni and Fe in the alloy. The results imply that the metal dusting resistance of industrial equipment can be improved in a scalable and practical way, and the method is under patenting.



SEM micrographs of Fe-based alloy after thermo-mechanical pretreatment (a), and after 20h exposure to metal dusting corrosion conditions of infinite carbon activity(b); right region subjected to pretreatment.

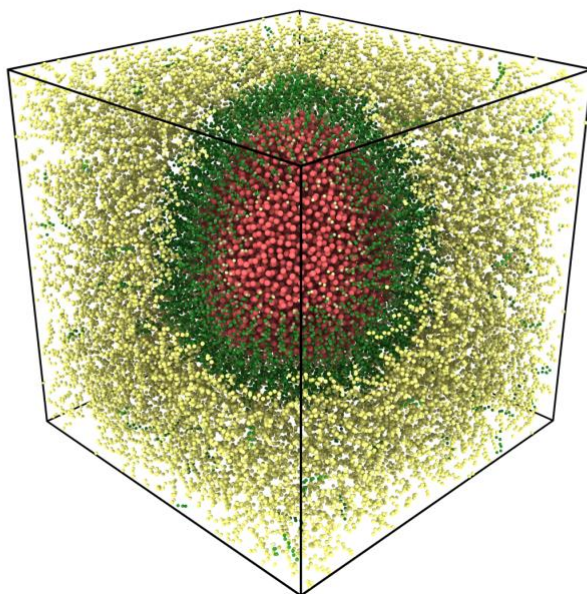
Deformation Mechanics of Microemulsion Droplet by Molecular Modelling

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Microemulsion exists extensively in natural environment, daily life, and countless commercial manufacturing including petroleum production, food processing and new materials fabrication. The properties of microemulsion attract increasingly intensive interest in multiple research fields. In this work, coarse-grained models of microemulsion are developed for studying the deformation mechanics of microemulsion droplets, aiming for the first time revealing the explicit steps in rupturing a surfactant coated water droplet in oil. With applying counter forces on the water core and surfactant shell in molecular dynamics simulations, the determinants of mechanical stability of microemulsion droplets are probed at different ambient temperature for the thermal-dependent effects. The results of this work can shed light on understanding the nanoscale mechanics in active demulsification in related application fields including oil recovery, industrial waste purification, and many others.



Challenges with FeS₂ Thin-Film Solar Cells

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Owing to the limitation of photovoltage generation above 200 mV, the conversion efficiency of experimental solid-state and photo-electrochemical pyrite (FeS₂) based solar cells have never exceeded 3%. A sulphur deficiency (S-deficiency) in the pyrite structure has commonly been discussed in the literature to be responsible for this limitation. However, there is no unambiguous evidences to correlate the low photovoltage with S-deficiency. With debates and inconsistent scientific findings, we here present a deductive reasoning from the electronic structure of FeS₂ and the vacancy formation energies to dissect the pragmatic view of associating the sulphur vacancy (S-vacancy) with poor photovoltage of FeS₂ solar cells. For a path forward research, we suggest a few key questions that have to be resolved to find the genuine causes behind the low performance, rather than a direct or indirect association with S-vacancies.

Cellulose-based Separators in Lithium-Sulfur Batteries: an XPS Study of the Lithium-metal Anode

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One of the major challenges for the realization of Li-S batteries is to minimize the spontaneous reactions between the lithium- (Li) metal electrode and the cathode reaction intermediates in the form of dissolved polysulfides (Li_2S_n or PS). These reactions give rise to the so called “polysulfide redox shuttle”, which results in rapid self-discharge reaction. The shuttle effect will further lead to the reactivity of Li metal means fast decomposition of the electrolyte, which results in short cycle life [1].

In this work, the use of a cellulose-based separator with a carbon nanotube (CNT) interlayer was investigated in Li-S batteries. In the latter, the sulfur electrode was fabricated using an optimized recipe (involving sulfur loadings of $2\text{--}2.5\text{ mg cm}^{-2}$) [2]. Compared to a conventional porous polypropylene separator, e.g. Celgard 2400, the unmodified cellulose separator and CNT-coated cellulose (CCC) separator both yielded a prolonged cycle life. Interestingly, however, a substantial decrease in the coulombic efficiency was observed in cells equipped with the CCC separator, contrary to expectation.

Surface analysis by X-ray Photoelectron Spectroscopy (XPS) indicates that the surface composition of the interphase formed on the Li-metal electrode was separator dependent. A higher fraction of reduced sulfur species was observed on the surface for the cells cycled with the cellulose-based separators. Moreover, a higher rate of electrolyte decomposition on the Li electrode was in evidence with the Celgard as the separator. The latter could be concluded from the higher photoelectron signal intensity found for salt degradation products on the Li surface. This finding corroborates the shorter cycle life seen for the cell with Celgard separator.

This work demonstrates the complexity of the interplay between several approaches that are commonly used to optimize Li-S cells, namely cellulose-based separators, porous carbon interlayers and the LiNO_3 additive. The results of this study deliver significant insights regarding further development of functional separators for high-performance Li-S batteries.

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