MATERIALS SCIENCE INITIATIVE SEMINAR:

MATERIALS FOR TOMORROW

1st Avancell Conference

October 18-19, 2011
Welcome to Materials for Tomorrow 2011 and Avancell Conference!

Dear Colleagues,

We are happy to welcome you to the events taking place October 18/19 2011 in the Chalmers kårhus. “Materials for Tomorrow 2011” is the 2nd Initiative Seminar of the Materials Science Area of Advance, a crucial meeting place for people representing research, innovation and society. At the same time, the first open “Avancell conference” following internal seminars invites academia and industry interested in making a future benefit to the Swedish forest resources.

Both conferences are free of charge and open for everybody. We have a common panel discussion on Oct 18 10.30-12.00 about “Future trends in Materials Science” where Chalmers and GU researchers from different scientific areas try to predict and discuss what is going to happen in the materials science field in the next 5 to 10 years. The poster session and following dinner with entertainment and mingling is also and gives excellent opportunity to continue scientific discussion and make plans for collaborations.

On Wednesday Oct 19, we warmly invite you to the special Arrhenius medal ceremony with following prize lecture on “Materials for polymer solar cells” by Mats Andersson, Chalmers professor at the Department of Chemical and Biological Engineering. He will be rewarded for his work on conducting polymers by the Swedish Chemical Society.

In this booklet you can find programs, some background information about both Avancell and the Materials Science Area of Advance as well as poster abstracts of the joined poster session.

We hope you have a stimulating time, find inspiration, build new collaborations and get excited to come back to next years material’s symposia.

Krister Holmberg Åsa Östlund Aleksandar Matic Mats Wallin
PROGRAMME

All presentations and panel discussions are open for everybody without prior registration.

TUESDAY, OCTOBER 18

Time: 9.00 – 22.00
Place: Runan, Kårhuset

SESSION 1: SPORTS AND TRENDS IN MATERIALS SCIENCE

9.00 - 9.20 Welcome
KRISTER HOLMBERG, AREA OF ADVANCE DIRECTOR

9.20 – 10.00 Has Sport a role to play in Material Science?
JAN-ANDERS MÂNSON, EPFL LAUSANNE, SWITZERLAND, LABORATORY OF COMPOSITE AND POLYMER TECHNOLOGY

10.00 – 10.30 Coffee

10.30 – 12.00 Panel discussion – “Trends in Materials Science” with
ANNE-MARIE HERMANSSON, CHALMERS, DEPT. OF CHEMICAL AND BIOLOGICAL ENGINEERING
LARS NYBORG, CHALMERS, DEPT. OF MATERIALS AND MANUFACTURING TECHNOLOGY
SESSION 2: BIO AND NANO IN MATERIALS SCIENCE

13.30 – 14.05 Biomaterials in orthopaedics - new demands based on changes of surgical techniques, diagnostics and new patient groups

HELENA BRISBY, GU, DEPT. OF ORTHOPAEDICS

14.05 – 14.40 Spinodal Decomposition in TiAlN thin films - a case of age hardening on the nano scale

LARS HULTMAN, LINKÖPING UNIVERSITY, DEPT. OF MATERIAL PHYSICS

14.40 – 15.10 Coffee

15.10 – 15.45 Atomic-scale theory for sparse matter

ELSEBETH SCHRÖDER, CHALMERS, DEPT. OF MICROTECHNOLOGY AND NANOSCIENCE

15.45 – 16.20 Nanostructured biocomposites - does the "nano" aspect really matter?

LARS BERGLUND, ROYAL INSTITUTE OF TECHNOLOGY, DEPT. OF CHEMICAL SCIENCE AND ENGINEERING

POSTER SESSION & DINNER

16.20 – 18.30 Poster session, including oral presentations

18.30 – 22.00 Dinner and entertainment
**WEDNESDAY, OCTOBER 19**

**Time:** 9.00 – 13.30  
**Place:** Runan, Kårhuset

**SESSION 3: MATERIALS SCIENCE IN A GREATER PERSPECTIVE**

9.00 – 9.30  Large scale facilities  
*LARS BÖRJESSON, CHALMERS, DEPT. OF APPLIED PHYSICS*

9.30 - 10.00  How X-ray free electron laser pulses interact with samples; from single molecules to bulk solids  
*JAKOB ANDREASSON, UPPSALA UNIVERSITY, LABORATORY OF MOLECULAR BIOPHYSICS*

10.00 – 10.05  Presentation of Arrhenius medal 2011 to MATS ANDERSSON, CHALMERS, for his work on conducting polymers

10.05 – 10:30  Prize lecture – Materials for polymer solar cells  
*MATS ANDERSSON, CHALMERS, DEPT. OF CHEMICAL AND BIOLOGICAL ENGINEERING*

10.30 – 11.00  Coffee

11.00 – 12.25  Panel discussion: “How should industry and Chalmers interact in order to optimize collaboration?” with  
*CLAES AHLNECK, ASTRAZENECA*  
*HANS PERSSON, VOLVO TECHNOLOGY*  
*ROLL ANDERSSON, SUMO BIOMATERIALS AND SCA*  
*ULF CARLSON, CHALMERS, DEPT. OF CHEMICAL AND BIOLOGICAL ENGINEERING*  
*HÅKAN GRUBB, XYLOPHANE*  
**Moderator:** LARS ROKKJAER, EQUILIBRIO

12.25 – 12.30  Summary of Panel discussions & concluding remarks  
*ALEKSANDAR MATIC, AREA OF ADVANCE CO-DIRECTOR*

12.30 – 13.30  Lunch
A closed session targeted at high school students from the Gothenburg area. Short presentations by young scientists from Chalmers as well as from industry will be followed by practical demonstrations and hands-on experiences of new materials.
Research spans five departments and includes several world-leading excellence centres and research programmes. The Department of Biomaterials at the University of Gothenburg is also part of the government-funded initiative.

Vision
Our vision is to make an impact on society and contribute to sustainability through excellence in materials research.

Design
Materials Science at Chalmers is structured into three thematic and two generic excellence profiles. In the thematic profiles, Materials for Energy Applications, Materials for Health and Sustainable Materials, multi-disciplinary research is carried out and spans natural science to engineering, and materials theory to processing.

The generic excellence profiles, Theory and Modelling and Experimental Methods, focus on developing new methodology and research infrastructures, which form the basis for thematic research. Staying at the forefront of materials theory, modelling, and experimental tools lays the foundation for breakthroughs in materials science.

Outstanding research
Research is primarily carried out at the departments of Applied Physics, Applied Mechanics, Chemical and Biological Engineering, Microtechnology and Nanoscience, and Materials and Manufacturing Technology. There are several excellence centres in the materials science area that span departmental boundaries and have strong industrial involvement. The main centres are the VINN Excellence Center Supramolecular Biomaterials, Wallenberg Wood Science Centre, the Competence Centre for High Temperature Corrosion, the Competence Centre for Catalysis and the Center of Excellence in Railway Mechanics. Chalmers is also involved in the VINN Excellence Center BIOMATCELL, which is hosted by the University of Gothenburg.

Innovation and impact on society
The combination of scientific excellence and relevance for society guides activities for the Area of Advance. Research aims to achieve new breakthroughs in materials science and to increase the competitiveness of industrial partners through new processes and products, thus creating a base for new companies through research ideas and
becoming a competence resource for society and industry. The means to reach the aims include:

- Supporting the development of young, talented scientists
- Giving excellence grants to selected, internationally recognized scientists
- Funding seed projects to develop new research lines and collaborations
- Establishing exchange with academia and industry
- Collaborating with large-scale facilities and research centres
- Organising outreach activities

**Integrated education**

Several of the master’s programmes at Chalmers directly relate to materials science. All of the master’s programmes are taught in English and there are a large number of international students from Europe, North America and Asia. On the PhD level, the cross-departmental graduate school in Materials Science provides genuine cross-disciplinary training and a common curriculum in materials science for PhD students from five different departments. Chalmers also hosts the graduate school in Soft Matter, with a national responsibility to provide specialised courses in the field of soft matter.

**Interdisciplinary research between Materials Science and other Areas of Advance**

Materials Science has links to several other Areas of Advance, in particular Energy, Production, Transport, and Nanoscience and Nanotechnology. A prime example is the Materials for Energy Applications profile which is shared with Energy.

**A sustainable future**

Materials Science contributes to the development of a sustainable future by enabling new technologies, as well as by increasing efficiency and decreasing the environmental impact of existing technologies. Examples of current research include new materials for batteries and fuel cells, lightweight materials, improved catalysts for emission control and for sustainable energy systems, and materials based on renewable feedstock.
Södra Skogsägarna started Avancell in 2005 as a research and idea network between Chalmers and industrial partners. The focus of Avancell is on wood fibres and aims to:

- Create a toolbox for fibre modifications
- Control fibre-water interactions
- Develop processes for produce textile fibres from wood

In 2008, the network was expanded with new companies: SCA Hygiene, Tetra Pak and Korsnäs, as well as the WooDi and Formulosa projects. In total, the Avancell network now includes 11 PhD students, 5 postdocs, 7 professors and more than 10 people from the partner companies.
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<td>Registration</td>
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<td>09.00 - 09.15</td>
<td>Welcome</td>
<td>Mats Wallin</td>
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<td>09.15 - 10.00</td>
<td>Dissolving pulp</td>
<td>Herbert Sixta</td>
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<td>09.50 - 10.30</td>
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<td>10.30 - 12.00</td>
<td>Panel discussion – trends in material science</td>
<td>Runan</td>
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<td>12.00 - 13.00</td>
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<td>13.00 - 13.45</td>
<td>Solvents for cellulose – strategies and controversial thoughts</td>
<td>Bruno Medronho</td>
<td>University of Coimbra</td>
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<td>13.45 - 14.30</td>
<td>Man-made textile fibres</td>
<td>Carl-Axel Söderlund</td>
<td>CAS Fibre Consulting</td>
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<td>15.00 - 15.45</td>
<td>From fibres to textile fabrics</td>
<td>Erik Bresky</td>
<td>The Swedish School of Textiles</td>
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<td>Intelligent textiles</td>
<td>Anders Bergner</td>
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<td>16.30 - 17.15</td>
<td>Design strategies for sustainable fashion &amp; textiles</td>
<td>Rebecca Earley</td>
<td>University of the Arts London</td>
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## Program Day 2

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<td>08.30 - 09.00</td>
<td>Processing and mechanical properties of thermoplastic composites based on cellulose fibres and ethylene - acrylic acid copolymer</td>
<td>Ruth Ariño</td>
<td>Chalmers University of Technology</td>
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<td>09.00 - 09.30</td>
<td>Modification of fluff pulp fibres: Cross-linking and alkali extraction</td>
<td>Kristoffer Lund</td>
<td>Chalmers University of Technology</td>
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<td>09.30 - 10.00</td>
<td>MFC/nanocellulose – chemical modifications of cellulose</td>
<td>Tom Lindström</td>
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<td>10.00 - 10.30</td>
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<td>10.30 - 11.00</td>
<td>NMR for moisture measurements in wood</td>
<td>István Furó</td>
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<td>11.00 - 11.30</td>
<td>The usage of cellulose and cellulose derivatives in pharmaceutical applications</td>
<td>Anette Larsson</td>
<td>Chalmers University of Technology</td>
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<td>11.30 - 12.30</td>
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<td>Visit to the Borås Museum of Textile History</td>
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<td>15.15 - 16.45</td>
<td>Visit to the Swedish School of Textiles</td>
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Novel Aspects in Dissolving Pulp Chemistry

Herbert Sixta
Department of Forest Products Technology, Aalto University, Espoo, Finland

Dissolving pulps are currently experiencing a significant market demand largely triggered by an increase in viscose fiber capacities in Asia. Conventional dissolving pulp production routes suffer from the significant yield losses owing to the conventional purification processes. An alternative approach for the manufacture of dissolving pulp is suggested in which hemicelluloses are selectively removed by an alkali post-treatment. Further, possible routes for adjusting pulp viscosity and improving pulp reactivity are introduced. The dissolution of a dissolving pulp in novel ionic liquids and its regeneration upon the addition of water is subject of the second part of the lecture. Solvatochromic parameters of cellulose solutions are related to the dissolution and regeneration behavior of cellulose. The latter is monitored by turbidity and rheological measurements.

“Greener” Solvents for Cellulose Dissolution: Strategies and Controversial Thoughts

B. Medronho¹,²*, M. G. Miguel¹, B. Lindman.¹, ³, L. Stigsson⁴

¹Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal
²University of Algarve, Laboratory of Plant Biotechnology, Campus de Gambelas, Faro, Portugal
³Lund University, Division of Physical Chemistry, Center for Chemistry and Chemical Engineering, SE-22100 Lund, Sweden
⁴KIRAM AB, Norra Villavägen 17, 23734 Bjärred, Sweden

*bfmedronho@portugalmail.pt

Cellulose is the most abundant natural polymer on earth and has numerous applications. In several processes one of the hardest tasks faced is related to cellulose dissolution. Traditional dissolution methods have important limitations especially allied to costs and environmental issues. The current understanding of cellulose (in)solubility in aqueous based solvents (or others) is based on the ability of a solvent to break down the strong cellulose inter and intra hydrogen bonds. This is widely accepted by the world leaders in the field. However, such mechanism is highly questionable since hydrogen bongs are not expected to the promote association in water. In this work we investigate the influence of amphiphilic-like molecules in different cellulose solvent systems. The addition of amphiphilic molecules decreases the hydrophobic interactions responsible for cellulose insolubility in aqueous media thus decreasing the viscosity of the resulting dopes. The data elucidates the amphiphilic character of cellulose.
Man-Made Textile Fibres

Carl-Axel Söderlund
CAS Fibre Consulting, Karlstad

Man-made fibres could be classified into two groups, natural polymer fibres and synthetic fibres.

**NATURAL POLYMER FIBRES**, such as Viscose (HMW), Lyocell/Tencel, and acetate, are man-made fibres from wood cellulose origin. The most used natural textile fibre is cotton. Mixed with man-made cellulose fibres or synthetic ones improved textiles are possible, but the future of cotton could be limited by ecological aspects. The Viscose process with staple fibre production is expanding in Asia where modern plants are more environmentally designed. Viscose fibres are very versatile with simple renewable raw materials. The Lyocell or Tencel process is mainly expanding in Europe and is a high tenacity fibre with minimal environmental impact. The Tencel and ionic liquid processes will expand dramatically if cheaper solvents and patent restrictions are solved. New processes like Carbamate or Biocelsol with direct dissolving of cellulose in NaOH is under development to be environmentally friendly, but the fibre properties still to be improved.

**SYNTHETIC FIBRES** are hydrophobic, such as polamides, polyesters, polyvinyl derivatives (polyacrylonitrile), polyethylene, polypropylene, and polyurethanes, and are dependent on the polymer development. Polyester is the largest one, versatile as a blending partner and will grow. The polyamides, polyolefins and acrylics will expand their use when the use of cotton decreases.

For the future the hydrophilic man-made cellulose fibres has a great challenge. One is if the fibre production is in fully integrated pulp plants (fibre clusters), with the whole chain from trees to the man-made cellulose fibres. The second challenge is as replacement and completion of cotton.

**From fibres to textile fabrics**

Erik Bresky
*The Swedish School of Textiles, Borås*

(Abstract missing)
Intelligent textiles

Anders Bergner  
*Swerea IVF, Mölndal*

New and coming fibers create extensive possibilities for innovations and totally new products in the textile sector. There are a range of relatively new high performance fibers giving opportunities for personal protective equipment with a new level of performance. Fascinating results and interesting products illustrating protection against water-jetting and textiles with excellent puncture resistance will be demonstrated. Ongoing research in the field of sustainable fibers for replacing cotton and traditional polymer fibers will complement in future high volume products. Together with new technologies for functionalization of materials and surfaces, the textile innovators will meet a thrilling future where functionality, sensors and actuators could contribute positioning textile technology as a future high-tech business with exciting possibilities involving advanced medical technology and IT-solutions.

TED’s TEN: Design Strategies for Sustainable Fashion and Textiles

Rebecca Earley  
*Textiles Environment Design (TED), Chelsea (CCW), www.tedresearch.net, University of the Arts London (UAL)*

Key words: *Design strategies, Consumer behaviour, Layered Thinking, Sustainability & Innovation, Product Development*

Through individual practice and group research at CCW, the TED group has developed TED’s TEN – a set of strategies which intend to help individuals and SME’s make more informed fashion/textile design decisions. These are currently being explored through a broad portfolio of research and consultancy projects, which ultimately ask the designer to consider several strategies at any one time, using design thinking to achieve a layered and interconnected approach. The resulting fashion/textile concepts often combine theoretical thinking with material, technical, and social innovations, and aim to connect and inform the fashion consumer with the fashion/textile product in new ways.

**TED’s TEN:**

1. Design to Minimise Waste  
2. Design for Recycling / Upcycling  
3. Design to Reduce Chemical Impacts  
4. Design to Reduce Energy and Water Use  
5. Design that Explores Clean / Better Technologies  
6. Design that Looks at Models from Nature & History  
7. Design for Ethical Production  
8. Design to Replace the Need to Consume  
9. Design to Dematerialise and Develop Systems & Services  
10. Design Activism
PROCESSING AND MECHANICAL PROPERTIES OF CELLULOSE FIBRES AND ETHYLENE – ACRYLIC ACID COPOLYMER COMPOSITES

Ruth Ariño*, Antal Boldizar
Department of Materials and Manufacturing Technology, Chalmers University of Technology, SE- 41296 Göteborg, Sweden

The melt processing and the tensile mechanical properties of composites consisting of 30 wt% cellulose fibers and ethylene-acrylic acid copolymer were studied. The compounding techniques used were extrusion mixing performed with a single screw extruder and elongation dispersive mixing performed with the injection-molding machine. All blends were injection-molded in a final step. Fiber length, fiber content and mechanical properties were studied and the number and the size of fiber aggregates in the samples were determined by microscopy analysis. Two passes of elongation dispersive mixing had a beneficial effect on the mechanical properties, which could be related to the fewer and smaller amounts of aggregates. The processing had a small or insignificant effect on the fiber length since the fiber lengths measured were within the same range as that of the starting material.

Modification of fluff pulp fibres: Cross-linking and alkali extraction

Kristoffer Lund
Chalmers University of Technology

Fluff pulp has been one of the key components of hygienic products, such as diapers, for many years. However, the introduction of superabsorbent polymers (SAPs) as the main absorbing material has decreased the dependence on fluff pulp. In order to decrease reliance on oil-based SAPs, it is of interest to investigate and improve on fluff pulp properties. In the first part, softwood kraft pulp fibres were cross-linked with a diepoxide. Results showed that the wet bulk under load of the low-density fibre networks increased as a result of the modification. In the second part, softwood kraft pulp and birch kraft pulp were alkali extracted with NaOH. It could be seen that the alkali extraction had a positive effect on the defibration properties of the pulps. Furthermore, softwood kraft pulp fibres alkali extracted at the highest concentration of NaOH seemed to render a more flexible low-density fibre network.

NanoFibrillar Cellulose (NFC)-an emerging material for large-scale applications

Tom Lindström
Innventia AB, Stockholm

There has been extensive research and development activities in the field of nanocellululosic materials during recent years, although microfibrillated cellulose was developed already during the late 70s at ITT-Rayonier in USA.
A major impediment for the large scale use of NFC has been the high energy use (excess of 25000 kWh/tonne NFC) for its energy use. This problem has now been alleviated by a series of different pre-treatment procedures of the fibres prior to the subsequent mechanical cell wall delamination.

Today, there are many companies in the process of commercializing MFC and several pilot plants are available are companies are planning up-scaling. A pilot plant for the nominal production of 100 kg/day (dry based NFC) has also been taken into operation at Innventia AB.

The current contribution will highlight critical issues in the production of NFC and discuss various applications and hurdles to overcome in order to make NFC production for various end-use applications viable.

NMR and MRI of water in wood and cellulosic materials

Sergey V. Dvinskikh, Guilhem Pages, Camilla Terenzi, and István Furó
Department of Chemistry and Industrial NMR Center, Royal Institute of Technology, Physical Chemistry, Teknikringen 30, SE-10044, Stockholm (furo@kth.se)

Water defines many properties of wood and cellulosic materials.\(^1\) Hence, methods for characterizing its molecular state in such matrices are in demand. Here, various approaches based on nuclear magnetic resonance (NMR) and NMR microimaging (MRI) are presented. It is also illustrated how \(^1\text{H}/^2\text{H}\) isotope selectivity can be exploited for mapping water distribution. Besides high-field NMR and MRI, low field portable open access (unilateral) magnets are explored for in situ and non-invasive monitoring of local moisture content in extended wood specimens.


The usage of cellulose and cellulose derivatives in pharmaceutical applications

Anette Larsson
Chalmers University of Technology

This seminar should show some new examples where cellulose based materials have been used to control the drug release rates. Our new film coating based on micro fibrillated cellulose, MFC, and hydroxipropyl methylcellulose, HPMC, has shown that an increase in the amount HPMC resulted in decreased water permeability; opposite to what expected. This was explained by that MFC self-aggregated into thin layers, which resulted in a structure that gives longer diffusion partway and thus decreased permeability. We have recently shown that modified nanocrystalline cellulose can be used to control the drug release rate. These observations indicate an extended usability of cellulose based materials for controlled drug release.
1. Development of methodology for Surface Analysis of Soft Magnetic Composite Powders

C. Oikonomou¹, E. Hryha¹, L. Nyborg¹

¹Department of Materials and Manufacturing Technology, Chalmers University of Technology, SE – 41296 Göteborg, Sweden

Soft Magnetic Composites (SMCs) are designed for sustainable industrial production of uniform isotropic components with 3D magnetic properties, which makes innovating electrical machine designs industrially feasible. Soft magnetic composite powders are based on water-atomized iron powders. The addition of an insulating coating formed by nano-layer of inorganic compounds with high resistivity is needed in order to minimizing the negative effect of eddy-currents. Obviously, the insulating coating is the paramount feature of the SMC technology. Analysis of its initial state/composition on the micro-level, as well as any changes in that context during further compaction and heat-treatment, are thus of great importance for a successful development and industrial applications of the SMCs. Therefore there is a need for the development of a reliable method to evaluate the composition and thickness of such insulating coatings. High resolution imaging combined with surface analytical and depth profiling techniques (High-Resolution Scanning Electron Microscopy combined with Energy Dispersive X-ray Spectroscopy and X-ray Photoelectron Spectroscopy) were used. Analyses were performed on commercially available SMC powder grades, having a phosphate based coating.

The presence of electrical insulating layer unavoidably leads to charging effects that have to be taken into account starting from the specimen preparation step. Charge compensation thus is of critical importance for the precision and validity of the results. Charging effects were confronted by both adding slow electrons with a neutralizer and by software correction. A non homogeneity of the charging effects at the specimen’s surface, in both the same and different sputtered depths, favored the usage of software correction.

Specimen preparation is essential to the methodology development as it has to provide maximal electrical conductivity and have a minimal effect on the coating’s integrity. Two commonly used techniques were implemented and compared. Slight pressing of the powder on a conductive substrate (soft aluminum plates) and mounting of the loose powder on a double sided adhesive carbon tape. The results indicated that the latter technique is more suitable for the XPS measurements while the former is needed to be used in HRSEM and EDX analysis.

Depth profiling was carried out by ion sputtering in XPS. The analyses revealed the presence of oxygen (O1s), iron (Fe2p) and phosphorous (P2p) on the as-received powder surface, indicating these elements as the main components of the insulating coating. Traces of silicon (Si2p) and nitrogen (N1s) and a strong presence of carbon (C1s) at the top layers of the coating were also noted.

Two approaches were followed for the evaluation of the coating thickness. One, based on the relation between the normalized intensity of iron metal peak and etching depth and a second, using the etch depth where the phosphor and oxygen intensities reach half the difference of their respective maximum and minimum values. Results indicated that the thickness of the coating extends to approximately 30 nm depth from the surface.

In addition, a HRSEM and EDX methodology for the observation of the coating’s surface morphology at high magnifications and more accurate elemental analysis was developed. Inlens detector and low acceleration voltages (~5 kV) with the minimal electron current, aiming in reducing the interaction volume and still excite all elements present on the surface, are recommended.
Electrodeposition is an advanced synthesis method for making nanocrystalline materials. It is a non-line-of-sight deposition technique that can be used to create a wide set of sample geometries from thin coatings to large free-standing electroforms. Electrodeposition can also be used to create new types of metal/metal nanocrystalline cellular metals by reinforcing conventional open cell metal foams or microtruss materials. These composite cellular materials can offer enhanced mechanical strength at low density. Fracture in the reinforcing nanocrystalline sleeve is a key part of the overall cellular failure mechanism. The amount of plastic deformation that can be supported by the nanocrystalline material before fracture is controlled by factors such as the grain size and grain size distribution. In that connection, also the texture plays an essential role. The amount of plastic deformation can also be controlled by mesoscale alloy and impurity compositional fluctuations that are typically seen in the form of bands that are oriented perpendicular to the growth direction.

EBSD analyses were performed and revealed that the banded structure is not affecting grain growth and texture development upon annealing. Grown grains were found to be random in shape and no preferential sites for grain growth were observed. Mechanical testing is on-going.
3. Solid-State NMR, A solution for structure elucidation

Alexander Idström* and Lars Nordstierna

Applied Surface Chemistry, Chalmers University of Technology, Göteborg, Sweden
*Corresponding author: idstrom@chalmers.se

Even though its solution-state counterpart is more widely used in elucidation of chemical structures, solid-state NMR spectroscopy has become increasingly important for analytical chemists. With hardware development, solid-state NMR resolution is now comparable to that of solution-state NMR [1]. In addition, phenomena which are not detectable by solution-state NMR, e.g. anisotropic nuclear spin interactions, can be studied or effectively utilized with solid-state NMR, giving rise to new possibilities when designing NMR-experiments [1].

A wide range of information can be acquired using solid-state NMR. In studies of cellulose; degree of crystallization, fibril and aggregate size, and relative amounts of cellulose allomorphs (I_a, I_β, II etc) can be investigated [2] as seen in Figure 1. As a tool for elucidating crystal structures the technique has become invaluable and when studying conformation, bond angles and bond lengths, solid-state NMR shows benefits concerning the ability to analyze inhomogeneous and amorphous samples, compared to traditional methods such as XRD [1]. When studying metal-ion coordination, solid-state NMR gives information about coordination location [3].

![Figure 1. Spectrum (red) showing the C-4 area from a sample of microcrystalline cellulose. Line-fitting (blue, pink) gives information about degree of crystallization, fibril and aggregate size, and relative amounts of cellulose allomorphs.](image)

References
4. Self-Assembled Single Molecule Electronics

Kasper Moth-Poulsen*,1 Titoo Jain2, Asger Petersen2, Erling Thyraug2, Fredrik Westerlund1, Erik Johnson2, Tue Hassenkam2, Kristine Kilså2, Mikael Bols2, Niels Harrit2, Thomas Bjørnholm2.

1) Chalmers University of Technology, SE-412 96 Gothenburg, Sweden. 2) University of Copenhagen, 2100 Copenhagen Denmark * E-mail: Kasper.Moth-Poulsen@Chalmers.se

The impressive degree of miniaturization of electronic components during the last 40 years has substantially improved the capabilities of computers and electronic devices and revolutionized the way we use electronics in our everyday life. The utmost degree of miniaturization of electronic components is the realization of single molecule electronic components. One limiting factor in fabrication of single molecule electronic devices is the electrode structure needed for contacting individual molecules, more specifically conducting leads separated by a few nanometers, long enough to be contacted by conventional methods. Since the nanogap between the electrodes is of the size of molecule, fabrication of these structures cannot be done by conventional lithography. As a consequence a number of techniques have been developed to contact the single molecule (mechanical break junction, electromigration and scanning probe techniques to name a few), these techniques are limited to measurements on one molecule in each experimental realization.

Therefore, new ideas are required to overcome the challenge of bridging the gap between the molecular length scale (1-2 nm) and the length scale accessible by top down lithographic techniques (20-30 nm) in a more parallel way. Another challenge is the basic physical understanding of the electron transport through single molecules, in particular the transport mechanism and the position of the energy levels. This presentation present our most recent results towards parallel fabrication of single molecule electronic devices and also discuss our effort to contribute to a general understanding of the molecular and interface structures that control the electronic transport on the single molecule level.

Figure 1. left/middle Nanogap between two gold nanorods assembled around a single poly ethylene polymer.[4] Right) self assembly strategy for a single molecule supramolecular complex embedded in a nanogap.
5. Glass Transition and Relaxation Processes in Xylitol-Water Mixtures

Khalid Elamin, Johan Sjöström, Helén Jansson and Jan Swenson

*Department of Applied Physics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*

Broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC) were employed to study supercooled xylitol mixed with water in a wide frequency range (10-2 – 106 Hz) and at different temperatures (120 – 365 K). The presence of water clearly has an effect on both the cooperative $\alpha$-relaxation and the secondary $\beta$-relaxation. The $\alpha$-relaxation, which shows non-Arrhenius temperature dependence, becomes faster with increasing concentration of water. The secondary $\beta$-relaxation shows Arrhenius temperature dependence and the intensity increases dramatically with increasing water concentration. We find one calorimetric glass transition over the whole concentration range. It decreases from 247 K for pure xylitol to about 181 K at a water concentration of about 37 wt%. At higher water concentrations ice is formed and the glass transition temperature increases to a steady value of about 200 K for all higher water concentrations. This Tg corresponds to an unfrozen xylitol-water solution containing 20 wt% water. In addition to the true glass transition we observed a glass transition-like feature at 220 K for all the ice containing samples. However, this feature is more likely due to ice dissolution [1].

References:

6. Laboratory preparation of viscose

-Equipment and processes at Karlstad University

L. Östberg, U. Germgård

Department of Chemical Engineering, Karlstad University, SE 651 88 Karlstad, Sweden

Karlstad University has a long tradition in performing research in the area of regenerated cellulose and cellulose derivatives due to the earlier local presence of several industries that produced this kind of products. There has also been a large number of dissolving sulfite pulp mills in Värmland and Dalsland and a substantial part of the pulp production in the Billerud company up to 1970s was in fact dissolving pulp.

At Karlstad University we have unique laboratory equipment for producing viscose up to the spinning stage but we have unfortunately not a spinning machine. However, we can produce all stages up to this point i.e. from dissolving pulp to viscose; the final analysis of the viscose solution is usually done as Fock’s test, Gamma number, Viscosity and Filtration clogging value. In the presentation we are demonstrating the laboratory equipment and the process technique that we use. We have also been active in research projects where the objective has been to increase the reactivity of the pulp prior to mercerization. The pretreatment methods used has been either an enzymatic or a chemical pretreatment and the influence from the wood raw material has also been studied [1,2].

Viscose research has during the last five years become very interesting for the pulp industry, for textile producers and final consumers. We are therefore preparing for new research projects in this area where our lab equipment will be very useful.


7. Conformational motions in hydrated myoglobin by dielectric relaxation spectroscopy

Guo Chen\textsuperscript{a,b}, Paul W. Fenimore\textsuperscript{b}, Hans Frauenfelder\textsuperscript{b}, Benjamin H. McMahon\textsuperscript{b}, Ferenc Mezei\textsuperscript{b}, Jan Swenson\textsuperscript{a}, and Robert D. Young\textsuperscript{d}

\textsuperscript{a}Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden; \textsuperscript{b}Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA; \textsuperscript{c}LANSCE, Los Alamos National Laboratory, Los Alamos, New Mexico, USA; \textsuperscript{d}Department of Physics, Arizona State University, Tempe, Arizona, USA

Protein function requires conformational motions; conformational protein dynamics are coupled to the dynamics in the bulk solvent and the hydration shell. In this study we investigated the protein-hydration shell interactions by measuring the dielectric response of myoglobin embedded in solid poly(vinyl) alcohol and hydrated at different levels. The hydration-shell relaxations depended sensitively on hydration. We found that the internal motions of myoglobin can be predicted from the hydration-shell relaxations using a simple model. Here we report two examples: the temperature dependence of the Mössbauer elastic fraction in myoglobin and the msd of all the non-methyl hydrogen atoms in myoglobin measured by neutron scattering. The rapid decrease in the elastic fraction and the rapid increase in the msd at $\sim200$ K are both predicted from the dielectric data [1,2]. This quantitative connection of dynamics between myoglobin and its hydration shell manifests the essential role of water for the functions of proteins.


8. Regenerated cellulosic fibres for textile applications

M. Kihlman¹, L. Stigsson², M. Westin³, U. Germgård¹

¹ Department of Chemical Engineering, Karlstad University, SE-651 88 Karlstad, Sweden.
² Kiram AB, SE-237 34 Bjärred, Sweden.
³ SP Trätek, SE-501 15 Borås, Sweden.

Cellulose is a highly interesting polymer for bio-based products and can be utilized in a wide variety of products, either in its native form or derivated. One application that is predicted to grow remarkably for cellulose is related to the textile fibre industry. The demand in this industry is being fueled mainly by the steady growth of the world population and the upcoming lack of crude oil. Thus, it is believed that in the future forest based raw materials can play a major role in replacing fossil oil based fibres and cotton to new ecological man-made fibres in both woven and nonwoven end applications.

The CelluNova project was initiated in January 2010 with the objective of developing a new environmentally friendly process for the production of cellulose-based textile fibres [1]. Regenerated cellulose fibres, based on dissolving pulp, have recently successfully been prepared from small pilot scale trials in a stepwise procedure as shown in Figure 1. Until this stage of the project various types of dissolving pulps, pretreatment methods, aqueous solvent systems and coagulation baths have been investigated.

![Figure 1: Process steps for preparation of textile fibres based on dissolving pulp.](image)

9. Crystallization and structural transformation of mol% 50Li$_2$O:(50-x)P$_2$O$_5$:xB$_2$O$_3$ glass (0≤x≤50)

Benson K. Money$^1$, K. Hariharan$^2$ and J. Swenson$^1$

$^1$Dept. of Applied Physics, Chalmers Institute of Technology, Goteborg, Sweden
$^2$Dept. of Physics, IIT Madras, Chennai – 600 036, India

Ion-conducting glassy electrolytes tends to devitrify, under favorable thermodynamics, to an ordered stable crystalline phase. Though the glass mol% 50Li$_2$O:50P$_2$O$_5$, exhibits high ionic conductivity, the low thermal stability hampers its high temperature applications. DSC studies show that Li$_2$O:P$_2$O$_5$ glass undergoes internal (bulk) crystallization, with the crystallization mechanism closely associated with JMA model [1]. Incorporation of B$_2$O$_3$ has enhanced the thermal stability of the glasses, as the glass transition temperatures (T$_g$) of mol% 50Li$_2$O:50P$_2$O$_5$ increased from 330 °C to 417 °C in mol% 50Li$_2$O:25P$_2$O$_5$:25B$_2$O$_3$. Also, the crystallization temperatures (T$_c$) of the “mixed former” glasses are higher compared to that of Li$_2$O:P$_2$O$_5$ glass. Vibration spectroscopy indicates the conversion of trigonal BO$_3$ units into tetrahedral BO$_4$ bridging units, which increases the cross linking and network dimensionality, thus enhancing the thermal stability of the glasses. To probe the local environment associated with Li$^+$ ions and structural modification with the introduction of second glass former, Co$^{2+}$ transition metal have been doped in glasses for the Optical absorption studies. The absorption spectrum showed variation in spectra suggesting transition between octa- and tetrahedral coordination of Li$^+$ ions as second glass former B$_2$O$_3$ replaces P$_2$O$_5$.

10. B(CN)₄⁻ based Ionic Liquids, Salts, and Lithium Battery Electrolytes

J. Scheers¹, J. Pitawala¹, F. Thebault¹, J.-K. Kim¹, P. Johansson¹, A. Matic¹, J.-H. Ahn², and P. Jacobsson¹

¹ Applied Physics, Chalmers University of Technology. ² ITRC for Energy Storage and Conversion, Gyeongsang National University, Republic of Korea.

Intrinsic safety problems of commercial Li-ion batteries, based on LiPF₆ and carbonate solvent electrolytes, prevent these from being up-scaled and applied to new markets, for example electric and hybrid electric vehicles. Therefore, attempts are made to identify new salt and solvent combinations that are safer, but still competitive with the performance of conventional LiPF₆ electrolytes. In this work [1] we focus on the properties of electrolytes based on Bison [B(CN)₄⁻] – a thermally stable and fluoro-free anion component of alkali salts and ionic liquids (IL).

The conductivities of Bison based ILs are found to be high, but poor LiBison solubility excludes their use as main solvents for Li⁺ conducting electrolytes. These results are surprising, since strong Li⁺–Bison coordination contradicts computational predictions of ion pair energies. However, a refined model using larger ionic clusters suggests that Bison preferentially coordinates Li⁺ monodentately, which promotes the formation of extended ionic networks.

In ethylene oxide (EO) based oligoethers, the strong Li⁺ coordinating ability of the EO unit overcomes the ion-ion interaction and enables the preparation of LiBison electrolytes. Here we report several properties of a 1M LiB(CN)₄ polyethylene glycol dimethyl ether (PEGDME) electrolyte, for example electrochemical stability and preliminary battery cycling results with a Li and LiFePO₄ electrode configuration (Fig. 1).

Fig. 1: Discharge capacity of coin-cells with a 1M LiB(CN)₄:PEGDME or 1M LiBF₄:PEGDME electrolyte in a Li and LiFePO₄ electrode configuration. Repeated charge/discharge (25°C; 2.5 - 4.0 V; 0.1 C-rate).

11. Strategic Research Support at Chalmers


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Email: sfs.aos@chalmers.se
12. Soft matter: an atomic-scale condensed matter starting point

E. Londero, E. Schröder, P. Hyldgaard

Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology

Full quantum physical calculations of biomolecular forces hold promise for predicting structure and function without input and in the presence of charge transfer. Being non-empirical, they deliver an atomic scale characterization of binding and relaxations, for example at material interfaces where few other detailed probes are available. Until recently however, our best condensed matter tool for non-empirical description, Density Functional Theory (DFT) was not capable of addressing soft matter and biomolecular problems. The issue is not only a huge number of atoms but also a failure of traditional approximations for the density functional.

The DFT functional vdW-DF [1] has proven to be a strong candidate for a new predicting condensed matter description [2]. It includes an account of dispersive interactions by introducing a true non-locality in the density functional. We show that our functional has the potential to describe extended systems with the accuracy of DFT, thus opening the way to the description of complex soft phenomena, such as adsorption/adhesion, catalytic reactions or nanoscale lubrication.


13. Regeneration of cellulose from ionic liquid solutions

Carina Olsson and Gunnar Westman

Chemical and Biological Engineering, Chalmers University of Technology

Native cellulose is arranged by intra- and intermolecular hydrogen bonds forming two-dimensional sheets. Stacking of these sheets results in a semi crystalline three-dimensional structure (Baird, O'Sullivan et al. 1998) with poor solubility in most common aqueous and organic solvents. Furthermore, few efficient cellulose solvents are sustainable in the sense of being mild, reusable agents disinclined to spread to air, soil and water. In this work the focus solvents are ionic liquids, shown to be very useful for wood polymers. (Swatloski, Spear et al. 2002)

Once the cellulose is dissolved, new cellulose materials can be formed by controlled precipitation in a non-solvent such as water. The properties of the regenerated material depend on starting material, solvent and the conditions during dissolution and precipitation.

Figure 1. Regenerated cellulose fibre.

Continuous regenerated cellulose fibres (see Figure 1) were produced from imidazolium IL solutions via a wet-spinning technique. Characteristics of the material were found to be comparable to those of a reference cotton fibre.

References.


14. Physicochemical properties and interactions of alkyl-phosphonate ionic liquids

Jagath Pitawala,* Aleksandar Matic, Per Jacobsson

Department of Applied Physics, Chalmers University of Technology, SE-41296, Göteborg, Sweden.

Jagath@chalmers.se

We report on the physicochemical properties, structure and interactions of ionic liquids based on traditional imidazolium cations and new alkyl-phosphonate anions (Figure 1). We have investigated the conductivity by dielectric spectroscopy whereas the phase behaviour and the thermal stability were studied by differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA) respectively. The structure and interactions were investigated using Raman spectroscopy.

All three ionic liquids show very similar and high conductivities, with DiMIm(MeO)(H)PO2 having the highest value with $8.7 \times 10^{-3}$ S cm$^{-1}$ at 30 °C. The conductivity values are well reflected in the glass transition temperature, $T_g$, which does not change upon increasing the cation and/or anion size. However, there is a slight dependence of the temperature behaviour of the conductivity as seen from the D-parameter obtained from fits to the Vogel-Fulcher-Tamman equation. The change in the D-value can be related to slightly change of the fragility (D) of the liquids with the size of the ions.

Figure 1. Name, Acronym, molecular structure, glass transition temperature ($T_g$), and fragility (D) of the studied ionic liquids (Left). Ionic conductivity of them as a function of inverse temperature (Right).
Graphene is a novel material which could have applications in many fields such as nanoelectronics. To fabricate large area single layer graphene is challenging. Chemical vapor deposition (CVD) of graphene on transition metals is recently developed for this purpose. We have grown single layer graphene on copper foils or evaporated thin films on silicon substrate. [1, 2] The graphene can be transferred onto other substrate by etching away the copper catalyst. Raman spectrum and electrical measurements are shown. Optical and scanning electron microscope images are presented. C$_2$H$_2$ or CH$_4$ have been used as the precursor. The growth temperature is 650 °C-1000 °C. Our future goal is to further optimize the electrical properties of as-grown graphene and apply it to functional nanoelectronic devices.


Polysaccharides are polyhydroxylic polymers, which can be functionalized by a wide selection of chemical reactions. The physical and chemical properties obtained are highly dependent on how and where substituents are located along the polymer chains, an issue which has been investigated by several research groups [1]. These findings and the increased attention on new sustainable wood-based materials have thus resulted in a growing interest in characterization methods appropriate for modified polysaccharides.

In this study, nuclear magnetic resonance (NMR) spectroscopy have been used to characterize nanocrystalline cellulose, cotton linters and softwood kraft pulp reacted with the cationic epoxide 2,3-epoxypropyltrimethyl ammonium chloride (EPTMAC). The cationization was accomplished using two different procedures, whereof one was a solvent and reagent minimizing spray technique.

The NMR results proved substitution primarily at positions O-2 and O-6 for all three types of cellulosic materials. Furthermore, the NMR spectra showed that the softwood kraft pulp, which was cationized with the spray technique, demonstrated a higher preference for O-6 (83%) on the expense of O-2 substitution (16%). In addition to the recognized 9 ppm shift change of carbons attached to substituted hydroxyl groups, the 2D NMR spectra also indicated that other neighboring atoms are affected by substitutions resulting in other types of shift changes. [2]

Lithium ion batteries are considered as the main power source for electric vehicles (EVs) because of high operating voltage and good cycle performance. However, low safety and low energy density of the system are obstacles to practical use in the EVs, or for use in large-scale energy storage systems. To improve the safety of lithium ion batteries, room temperature ionic liquids (RTILs) can be an alternative to the traditional organic liquid electrolytes, which are volatile and flammable. This is because the RTILs have negligible volatility, non-flammability, and high temperature stability [1]. In addition to the safety issue, for large-scale energy storage systems, a new battery system with high energy density and inexpensive active material is required. Sulfur-based lithium batteries such as Li/S and Li/MS\textsubscript{2} (MS\textsubscript{2}, M=Cu, Fe, Ni, Ti) are very attractive candidates for next generation energy storage systems due to their high theoretical energy densities (e.g. 2600Wh/kg for elemental sulfur and 1273Wh/kg for FeS\textsubscript{2}). Furthermore, the cathode active materials are abundant, cheap, and environmentally friendly. In this study, we investigate the physicochemical and the electrochemical properties of ionic liquids used in lithium/IL/iron disulfide cells.
18. Rigid Lightweight Paperboard

Mikaela Börjesson

Chemical and Biological Engineering, Chalmers University of Technology

The project **Rigid Lightweight Paperboard** is one of four sub-projects within the Formulosa research cluster. The aim with Formulosa is to develop new cellulosic materials and composites for packaging applications, this by keeping the strength and stiffness and at the same time introducing formability to the fibre.

The aim with the sub-project **Rigid Lightweight Paperboard** is to develop cellulosic fibres that can improve paperboard stiffness. This could be achieved by modifying the cellulose fibres. Earlier studies in the project have shown that modification of N-methylmorpholinium (NMM) cellulose by heat forms covalent crosslinks between cellulose chains due to the NMM moiety (Fig.1.), which makes the NMM cellulose to be considered as a reactive cellulose derivative [1]. The continuation of the project is to explore alternative substituents that can act as “on-demand” crosslinkers.

![Fig.1: Suggested reaction scheme for heat induced self-crosslinking of NMM-cellulose.](image)

19. Morphogenesis of Nanostructured Calcium Phosphates Using Liquid Crystalline Templates

W-X. He\(^1\), J. Bielecki\(^2\), C.S. Knee\(^3\), M. Andersson\(^1\)

\(^1\)Chemical and Biological Engineering, \(^2\)Applied Physics, Chalmers University Of Technology
\(^3\)Chemistry, University Of Gothenburg

Liquid crystalline (LC) phases having water domains in the size range 5-10nm can be used as templates for the formation of nanoscale calcium phosphates (CaPs). [1] In the present study, LC phases have been utilized to synthesize amorphous calcium phosphates (ACP) with different morphologies. Furthermore, a controllable aging route has been performed on ACPs for the formation of bone-like apatite. [2]

Fig. 1 shows the proposed mechanism of CaPs morphogenesis in LC templates. CaPs synthesized within the H\(_2\) LC phase, are ACP spherules with a narrow size distribution (diameter 8–12 nm) and ACP rods (diameter 6 nm), with a specific surface area (SSA) in the range of 150–170 m\(^2\)/g. Where the ACPs synthesized using the L\(_\alpha\) LC phase present sheet-like morphology. After the H\(_2\)O-aging route, ACP spherules evolved into elongated apatites (1.5–4 nm wide) with an ultrahigh SSA of 356 m\(^2\)/g and bone-resembling features (namely calcium and hydroxyl deficiency, carbonate substitution and poor crystallinity).

Fig. 1: Schematic illustrations of CaP morphogenesis in LC templates: A. ACP nano-spheres, B. ACP nano-rods prepared in a H\(_2\) LC phase; C. ACP nano-sheets prepared in a La LC phase.

Within the confined space offered by the LC phases, CaPs with different morphologies (sphere, rod, sheet, wire, and even mesoporous structures) were formed. Furthermore, the conversion of ACP to crystalline apatite in aqueous media was observed as well and nanocrystalline apatite with ultrahigh SSA and bone-resembling features were prepared.

20. Transmission electron microscopy study of the evolution of the structure of AlO$_x$ barriers in Al/AlO$_x$/Al tunnel junctions

Lunjie Zeng$^1$, Tine Greibe$^2$, Samira Nik$^1$, Per Delsing$^2$, and Eva Olsson$^1$

$^1$ Microscopy and Microanalysis, Applied Physics, Chalmers University of Technology
$^2$ Quantum Device Physics, Microtechnology and Nanoscience, Chalmers University of Technology

The effect of partial oxidation pressure (P$_{ox}$) and oxidation time (O$_t$) during fabrication on the structure of the AlO$_x$ barrier in Al/AlO$_x$/Al Josephson junction has been investigated using transmission electron microscopy (TEM). The thickness of the barriers is inhomogeneous as determined by high resolution scanning (S)TEM imaging. Comparing the thickness distribution of the barriers grown at different conditions, it was found that the distribution showed little variation among different junctions where the average thickness varied between 1.3 and 1.5 nm. The structure of the barriers was studied using imaging and electron energy loss spectroscopy (EELS). The barriers with P$_{ox}$/O$_t$ being 0.1 mbar/3 minutes were not fully oxidized and Al$_2$O$_3$ and Al coexisted in the barrier. At higher P$_{ox}$ and larger O$_t$ the barriers consisted of stoichiometric amorphous Al$_2$O$_3$.

A. Bergstrand, J. Cramby, S. Uppström and A. Larsson

Pharmaceutical technology, Chemical and Biological Engineering, Chalmers University of Technology

Resorbable polymers have received much attention in the past decades due to their potential as implant materials for controlled drug release or tissue engineering. The implants act as a drug delivery device or as a temporary support for transplantation of cells and tissue. Depending on the function of the material, the biodegradable implant may be dense or porous materials. A porous material may facilitate the flow of nutrients, degradation and waste products. A simple and straightforward method is to use emulsions in order to template porous structures in materials. We report on water-in-oil emulsion templating in combination with solvent casting to fabricate highly porous and permeable poly(hydroxy butyrate), PHB, material.

Figure 1. SEM micrograph of the surface of a Poly(hydroxy butyrate) film made porous by water droplets from an oil-in-water emulsion. Adjacent droplets are forming interconnected structures during film formation.

PHB is naturally occurring polyester which is degraded into normal mammalian metabolites and resorbed when implanted in the body. With this template method we can fabricate PHB materials with different degree of porosity and pore interconnectivity. We can also combine PHB films of different porosity. This enables us to design and fabricate resorbable PHB materials with different molecular permeability.
22. Molecular Weight Dependence on Structure-Property Relations in Ethyl-Hydroxypropyl-Cellulose Films

Helene Andersson¹, Johan Hjärtstam², Mats Stading¹,³, Christian von Corswant², Anette Larsson⁴

¹Structure and Material design, SIK – The Swedish Institute for Food and Biotechnology
²AstraZeneca R&D Mölndal, ³Materials and Manufacturing Technology, Chalmers University of Technolog, ⁴Pharmaceutical Technology, Chalmers University of Technology

Ethyl cellulose (EC) and hydroxypropyl cellulose (HPC) are commonly used for pharmaceutical coatings in oral extended release formulations. The coatings are formed by spraying an EC-HPC-ethanol solution onto drug cores, during which solvent evaporation allows EC and HPC to phase separate. After oral ingestion the water soluble HPC leaches out and leave a porous film of predominantly EC, though which the drug can be released by diffusion and/or convection [1]. In a preliminary study on cast films of EC and HPC, we showed that the phase separated microstructure of EC/HPC-films is highly dependent on the M_w of EC (Fig. 1). We hypothesize that the rate of drug transfer during diffusion is strongly related to the microstructure of the film. Thus, in the present study we have investigated the functional and structural effects of EC M_w on sprayed EC/HPC-films (70:30 w/w).

Results showed that upon increasing the M_w of EC the permeability of water and a model substance decreased. Smaller pore structures were found in films with high M_w EC, as well as film sections exposed to rapid drying. Moreover, the total HPC leaching was significantly lower for the film of highest EC M_w. In conclusion, diffusional mass transfer in films are influenced by the M_w of EC, due to differences in microstructure and HPC leaching. This is likely a result of the effects of M_w on kinetics and mechanisms of phase separation, for which smaller pores could stem from an earlier viscosity related retardation of the phase separation process.

23. Variations in profiles of sodium ion concentration during Kraft cooking – Influence on delignification and carbohydrate removal

Binh Dang, Harald Brelid, Johannes Bogren and Hans Theliander

1Forest Products and Chemical Engineering, Chalmers University of Technology, SE-41296, Gothenburg, Sweden
2Södra Innovation, SE-43286 Väröbacka, Sweden

The goal of this study is to investigate the influence of different sodium ion concentration profiles on the delignification rate and carbohydrate degradation under kraft cooking conditions. Cooking experiments were performed in a small scale flow-through reactor in which the resorption of xylan and lignin was minimized through the continuous replacement of the cooking liquor. The sodium ion concentration was controlled by the addition of sodium carbonate.

The obtained data from the reference experiments with a constant sodium ion concentration throughout the whole cook showed that an increase in sodium ion concentration in the cooking liquors gave a decrease in the rate of delignification and xylan removal. The obtained results indicate that the delignification rate and xylan removal in the latter part of the kraft cook were affected by the sodium ion concentration in the early part of the kraft cook. Variations in the profiles of sodium ion concentration had different impacts on the delignification rate and the removal of xylan. The results imply that the understanding of the kinetics of kraft cooking is far from complete.
24. In vivo study of lipid-water cubic formulation for drug delivery in photodynamic therapy

Hanne Evenbratt*1, Charlotte Jonsson4, Jan Faergemann3, Marica B Ericson2, Sven Engström1

1 Department of Chemical and Biological Engineering, Chalmers University of Technology
2 Department of Physics, University of Gothenburg
3 Department of Dermatology, Sahlgrenska University Hospital
4 Department of Chemistry, Dermatochemistry and Skin Allergy, University of Gothenburg

The objective of this study was to evaluate ways of obtaining cubic phases and to show the efficiency of the new instantly formed lipid-water cubic formulation as drug delivery system for δ-aminolevulinic acid (ALA) and methylaminolevulinate (MAL) in vivo. The commercial drug Metvix® and a traditional cubic formulation served as control.

The ability to form a cubic structure with little effort within minutes opens up new and interesting opportunities for drug delivery. Stability problems could be circumvented by employing an in situ produced system. The cubic phase has a bicontinuous structure, suitable for accommodating hydrophilic, hydrophobic or amphiphilic substances. These systems has been shown to have interesting properties when used in photodynamic therapy (PDT) with ALA or MAL as photosensitizers [1]. PDT is based on photosensitization of skin cells and has become an important tool for cancer treatment [2].

The formulations were topically applied to nude mice and the subsequent formation of photosensitive substance was monitored by fluorescence measurements. It was found that particularly one instantly formed cubic formulation was a possible alternative to use in PDT. Higher fluorescence levels were observed compared to mice treated with conventional drug.

Next step is clinical trials evaluating this instantly formed cubic formulation further.

25. Different types of microfibrillated cellulose as filler materials in polysodium acrylate superabsorbents

Mikael Larsson¹, Qi Zhou² and Anette Larsson¹

¹Department of Chemical and Biological Engineering, Chalmers University of Technology, 41296 Gothenburg, Sweden
²Wallenberg Wood Science Center, Royal Institute of Technology, SE-100 44 Stockholm, Sweden and School of Biotechnology, Royal Institute of Technology, SE-106 91 Stockholm, Sweden.

Microfibrillated cellulose (MFC) is known to provide strong reinforcing effect in polymer nanocomposites. We have previously shown that MFC is highly efficient as a filler material in swelling polysodium acrylate superabsorbents (SAPs), strongly influencing swelling and mechanical properties of the materials [1]. We proceeded to investigated how low concentration of MFCs, prepared by three different methods, differed in their effect on swelling and mechanical properties when used as fillers in previously mentioned SAPs. Furthermore, the ability to retain those effects after washing was investigated [2].

The results confirm that MFC holds great potential as a filler material in superabsorbents, especially as the “filler effects” were reasonably retained after washing and drying. Furthermore, the results provide some insight on how the structural properties and surface charge of used MFC will affect gel properties depending on swelling conditions.

26. Efficient coating protection through controlled release of actives from microparticles

L. Nordstierna, J. Borg, A. Mok, A. Movahedi, M. Nordin, and M. Nydén

Division of Applied Surface Chemistry, Department of Chemical and Biological Engineering, Chalmers University of Technology

Current protective coating applications using biocides lose the protection quite rapidly as small molecular size renders a fast diffusional biocide leakage. We investigate a method for prolongation of the coating protection by reducing the release rate of biocides in a controlled manner. A promising improvement of can be achieved by the use of encapsulated biocides in the coating material. The biocide is placed into microparticles, from where it is slowly distributed into the coating. By different microscopic techniques the microparticles has been found to be compatible with the coating material. Biocide release from the coating has been recorded by various analytical techniques and it was shown that the release is considerably slower from coatings with microparticles compared to an ordinary formulation with freely dispersed biocides [1]. We suggest that microparticles are very efficient for controlling biocide release from protective coatings since they allow for optimization of biocide concentrations. They also increase the lifetime of the protective coating independent on the type of paint system used.

Polymer based organic photovoltaics is a field that has attracted a lot of attention in the last decades. Low cost and fast roll-to-roll production in combination with lightweight and flexible products are advantages that make polymer solar cells interesting and a potential competitor to traditional silicon-based devices. Currently, the best devices achieve a power conversion efficiency of about 8%. For polymer solar cells to become commercially viable the efficiency need to be increased to around 10% in modules.

The interest for diketopyrrolopyrrole (DPP)-based polymers and small molecules for photovoltaics has increased in the last few years, since they can be synthesized in a few simple steps from commercial products. A series of polymers containing Pyrrolo[3,4-c]pyrrole-1,4-dione, 2,5-bis(2-hexyldecyl)-2,5-dihydro-3,6-di-2-thienyl and three different phenylene-based donors were recently synthesized by our group. One of the polymers has previously been studied by Bijleveld et al. [1], reaching efficiencies above 5%. In an effort to increase the efficiency even further, alkoxy groups has been introduced onto the donor units. This was done to redshift the absorption and thereby be able to harvest a larger amount of photons from the solar spectra. The electronic and photo physical properties of the different polymers were evaluated and compared in respect to their structural differences.

References
28. Materials for tomorrow - by means of theory

Itai Panas

Energy & Materials, Department of Chemical and Biological Engineering
Chalmers University of Technology

Mechanistic insights into superconductivity, development of materials with improved corrosion resistance, novel catalytic strategies, and sustainable construction materials comprise some research themes of ours.

Catalysts for tomorrow:

Three platforms are currently explored:

1. Metal nanoalloys for co-generation of energy and valuable chemicals (with Jakub Jirkovsky et al)
A "guest-host" strategy is explored to achieve enhanced selectivity in O₂ reduction towards H₂O₂ formation avoiding formation of water. Theory predicts Pd, Pt, and Rh to be favorable at low concentrations. In case of Pd, this was validated by means of experiment (JACS, tentatively accepted). At higher Pd concentrations theory predicts segregation under oxidizing conditions, and re-alloying upon reduction. This was also confirmed by experiment (in manuscript).

2. Metal oxide nano-particles (with Michael Busch, Jakub Jirkovsky, Elisabet Ahlberg)
A mechanism for water oxidation was demonstrated on a binuclear manganese oxide cluster, and the rate limiting step determined (PCCP, in print). The finding was generalized, a "test rig" formulated, and the catalytic performances of binuclear Cr. Fe, Mn, and Co sites were evaluated. An ideal hetero-nuclear Fe-Mn catalytic site for water oxidation was identified (PCCP, in print). Usually water oxidation to produce H₂ has O₂ evolution as a necessary byproduct. In a recent study we demonstrate how the catalytic site can instead be regenerated by epoxidation of ethene², thus improving the overall economy of H₂ production (JACS, in print).

3. Graphene (with Angelica Lundin)
Various chemically modifications of graphene are being investigated, utilizing its robustness and electronic properties (in preparation).
Bulk hetero junction solar cells with conjugated polymers for solar cell applications have garnered a lot of interest over the last few years due to their light weight, flexibility and low cost. Recently solar cells with efficiency over 7% have been produced. In this study polymers were synthesized with the same backbone, but with differing side-chains. A series of seven polymers with the donor-acceptor-donor structured were obtained via Suzuki coupling. The structure of the polymers vary by the length of the alkoxy chain in the meta position of the 5,7-bis(5-bromothiophen-2-yl)-2,3-bis(3-methoxyphenyl)thieno[3,4-b]pyrazine monomer and the length of the alkyl chain of the 2,2'-(9,9-dioctyl-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)monomer. The polymers were characterized using UV-VIS spectroscopy, Square Wave Voltammetry, Size-exclusion chromatography and device fabrication with PCBM. Altering the length of the side-chains was expected to change the morphology of the bulk hetero junction, this was however not observed to the expected extent.
Electrospinning of cellulose nanofibres from ionic liquids. The effect of different co-solvents.

J. Thunberg¹,², L. Härdelin²,³, E. Perzon²,³, G. Westman¹,², P. Walkenström²,³, P. Gatenholm¹,³

¹Chemical and Biological Engineering, Chalmers University of Technology
²Wallenberg Wood Science Center, Chalmers University of Technology
³Department of Textiles and Plastics, Swerea IVF, Mölndal

Electrospinning is a solution spinning technique in which fibers of submicron scale diameter are formed. Using cellulose as raw material for solution spinning generates a dissolution problem since cellulose is a linear chain of β(1→4) linked D-glucose units and is crystalline due to inter- and intra-molecular hydrogen bonding. Therefore cellulose has poor solubility in conventional non-derivatizing solvents, but solutions with a cellulose content as high as 25 % can be obtained in imidazolium-based ionic liquids. Ionic liquids have low vapor pressure and do not evaporate and electrospinning from ionic liquid solutions can be be categorized as non-evaporating electrospinning. Therefore a precipitation bath was needed in the spinning process.

![Cellulose fibers electrospun from Ionic liquid 1-ethyl-3-methylimidazolium acetate (EmimAc)](image)

In this work a process-window where cellulose/ionic liquid solutions can be electrospun is presented. The focus this work was to correlate the characteristics of the spinning dopes physical properties, such as viscosity and surface tension, to the ability to form submicron regenerated fibers. Conventional solvents were used as co-solvent in the spinning dopes to optimize the spinning dopes processability.
One promising alternative to silicon based solar cells include polymers as the light harvesting material. Polymer based solar cells can offer a lower production cost but also a more flexible material and a light weight product. The main challenge with polymer based solar cells is that the efficiency is not as high as for the silicon. The research effort is very extensive within this area and the efficiencies are improving rapidly.

In polymer based solar cells the active layer often consists of a bulk hetero junction (BHJ). This BHJ include at least one conjugated polymer but also an electron transporting compound. This compound is also needed to get the charge separation that is wanted to generate a current. The electron transporting compound that has reached the highest efficiencies is fullerenes, or more correctly PCBM. Other examples are different kinds of metal oxides and electron transporting polymers.

This poster will present solar cells that use ZnO nanoparticles as the electron transporting material in the BHJ. The ZnO nanoparticles that are used in this project are synthesized according to published methods\textsuperscript{1} from zinc acetate dehydrate and different methods are used to analyze them, such as DLS and TEM. The polymer that is used is called TQ1\textsuperscript{2} and has given good results with PCBM. Different parameters are varied when doing the cells, for example spin speed and concentration of ZnO nanoparticles. Both regular and inverted cells are done and will be presented on the poster.

\textsuperscript{1} W. J. E. Beek, M.M. Wienk, M. Kemerink, X. Yang, R. Janssen; J. Phys. Chem. B 2005, 109, 9505-9516

\textsuperscript{2} E. Wang, L. Hou, Z. Wang, S. Hellström, F. Zhanf, O. Inganäs, M. R. Andersson; Advanced Materials 2010, 22, 5240-5244
Selective functionalization of nanostructures with nanometer resolution is important for the development of a broad range of applications ranging from single molecule electronics to advanced sensor technologies where the single molecule is used as the sensing unit. Today nano-scale functionalization is typically achieved using a combination of top-down lithographic techniques and chemical self-assembly. The resolution is therefore limited to the resolution of the lithographic technique – typically in the 30-100 nm range. Improved resolution and selectivity is highly desirable since it might lead to new opportunities in a broad range of applications ranging from single molecule electronics to sensors and nano medicine. This research project focus on the development of chemistries that allow for selective, lithography free functionalisation of nanostructures with sub nanometer resolution. The work takes it’s offspring from organic synthesis, and will also include nanoparticle and nanorod synthesis, surface functionalisation and characterisation.

Jain et al.¹ have recently shown (figure 1 left), that the build-up of gold nanorod dimers with one molecule in between is possible. By synthesizing new molecular bridges with functional chemical groups we hope to be able to use this approach to construct nanorod dimers attached to a single active functional molecule.(figure 1 right)

33. Potentiostatic Study of a Microbial Fuel Cell Based on Graphite/TiO₂ Spin-Coated Electrodes and *Shewanella oneidensis* Culture.

Davide Zanelli¹, Maurizio Furlani², Valeria Mapelli³, and Bengt-Erik Mellander²

¹ Environmental Biology Master, Faculty of Mathematics Physics and Natural Sciences, University of Trieste, Italy

² Dept. of Applied Physics, Chalmers University of Technology

³ Dept. of Chemical and Biological Engineering Industrial Biotechnology, Chalmers University of Technology

In the area of microbial fuel cells (MFCs) the interest is focused on the possibility to obtain electrical energy exploiting the bacterial metabolism and on the effect of electrical current on the products of the metabolism. Methane and hydrogen can also be obtained. In this work a new type of electrode is used: FTO-glass in combination with a mesoporous coating prepared with spin-coating technique and thermal treatment. Measurements of load curves (Fig 1) and voltammograms are compared.

Fig. 1: Potential variation and current variation for three external resistance load: 20000 Ω (× left in the graphs), 2000 Ω (square, center in the graphs) and 200 Ω (triangle, right in the graphs). The circuit is open at the first point, then closed until the potential is at a minimum, and after a few seconds the circuit is opened to let potential recover. Potentiostat set in ZRA mode.

The large capacitive effect of the system has been observed and to some extent analysed with different loads. This effect might be interesting in the MFC when a large impulse of energy is the required property, and it might offer ways to study the electron transfer process. The power density of the studied MFC (2.2 mW/m² and 7.0 mW/m³ in oxic cathode condition; 1.8 mW/m² and 5.7 mW/m³ in anoxic cathode condition) was much higher than that reported by Rabey and Verstraete [1] when expressed as function of the electrode surface (0.000032 mW/m²) and lower when expressed as function of the total batch volume (80 mW/m³).

Today, there is a large use of petroleum-based superabsorbents but recently the interest of renewable alternatives has increased. In this work, two new wood-based materials have been developed that are suitable in various absorption applications. These two materials were produced in a three step process comprising the steps of oxidation, fibre disintegration and drying. The starting material was a never-dried bleached softwood kraft pulp, which was chemically modified by TEMPO oxidation to introduce new carboxylate and aldehyde groups. It was found that the aldehyde groups contributed to the wet integrity of the absorbent materials possibly by formation of hemiacetal bonds. After the oxidation treatment, the pulp fibres were gradually disintegrated into a network of liberated fibrils. The disintegration was found to be more rapid for the oxidized pulp than for the non-oxidized pulp, possibly due to greater repulsive forces between the fibrils and the decoupling of the carbohydrate network.

Freeze drying produced a porous foam (see Figure 1) with a large surface area enabling a rapid absorption rate, as well as, a reasonably large absorption capacity also under load. Air drying formed a compact film with a slow absorption rate but with a high final absorption capacity.
Hydrogen storage in metal hydrides has been suggested as a way to overcome volume problems when storing hydrogen onboard vehicles. However, this approach suffers from too high stability of the metal hydrides and slow kinetics for loading and unloading of the hydrogen. A possible way to overcome these problems might be to use metal nanoparticles.

Indirect Nanoplasmonic Sensing (INPS) is a novel experimental technique which utilizes localized surface plasmons in Au sensor particles to monitor changes in the dielectric environment around the sensor particles. [1]

Here, we demonstrate how INPS, in a simple optical transmission experiment, can be used to monitor and quantify size effects in metal hydride formation on the particle ensemble in Mg and Pd nanoparticles, see Fig. 1, ranging in size from 1 nm to 80 nm. The latter are ideal model systems to scrutinize how nano-sizing of the hydrogen storage system influences phase diagram, thermodynamics and kinetics of nanoscopic metal hydrides. Furthermore, Mg is a very interesting system for commercial solid-state hydrogen storage due to its lightweight and low cost.

Fig. 1: Sketches and SEM images of the samples used to study hydrogen storage properties in Pd (a) and Mg (b) nanoparticles.

36. A new hydrophilic antifouling coating for marine applications

Ali Reza Movahedi¹, Nina Kann², Hans Blanck³ and Magnus Nydén¹

¹Applied Chemistry, Chalmers University of Technology
²Organic Chemistry, Chalmers University of Technology
³Plant and Environmental Sciences, University of Gothenburg

The protective coatings used today in marine applications such as ship bottoms have great problems with bio-fouling. Authorities have banned many of the substances that were discovered toxic to marine organisms but this has lead to the use of extreme concentrations of copper instead.

We suggest here by strongly adsorbing the natural abundant copper to a coating, an antifouling effect can be produced without any net emission of biocides into the sea. The adsorbed copper will be highly enriched in the coating compared to the concentration in the sea. Then a chemical process starts inside the coating in which Cu²⁺ is reduced to Cu¹⁺. Cu¹⁺ is not strongly bound to the coating, hence can act as natural biocide at the interface between the coating and the sea. It will rapidly oxidize back to the 2⁺-state afterwards due to the oxidizing environment of water, so quickly re-enter into the coating.

Here we have made a multifunctional host material which will act as a support for the copper ions within the coating. The host material has the ability to stabilize copper ions and it can further be tuned in a way which gives the control of copper ions exchange between the coating and the sea.
37. Atomic Scale Modeling of Precipitation in Metallic Alloys

Paul Erhart\textsuperscript{1} and Babak Sadigh\textsuperscript{2}

\textsuperscript{1}Chalmers University of Technology, Gothenburg

\textsuperscript{2}Lawrence Livermore National Laboratory, Livermore, California, USA

Technological progress continues to demand high-performance metallic alloys that are ever stronger, lighter, more resilient, or simply cheaper than existing materials. In this regard understanding and controlling microscopic features and mechanisms become ever more important. Atomic scale modeling can be one of the most powerful tools to provide such insight. In this contribution we provide an overview of some of our most recent work in this field. In the first part we study Cu precipitation in Fe, which pertains to the application of ferritic steels in nuclear environments. We map out in detail the temperature and size-dependence of the structure of the precipitates providing key information for understanding of embrittlement in these materials.

In the second part we address the role of oxygen impurities in alpha-Ti. In spite of their importance for the mechanical properties, available Ti-O phase diagrams do not provide a conclusive picture for the Ti-rich side. Using first-principles calculations in conjunction with Monte-Carlo simulations, we propose a revised phase diagram that features several long-range ordered Ti-O phases, two of which are stable up to approximately 600 K. Specifically, the Ti\textsubscript{8}O phase is predicted to precipitate already for very small oxygen concentrations intriguing implications for the mechanical properties.

![Figure 1: 9R-Cu precipitate in Fe.](image1)

![Figure 2: Ti-rich side of Ti-O phase diagram from simulation.](image2)
38. Phthalimide Based Donor-Acceptor Polymers as Ambipolar and Light Emitting Materials


1 Chalmers University of Technology, Department of Chemical and Biological Engineering, SE-412 96 Gothenburg, Sweden

2 University of Cambridge, Optoelectronics Group, Cavendish Laboratory, JJ Thomson Avenue, Cambridge, United Kingdom, CB3 0HE

E-mail: steckler@chalmers.se

Presently, most organic polymers offer either p-type or n-type charge transport, with only a few possessing the ability of being ambipolar with balanced hole and electron mobilities. Most of these polymers are thiophene based materials which are often combined with diketopyrrolopyrrole (DPP) acceptors [1]. Recently phthalimide based donor acceptor polymers have shown potential as solar cell materials [2] and as ambipolar charge transport materials in combination with bi-thiophene based donors [3]. However, very little has been published on the emissive properties of these types of polymers, with most involving poly(arylene ethynylene)s PAEs with phthalimide [4]. We have synthesized some phthalimide based donor-acceptor polymers using thiophene based donors in order to optimize the emissive and charge transport properties for use in OFETs and LFETs. We demonstrate the structure property relationships for the optimization of the molecular weight relative to the charge transport and emissive properties. Maximum hole and electron mobilities of 4 x 10^-3 cm²V⁻¹s⁻¹ and 1 x 10⁻² cm²V⁻¹s⁻¹ have been obtained, while polymer films have exhibited a PLQE of ~28 %.


In the strive for a more sustainable textile industry, it is crucial to have a holistic approach when assessing the sustainability of textile fibres. Apart from consideration of the entire fabric product life cycle, the three dimensions of sustainability and all relevant impact categories, it is also essential to account for the impacts’ dependency on the location of operations. We illustrate this location dependency of impacts by comparing Swedish and East Asian synthetic cellulose fibres. Novel environmental and social life cycle assessment methods are applied for characterising four seldom studied impact categories: water footprint, biodiversity impact of land use, working conditions and contribution to economic/technology development.

The result demonstrates location dependencies due to e.g. latitude, altitude and precipitation of the utilised forest, and working conditions and R&D efforts in the region of operation. Similar location dependencies can be expected for numerous other social and environmental impact categories. Hence, it is unfeasible to make precise claims about the sustainability of a textile fibre solely based on its material composition. Precision will depend on moving beyond generic fabric data, into specific supply chain data. The study also demonstrates that there are usable characterisation methods available for hitherto seldom considered impact categories.
40. Green production of biomaterials from hemicelluloses

Agnes Stepan,a,b, Gunnar Westman,a,b, Lisbeth Olsson,a,b and Paul Gateno-holma,b

a Wallenberg Wood Science Center

b Biopolymer Technology, Organic chemistry and Industrial Biotechnology

Department of Chemical and Biological Engineering

Chalmers University of Technology

Thermoplastic materials based on renewable raw materials are emerging biomaterials with great potential of large-scale industrial application. Plant hemicelluloses, the second most abundant biopolymers on the earth are attracting more attention as a source for value added product. Hemicelluloses are complex polysaccharides with large variations of chemical structures and molecule weight. In this research we are studying the effect of molecular architecture of chemo-enzymatically modified plant hemicelluloses on material properties. In this study mainly arabinoxylans are being investigated for these modern ways of modification and utilization. We found that the higher degree of arabinose substitution contributes to flexibility of acetylated films. Enzymatic modifications are evaluated as a more environmentally benign modification method. Esterification/acylation with enzymes has a potential, since lipase/cutinase has a proven record in biocatalytic reactions [1]. Green solvents such as ionic liquids can also aid more environmentally benign chemical or enzymatic modification methods [2].

As a final goal, fossil fuel based binders, coatings and composites are aimed to be replaced by these biooriginated and biodegradable plastics.

![Fig. 1. Acetylation of Arabinoxylan (AX)](image)

References.
41. New quinoxaline and pyridopyrazine-based polymers for solution processable photovoltaics


During the last decades, utilizing polymers as the light harvesting material in bulk heterojunction solar cells has been under intensive research. The main driving force for this is that polymers offer the advantage of cost efficient production of solar cells via a roll to roll process. Other advantages about polymer-based solar cell are that the devices can be light-weight and flexible, thereby opening up numerous commercial applications. One major hurdle still is the power conversion efficiency of these devices, which has to be around 10% efficiency in the lab before the concept becomes commercially viable. Currently, the best cells achieve an efficiency of about 8% in the lab.

Recently, an easy to synthesize quinoxaline-thiophene copolymer has been synthesized by our group. This so-called TQ1 polymer achieved excellent efficiencies (up to 6%) in solar cells that were based on a TQ1:fullerene blend.\[1\] In an effort to achieve even higher efficiencies and to investigate new possibilities with this type of polymer, the structure of this polymer has been slightly modified. This resulted in a series of new polymers in which their electronic and photophysical properties have been evaluated and compared in respect to the structural changes that have been made.

42. Voltage Stabilisers for Improving the Resistance to Electrical Treeing in XLPE

M. Jarvid¹, A. Johansson², M. Andersson¹, S. Gubanski²

¹Chemical and Biological Engineering, Chalmers University of Technology
²Materials and Manufacturing Technology, Chalmers University of Technology

Electrical treeing is a degradation phenomenon taking place in solid dielectrics when stress in form of strong divergent electrical field is applied. For high voltage equipment, this can be a big problem as small metal impurities or gas filled voids inside polymeric insulation can cause such local field enhancements. An electrical tree will, once initiated, eventually cause dielectric breakdown and it is therefore crucial to prevent them from occurring.

One method for inhibiting or slowing down the process of electrical treeing is to introduce additives, known as voltage stabilisers, into the polymeric insulation material. In this study, cross-linked polyethylene (XLPE) has been stabilised with three new voltage stabilisers based on a benzil core. Electrical treeing measurements made clear that all of the stabilised materials had improved resistance against electrical treeing compared to reference XLPE. It has also been shown that these additives only have a minor effect on the cross-linking of the polymer. Additionally, vinyl moieties can be used to bond the stabilisers covalently to the polymer matrix in the cross-linking process without the molecules losing their voltage stabilising effect. This prevents long term migration of the stabilisers out of the material.

Fig. 1: Electrical tree in XLPE, initiated at a needle tip
43. Flow-through nanoplasmonic biosensor for detection of low concentration bio-analytes

Mazzotta F. ¹, Jonsson M.P.², Höök F¹.

¹Chalmers University of Technology, Sweden
²Delft University of Technology, The Netherlands

The impact on society of diseases connected to the aging of the population, e.g. Alzheimer’s and Parkinson’s diseases, has triggered an increasing interest in the development of biosensors able to detect low concentration bioanalytes in small volumes.

In this work we developed a fabrication scheme which allows creating gold nanoplasmonic active structures of different sizes and shapes on the walls of nanochannels etched through a 220 nm thick silicon nitride membrane. Nanoplasmonic active structures are generally exploited in biosensors because of the high sensitivity of their resonances to local changes in the refractive index in the surrounding environment. However, the performances of the sensor will be greatly influenced by the mean of choice for transport of the molecules to the sensitive surfaces of the sensor, especially while operating in the low concentration regime.

In the presented system, the combination of gold nanoplasmonic structures and silicon nitride nanochannels ensure both that the sensitivity of the sensor is localized to within the nanopores and that the chance for the analyte to bind on the sensing elements is maximized. This novel setup could allow reaching the reaction-controlled regime with flow speed in the range of 0.01 µl/min for fast kinetic reaction while keeping the total volume consumption needed to reach a detectable signal in the nL range.
44. Characterization of the interaction between nanoformulated drugs and model lipid membranes towards improved drug delivery systems

Laura De Battice¹, Rickard Frost¹, Chantal Sevrin², Natalia Kuznetsova², Christian Grandfils², and Sofia Svedhem¹

¹Dept. of Applied physics, Chalmers University of Technology (Göteborg, Sweden)
²Interfacultary Research Center of Biomaterials (CEIB), Université de Liège (Liège, Belgium)

The development of nanoparticles (NPs) for the delivery of therapeutic agents has introduced new opportunities for the improvement of medical treatments. Among these opportunities, surface based analytical techniques are promising tools to improve our understanding of biointerfacial phenomena, such as NP interactions at biological barriers. Here, electrostatically assembled complexes made of polycationic polymers and biopharmaceutical drugs are being designed to promote delivery through non-invasive administration. These NPs loaded with human insulin (HI) were characterised by Dynamic Light Scattering (DLS) and Nanoparticle Tracking Analysis (NTA). Typically, NP size was about 200 nm with a relatively good agreement between these two techniques. In addition, zeta potential measurements showed that these NPs had a surface potential of around +25 mV. Using the Quartz Crystal Microbalance with Dissipation monitoring technique (QCM-D), we studied in real time the interaction between the NPs and different kinds of model lipid membranes, formed on SiO₂ coated crystals. We found that, on negatively charged membranes, NPs formed increasingly dissipative layers for increasing Mn of the polycation used to prepare the NPs. Thicker layers were formed on neutral membranes. NPs containing a ternary compound were also investigated. Interestingly, without modifying drastically the mean size or the zeta potential of the NP, the presence of this additional compound was shown to alter completely the adsorption profile and total amount of NP adsorbed on the negatively charged membranes, evidenced by a transient mass uptake. The difference in interaction profiles between binary and ternary NPs makes the study of those NPs very interesting in terms of drug release.

Fig. 1: Schematic drawing illustrating a potential mechanism for the interaction of ternary NPs with a negatively charged cell surface
45. Functional microstructure of tunable Ba_{0.25}Sr_{0.75}TiO_{3} thin film bulk acoustic wave resonators

Markus Löffler,1 Andrei Vorobiev,2 Lunjie Zeng,1 Spartak Gevorgian,2 Eva Olsson1

1Applied Physics, Chalmers University of Technology
2Microtechnology and Nanoscience, Chalmers University of Technology

The evolution of the Q-factor of tunable solidly mounted Ba_{0.25}Sr_{0.75}TiO_{3} (BSTO) thin film bulk acoustic wave resonators (FBARs) as a function of BSTO growth temperature shows an unexpected steep drop at high growth temperatures, which should favor BSTO crystallinity. Therefore, complementary methods such as TEM, EDX, EELS and AFM1 have been employed to study the microstructure of these thin films grown at different temperatures. Changes in microstructure including the grain size, texture misalignment, the presence of an amorphous interfacial layer at the BSTO/bottom electrode interface, and interface roughness have been investigated. A modification of the bottom electrode morphology and adhesion layer composition have been found, which are the cause for a drop in Q-factor at higher growth temperatures (Fig. 1). These changes are explained by grain boundary diffusion and the stress situation in the bottom electrode and adhesion layers. These findings can help to improve the device performance by optimization of BSTO growth conditions while taking into account the dynamic nature of adhesion layer/bottom electrode interaction.

Fig. 1: Left: Evolution of Q-factor with growth temperature. Right: TEM micrograph of the bottom electrode region of sample M79, showing adhesion layer/bottom electrode interaction after high temperature BSTO growth.
46. Atomistic Modeling of Graphene Using an Adaptive Quasi-Continuum Method as a Tool for Computational Homogenization

K. Runesson, A. Memarnahavandi, F. Larsson and R. Larsson

Dept. of Applied Mechanics, Chalmers University of Technology

Atomistic modeling of a graphene monolayer at zero temperature (static analysis) is carried out as part of a computational homogenization scheme to obtain macroscopic stress-strain relations, cf. [1]. A suitably calibrated Tersoff-Brenner potential is used for an atomic structure with divacancies, representing a typical type of defect. The relaxation analysis is carried out for zero macroscopic strain as well as for zero macroscopic stress. The desired stress-strain response is then obtained upon applying the appropriate deformation gradient, while Dirichlet-Taylor type of boundary conditions are imposed on the chosen “Representative Unit Volume”.

The Quasi-Continuum (QC) method for “model reduction in the Finite Element sense” is used in order to increase the computational efficiency, cf. [2]. As a means of controlling (and reducing) the induced model reduction error, an adaptive strategy for mesh refinement is devised based on control of the error in selected macroscopic stress components. The effect of choosing different strategies for computing these stresses is assessed.