The Materials Science Graduate Student Days 2014

Booklet

February 26-27, 2014
Virtual Development Laboratory (VDL), Chalmers
Programme

Wednesday, February 26

08.30 - 09.00  Registration and mounting of posters
Chair:  Mikael Rigdahl, Materials and Manufacturing Technology

09.00 - 09.15  Welcome

09.15 - 09.45  Invited:  Rapid transfer of research results into industrial use, some examples from Swerea IVF
Mats Lundin, Swerea IVF, Mölndal

09.45 - 10.30  COFFEE and Poster session

10.30 - 10.50  Theory meets experiment in surface science
Maxime Van den Bossche, Applied Physics
Chair:  Anna Clemens, Applied Physics

10.55 - 11.15  Fate of hydrogen upon oxidation of zirconium alloys by water: Mechanistic insights from first principles calculations
Mikaela Lindgren, Chemical and Biological Engineering

11.20 - 11.40  Organic modification of MMT for application in plasticized PVC
Henrik Petersen, SP, Borås / Materials and Manufacturing Technology

11.45 - 12.00  Presentation of Materials Science Area of Advance
Anders Palmqvist, Area of Advance Co-Director

12.00 - 13.00  LUNCH

13.00 - 15.00  Lab tour, Materials and Manufacturing Technology

15.00 - 15.30  COFFEE and Poster session
Chair:  Lena Falk, Applied Physics

15.30 - 16.00  Invited:  Time of light - from ion counter to metal former
Boel Wadman, Swerea IVF, Mölndal

16.00 - 16.20  At the interface between life science and materials science: atom probe tomography of osseointegration
Gustav Sundell, Applied Physics

16.25 - 16.45  Colour-changing textile coatings containing multilayered mica pigments
Veronica Malm, The Swedish School of Textiles, Borås / Materials and Manufacturing Technology

16.50 - 17.10  Nano-coated steels for solid oxide fuel cell (SOFC) interconnects
Rakshith Nugehalli Sachitanand, Chemical and Biological Engineering

17.10 - 18.00  Poster session

18.00  DINNER at Hyllan
Thursday, February 27

Chair: Sten Eriksson, Chemical and Biological Engineering

09.00 - 09.30 Invited: SP Technical Research Institute of Sweden - some aspects on providing capacity for innovation
Claes Tullin, SP, Borås

09.35 - 09.55 Highly conductive bicomponent fibers
Erik Nilsson, Swerea IVF, Mölndal / Materials and Manufacturing Technology

09.55 - 10.20 COFFEE and Poster session

10.20 - 10.50 Invited: The complex construction of food materials
Camilla Öhgren, SIK
Chair: Christos Oikonomou, Materials and Manufacturing Technology

10.55 - 11.15 Quantifying exosomes: a crossroads between physics, chemistry and biology
Deborah Rupert, Applied Physics

11.20 - 11.40 Chemical Looping Combustion
Sebastian Sundqvist, Chemical and Biological Engineering

11.45 - 12.00 Moleclues
Per Thorén, Materials Science Area of Advance Communications Officer

12.00 - 13.00 LUNCH
Chair: Rakshith Nugehalli Sachitanand, Chemical and Biological Engineering

13.00 - 13.20 Optical spectroscopy of single functional nanoparticles
Svetlana Syrenova, Applied Physics

13.25 - 13.45 Surface chemical analysis of soft magnetic composite materials
Christos Oikonomou, Materials and Manufacturing Technology

13.50 - 14.10 Heading towards eco-efficient surface protection:
Physicochemical modification of microparticles for controlled release of biocides in protective façade coatings
Jonatan Bergek, Chemical and Biological Engineering

14.10 COFFEE and Concluding remarks
# List of participants

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<td>Veronica Malm</td>
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<td>PhD student, The Swedish School of Textiles, Borås</td>
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<td>Viktor Nilsson</td>
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*TF = Teknisk fysik (Applied Physics),
KB = Kemi- och bioteknik (Chemical and Biological Engineering),
MoT = Material- och tillverkningsteknik (Materials and Manufacturing Technology)*
Posters

P01 Properties of LiFSI/LiTFSI doped ionic liquids for HT-LIB application  
  Manfred Kerner, TF

P02 Dynamic properties of water-xylitol solutions  
  Khalid Elamin, TF

P03 Deformation mechanisms in a WC-Co based cemented carbide during creep  
  Amine Yousfi, TF

P04 Monitoring catalyst sintering under operating conditions  
  Pooya Tabib Zadeh, TF

P05 Characterization of NaX (X=TFSI, FSI) - PEO based solid polymer electrolytes for Na+ battery application  
  Andrea Boschin, TF

P06 Atom probe tomography of thin carbide films  
  Sabrina Koch, TF

P07 Investigation of X750 Ni-Alloy  
  Silvia Tuzi, TF

P08 Metalion-exchange in small-pore zeolites for catalytic emission control applications  
  Anna Clemens, TF

P09 Characterisation of polycrystalline cubic boron nitride tool materials  
  Kristina Lindgren, TF

P10 The capability of ESEM in-situ techniques in evaluation of the initial corrosion stages of stainless steels at 450oC  
  Nooshin Mortazavi, TF

P11 The effect of surface treatment on the corrosion behavior of Ni-based alloys studied by high-resolution techniques  
  Haiping Lai, TF

P12 Interactions and mechanisms for surface sizing polymer particles  
  Frida Iselau, KB

P13 Catalysts for ammonia production - fundamental studies towards passive SCR systems  
  Emma Adams, KB
P14 Characterization and evaluation of surface functionalized silica nanoparticles
   Sanna Björkegren, KB

P15 Structural investigation of cellulose using solid-state NMR spectroscopy
   Alexander Idström, KB

P16 Developing a biomimetic water desalination device using mesoporous supported lipid bilayers with aquaporins
   Simon Isaksson, KB

P17 Zeolite SSZ-13 as NH3-SCR catalyst
   Alexander Shishkin, KB

P18 Atmospheric corrosion behavior of Mg-Al alloys in high pressure die cast and semi-solid casting forms
   Mohsen Esmaily, KB

P19 Nano-coated ferritic steel foils for SOFC interconnect applications
   Hannes Falk Windisch, KB

P20 Surface Engineering of Austenitic Stainless Steels
   Giulio Maistro, MoT

P21 Mechanical performance of wheel and rail materials
   Dimitrios Nikas, MoT

P22 Needle punching of wet cellulosic fibre structure
   Maria Klingberg, MoT

P23 Cellulose composite fibres spinning
   Tobias Moberg, MoT

P24 Recycling of plastics from electronic waste
   Erik Stenvall, MoT

P25 Delubrication of Powder Metallurgy Steels
   Seshendra Karamchedu, MoT
Abstracts – Oral presentations

O1 Theory meets experiment in surface science
Maxime Van den Bossche, TF

Understanding heterogeneous catalysts at the atomic scale is one of the main motivations for surface science. The use of well controlled model systems allows for fundamental understanding of molecular-surface interactions and reactions. Within the surface science approach, the combination of experiments and atomistic calculations have proven very powerful [1,2]. In particular, the use of the density functional theory enables calculations of several properties such as adsorption energies, energy barriers, vibrational frequencies, and shifts in electronic binding energies with reasonable accuracy. Comparing theoretical results with experimental data often allows for a detailed understanding of governing processes. Here, water formation, carbon monoxide adsorption and methane oxidation on palladium oxide surfaces will be given as examples [3,4] of the surface science approach.


O2 Fate of Hydrogen upon Oxidation of Zirconium Alloys by Water: Mechanistic Insights from First Principles Calculations
Mikaela Lindgren, KB

Design of corrosion resistant zirconium alloys in air-free water relies on a compromise between two opposing strategies, minimize the oxidation rate and minimize the hydrogen pick-up by favoring hydrogen evolution. Understanding these processes is of major importance to the nuclear industry where zirconium alloys are used as fuel claddings. In this study, the oxidation of zirconium by water is analyzed in terms of an anode reaction and a cathode reaction by means of first principle calculations. The anode reaction involves Zr oxidation by oxide ions resulting in release of electrons. Details in the complementary cathode reaction is of particular importance owing to the dramatic influence that transition metal additives have on the fraction of hydrogen picked up in the alloy. Efficient utilization of the exothermic Zr oxidation reaction by water is found to drive proton-electron recombination by forming reactive hydride ion intermediates. Once formed, the hydride ion can undergo hydride-proton recombination forming H2. The magnitude of the exothermicity of this recombination is found to be dependent on transition metal and correlates to the transition metal dependence of hydrogen pick-up fraction: Larger exothermicity implies smaller hydrogen pick-up fraction. ZrO2 is unstable in contact with Zr metal resulting in oxygen dissolution in the metal matrix. The impact of the high solubility of oxygen in Zr in the effective anode
potential is addressed. In particular, the ability of the anode reaction to form the hydride ion intermediate is evaluated for relevant suboxide concentrations.

**O3 Organic modification of MMT for application in plasticized PVC**

*Henrik Petersen, MoT, SP Borås*

Abstract Polyvinyl chloride (PVC) is one of the world’s most widely produced polymers and it is used in a wide range of areas such as building, transport, packaging, electrical/electronic and healthcare. Manufacturing of PVC products is dependent on several additives, e.g. plasticizers, heat stabilizers and flame retardants. To reduce the migration of additives in PVC products the incorporation of a nanofiller, mostly Montmorillonite (MMT) clay with high aspect ratio and large surface area, can be used to create physical barriers. There are also many results from literature showing that nanoclays have flame retarding qualities. Before MMT can be processed into a polymer matrix it has to be organically modified (OMMT), due to processability and compatibility issues. In many studies it has been shown that commercially available OMMTs are not suitable for PVC, hence they contribute to degradation processes [1]. In this paper the aim is to organically modify MMT for use in PVC. In an earlier project [2] the idea of chelating agents as organic modifiers was presented and here we combine theoretical studies using Hansen Solubility Parameters (HSP) with practical laboratory work to find out which parameters will have an influence on the final results. Various types of natural Montmorillonite clay were swelled in solvents with solubility parameters differing from each other. The clays were then treated with a proper organic modifier to increase interlayer spacing and improve compatibility with the polymer matrix. Thermogravimetric analysis (TGA), x-ray diffraction analysis (XRD) and scanning electron microscopy (SEM) were used to evaluate the outcome of the experiments.


**O4 At the interface between life science and material science: atom probe tomography of osseointegration**

*Gustav Sundell, TF*

In the field of biomedical technology a critical aspect is the ability to control and understand the integration of an implant device in living tissue. Despite the technical advances in the development of biomaterials, the elaborate interplay encompassing material science and biology on the atomic level is not very well understood. Within implantology, anchoring a biomaterial device into bone tissue is termed osseointegration. Due to the complex nature of the biological response that occurs at the interface, a detailed description of osseointegration on the smaller length-scales is still lacking. Herein it is
shown that atom probe tomography can be used to study the implant/tissue interaction, allowing for 3D atomic mapping of the interface region. Our analyses demonstrated that direct contact between Ca atoms and the implanted titanium oxide surface is formed, without the presence of a protein interlayer, meaning that a pure inorganic interface is being created. This type of atomic-scale examination of interfaces between living tissue and foreign material may add a new dimension to the field of biomaterials, helping the design of improved implant materials.

**O5 Colour-changing textile coatings containing multilayered mica pigments**

Veronica Malm, MoT

Angle-dependent colour-changing effects within the turquoise-blue-violet region has been achieved on textiles, using coating formulations added with multilayered mica pigments (EP) and a knife coating method. The multilayered metal oxide structure of these pigments lead to selective reflections of light (colours) at certain observation angles, provided that their parallel orientation to a flat substrate is achieved. Textile coatings with these types of pigments have a promising future for functional purposes, aesthetic eye-catching applications, product authentication as well as optical filtering for thermal management. The amount, distribution and orientation of EP-platelets (within a coated layer) and the light transmitted through their semitransparent structure highly influenced their optical effects. Therefore the surface structure and colour of the substrate as well as the coating formulation combined with different coating parameters is considered to influence on the colour-changing effects of textile coatings containing EPs. Multi-angle colour measurements showed that EP-coated black textile substrates with different structure characteristics exhibited angle-dependent colour changes, and, although the colour changes decreased with increased surface roughness (characterised by scanning electron micrographs (SEM)) they were highly visible for the human eye. No significant colour changes were visually seen on the white substrates due to intense reflections of the incident light from the white surface, transmitted back through the coated layer containing the semitransparent pigments. The gap (between knife and fabric) and coating speed strongly influenced the formulation viscosity during coating, resulting in coating deposit variations. Increased amount of coating deposits generated samples with larger amounts of EPs distributed within the coated layer and more horizontally oriented platelets. Thus, a more pronounced angle-dependent colour-change was achieved on smoother black substrates with increased solids deposit and a thicker coated layer.
O6 Nano-coated steels for solid oxide fuel cell (SOFC) interconnects
Rakshith Nugehalli Sachitanand, KB

Solid Oxide Fuel Cells (SOFCs) are electrochemical energy conversion devices that have the potential to achieve high efficiencies while using a broad range of fuels. Unlike other fuel cell technologies SOFCs do not require hydrogen as a fuel but can operate with high efficiency on hydrocarbon fuel from fossil- or renewable sources (e.g. natural gas, diesel, biogas). Today the main obstacle for their widespread implementation is a limited lifetime due to high degradation rates.

Two important degradation mechanisms in SOFCs are directly related to the ferritic steel based bipolar plate- which connects together single cells in series to form a ‘stack’. The first is the formation of volatile chromium oxides which commonly causes fast degradation in cell performance due to poisoning of the cathode. The other important lifetime limiting factor related to metallic interconnects is the ability to form a thin protective oxide under oxidation. Both issues have been addressed by the use of nano-coatings that have been applied to typical interconnect steel grades in order to minimise Cr evaporation and increase corrosion resistance. The samples are analyzed using SEM, TEM/EDX and XRD and the volatilization of Cr is measured using a recently developed denuder technique.

O7 Highly conductive bicomponent fibers
Erik Nilsson, MoT, Swerea IVF Mölndal

In order to improve the electrical properties of core conductive bi-component fibres, high amounts of a low surface area carbon black (CB) were incorporated into a high density polyethylene (HDPE) matrix. Composites were manufactured, characterized and utilized in the form of conductive bicomponent fibres. The spinnability, the melt elasticity and the electrical conductivity of the composite were evaluated. Bi-component fibres were produced with composite containing as much as 40 wt-percent CB. The fibers have a polyamide (PA6) sheath and CB composite as core material. Increasing the cold drawing temperature and introducing inline annealing has a favorable influence on fibres electrical properties without influence their mechanical properties. It is believed that the increased polymer chain mobility at elevated temperatures during cold drawing enable preservation of the conductive CB network in the composite, but also an re-agglomeration during annealing above the melting temperature of the HDPE matrix.
Exosomes are extracellular vesicles secreted from cells and can be isolated from body fluids such as blood and urine. They are constituted of a protein embedded lipid membrane enclosing a hydrated core containing soluble proteins and nucleotide material. Exosomes are nowadays largely investigated as increased evidence of the exosome important role in a broad range of physiological processes, pathological conditions and disease diagnostics. For example, they are seen as intercellular messengers to deliver biological material such as genetic information to other cells highlighting their potential to be part in cancer spreading. Accurate methods capable of quantifying exosome concentration in biological fluids remain lacking. We hereby present a novel method for exosome quantification using label-free surface based sensing with surface plasmon resonance read-out. As a model system, synthetic lipid vesicles were quantified were sued to mimic exosomes. Low concentration of CD63-positive exosomes (CD63+) released from human mast cells (HMC-1) was then measured with a detectable signal from below 4 µg/ml of total protein content. The sensing platform exhibited an excellent specificity with a non-specific signal <0.5% to the specific one. The uncertainty in the vesicle quantification using surface plasmon resonance may be as large as ±50% due to the complexity in sample composition. However, this method allows for the highly selective determination of the exosomal total mass with sensitivity of high signal to noise ratio (~100) for the low picoMolar regime and thus appears as complement more established nanovesicles quantification techniques.

In the world of today with rising climate problems while most of the energy used still comes from fossil fuels is not sustainable. This cannot continue if we are to avoid serious climate changes but all nations are dependent on the use of fossil fuels so what can be done. One part of a solution could be carbon capture and storage where the carbon dioxide (CO₂) would be captured from big point emission sources like power plants and then stored in the ground. This would prevent the emission of greenhouse gases to the atmosphere and still make it possible to operate on fossil fuel. One method of capturing the CO₂ is chemical looping combustion (CLC) which is a combustion process which splits the reaction in two parts, each one taking place in a different chamber. The combustion of fuel takes place in the fuel chamber which cut off from the normal air and supplied with oxygen by an oxygen carrier. The oxygen carrier is a metal oxide which takes up oxygen in the other chamber the air chamber where the normal air flows through. The metal oxide is transported to the fuel chamber where the oxygen can take part in the combustion reaction. Because of this internal separation a very pure product stream is obtained in which ideally only steam and CO₂ would be and the steam could easily be removed by cooling. This is one benefit with CLC.
compared with other methods of CCS which all require some sort of separation and separation always has an energy penalty. The penalty can be as high as 30% of the power produced which would drastically increase the price of energy.

O10 Optical spectroscopy of single functional nanoparticles

Svetlana Syrenova, TF

Today’s rapid progress in nanotechnology creates an increasing demand to obtain profound understanding of single functional nanoparticle behavior associated with strong size, shape and chemistry dependent properties. This challenging task is greatly facilitated by the phenomenon of the localized surface plasmon resonance (LSPR) in noble metal nanoparticles, and there is an increasing potential to use it as a tool to investigate processes in/on single functional nanomaterials in situ. In this work we demonstrate how to use plasmonic nanoantenna structures for optical spectroscopy of single functional nanoparticles. The model system is adsorption/desorption of H₂ in small Pd nanoparticle, monitored at a single particle level.

O11 Surface Chemical Analysis of Soft Magnetic Composite Materials

Christos Oikonomou, MoT

Soft Magnetic Composite (SMC) components produced based on traditional Powder Metallurgical (PM) techniques are strong candidate materials for electromagnetic applications. Their advantages are based on profitable and energy efficient production methods, shape complexity realization and uniquely uniform and isotropic 3D magnetic properties. SMC powder grades consist of encapsulated iron powder particles with an ultra-fine, electrically insulating surface coating. Component manufacturing procedure involves compaction of the admixed SMC powder with a lubricant to a final shape, as well as a subsequent heat-treatment that aims on the relaxation of stresses induced during the compaction. The concept of SMC is based on taking advantage of the dielectric properties of the surface coating and creating a laminated stack in a powder form. In this manner, products with superior magnetic performances can be produced as opposed to the more traditional laminated steels and ferrites, due to the higher reduction of core losses especially at high frequency applications. It is obvious that the insulating coating is the paramount feature of the SMC technology. Its morphology, thickness, cohesion to the powder particles, durability and chemical stability during compaction and heat-treatment, are critical for the properties of a finished component. The aim of this work is to analyze the behavior of such type of insulating coatings in order to model and tailor the process and optimize the performance of the product. For this reason, a methodology was developed based on a combination of surface and volume sensitive analytical techniques, namely X-ray photoelectron spectroscopy (XPS) and high resolution scanning electron microscopy (HR SEM) coupled with energy dispersive x-ray spectroscopy (EDX). The proposed methodology was implemented on both as-received powder and on finished components that
were treated at different temperature regimes in order to investigate the effect of the heat treatment to the nature of the surface coating.

O12 Heading towards eco-efficient surface protection: Physicochemical modification of microparticles for controlled release of biocides in protective façade coatings
Jonatan Bergek, KB

Biocide-containing façade paint loses its protective ability after a short period of time due to fast and premature leakage of the biocides. A promising improvement can be achieved by encapsulating the biocides and thereby reducing the release rate from the coating. The biocide is formulated into microparticles and the biocide release from the protective coating is controlled by the rate-determining diffusion from the microparticle into the surrounding coating matrix. In this work, long-term extended release has been obtained by two types of physicochemical modification of core-shell microparticles, formulated using the internal phase separation methodology. In the first modification route, the mode of solvent evaporation during the formulation step was altered. The second modification involved assembly of polyelectrolyte multilayers attached to the microparticle surface. Biocide release from a number of formulations of microparticles and coated films of paint has been studied by various analytical techniques. In addition, mathematical diffusion models have been applied to describe the biocide leakage.
Abstracts – Poster presentations

P1 Properties of LiFSI/LiTFSI doped ionic liquids for HT-LIB application

Manfred Kerner, TF

There is an increasing interest in lithium batteries for high temperature applications – HT-LIBs (≤150°C). To comply with these conditions, all battery parts have to be stable at high temperatures, without becoming a security problem – or their properties being deteriorated. Here we focus on HT-LIB electrolytes. Ionic liquids (IL) is a class of materials offering several important advantages: they are thermally stable, nonflammable, liquid over wide temperature ranges, have high ionic conductivities, and wide electrochemical windows. Furthermore, they have very low vapour pressures, which make them ideal candidates for HT-LIBs. Recently, there has been a lot of research focusing on ILs incorporating the anions bis(trifluoromethanesulfonyl)imide (TFSI-) or bis(fluorosulfonyl)imide (FSI-), because of their high thermal stabilities and conductivities. Also, it is known that the ILs incorporating FSI- prevent aluminium current collector corrosion. We have investigated the ILs 1-ethyl-3-methylimidazolium FSI (EMIFSI) and EMITFSI in combination with the Li-salts LiTFSI and LiFSI. – used at mole fractions of x=(0), 0.1, and 0.2. All investigated ILs and mixtures are thermally stable liquids in the temperature range -15°C to 150°C, which is a basic requirement for HT-LIBs. The highest room temperature ionic conductivity, 15 mScm⁻¹, which could be further increased with temperature, was found for the pure EMIFSI IL. Thermogravimetric analysis showed an increasing thermal stability with Li-salt mole fraction for EMIFSI electrolytes. The thermal stability of EMITFSI was unaffected by inclusion of LiTFSI, but exhibited a higher thermal stability in general. For both ILs the conductivity decreased when Li-salt was added. Also, distinct drops in conductivity were observed at the materials glass transition temperatures, Tg. These initial fundamental property studies have identified specific electrolytes to be tested vs. novel electrodes developed at Uppsala University within the common SSF project „From road-to-load“.

P2 Dynamic properties of water-xylitol solutions

Khalid Elamin, TF

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Differential scanning calorimetry (DSC), broadband dielectric spectroscopy (BDS), dynamic light scattering (DLS) and small-angle neutron scattering (SANS) were employed to study water-xylitol solutions. From DSC and dielectric spectroscopy we find that the glass transition temperature, Tg, decreases with increasing water content up to 29 wt.% water [1]. From BDS
the similarities in the peak shape, time scale and activation energy between the water (w) relaxation and the intrinsic $\beta$-relaxation of xylitol at water contents below 13 wt.% water suggest that the $\beta$-relaxation of xylitol determines the w-relaxation at such low water contents. The structural $\alpha$-relaxation and the w (or $\beta$)-relaxation are strongly dependent on the water concentration of the xylitol-water mixture [1]. The SANS measurement showed that none of the solutions exhibit any significant scattering in the low-q-range, below $q=1$ nm$^{-1}$. The DLS data show an ultraslow relaxation process with a $1/q^2$- dependent relaxation time, as expected for long-range diffusion. Two different approaches were used to estimate the hydrodynamic radius RH of the self-diffusing particles by using the Stoke-Einstein relation. In the first approach we assumed that xylitol undergoes Brownian self-diffusion in a medium of water and in the second approach we assumed that the diffusing xylitol particles feel the macroscopic viscosity of the solution. The first approach gives at very low water concentrations a particle size that is not consistent with the SANS data (i.e. a too large size), and in the case of the second approach the particle size becomes unrealistically small, particularly at low water concentrations, indicating that this approach overestimates the relevant microscopic viscosity of the Brownian medium [2]. Therefore, the most correct microscopic viscosity to use is probably somewhere between the viscosity of bulk water and the bulk viscosity of the given solution. However, by combining SANS and DLS data, we can conclude that the observed ultraslow DLS-process is not due to long-range concentration fluctuations, as often thought for sugar solutions, but due to the Brownian motion of single xylitol molecules or possibly very small clusters of a few xylitol molecules and associated water [2].


P3 Deformation mechanisms in a WC-Co based cemented carbide during creep

Amine Yousfi, TF

The microstructure of a WC-Co based cemented carbide has been investigated before and after plastic deformation at high temperatures. The material was fabricated with a Co binder phase content of 15 vol% and smaller additions of Cr. Hot compressive creep tests were performed under an applied load of 900 MPa at 1000 and 1100°C. The test bars were deformed to 10 or 20% strain at 1000°C, and to 7% strain at 1100°C. Quantitative microscopy using SEM suggests that WC grain growth took place during the creep tests, and that the growth took place preferentially in the plane perpendicular to the load axis. Deformation was also associated with a redistribution of the WC grains resulting in the formation of intergranular Co lamellae and cavities. Detailed studies of grain boundaries and defect densities in the Co binder and the hard phase grains were carried out using TEM. EBSD showed that there was an increased spread in the crystallographic orientation of the binder phase after deformation.
P4 Monitoring catalyst sintering under operating conditions

Pooya Tabib Zadeh, TF

Heterogeneous catalysts are often realized as nanometer sized metal particles dispersed on high surface area oxides, such as Al₂O₃. However, due to the excessive surface energy of small metal particles they are prone to sinter (i.e. coalesce into large particles) during operating conditions. This is a major cause of catalyst deactivation leading to additional costs associated with either metal overloading or regeneration procedures. Understanding the kinetics and mechanisms of sintering could pave the way to design a sintering-resistant catalyst. We used TEM and indirect nanoplasmonic sensing (INPS) to monitor the kinetics of Pt nanoparticle sintering on different flat support materials (model catalyst) and different atmosphere. Remote read out of changes in plasmonic signal upon sintering (in an INPS measurement) made it possible to follow the events under operating conditions with high temporal resolution. Our results show different mechanisms behind sintering of Pt particles in different atmospheres.

P5 Characterization of NaX (X=TFSI, FSI) - PEO based solid polymer electrolytes for Na+ battery application

Andrea Boschin, TF

At present sodium ion batteries represent a possibly cheaper alternative to lithium ion batteries. Indeed sodium is more abundant than lithium and still shows similar chemical and electrochemical properties. The sodium-ion battery electrolyte research is diverse; organic solvents, polymers, and ionic liquids as matrices are all being used (1,2). Ion conducting solid polymer electrolytes (SPEs) avoids the use of organic liquids and thereby enables fabrication of flexible, safe and compact solid-state structures. The ionic conductivities of sodium and lithium SPEs based on poly (ethylene oxide), PEO, are comparable (3,4), however, both having low conductivity values: 10^-5-10^-6 Scm⁻¹ at room temperature. The main part of the research performed so far on Na⁺ conducting SPEs was carried out during the 1980-90’s (3,5). Here we focus on PEO SPEs with NaTFSI or NaFSI as the sources of Na⁺ and with O:Na⁺ ratios (n) of 20, 9, and 6. Characterization has been carried out using dielectric spectroscopy, differential scanning calorimetry (DSC), Raman and ATR-IR spectroscopy, in order to evaluate possible differences due to employing different anions and/or different O:Na ratios. The highest ionic conductivity at 20°C (5•10^-6 Scm⁻¹) is obtained for NaTFSIPEO9. The conductivity increases up to 3•10^-4 Scm⁻¹ at 70 °C.

P6 Atom probe tomography of thin carbide films

Sabrina Koch, TF

Atom probe analysis (APT) is a physical analysis method where a chemical 3 dimensional volume of a material can be displayed with atomic resolution. During the analysis a needle shaped specimen (50-100 nm in diameter) is field evaporated in high vacuum under laser bombardment. As a result of this “treatment” the atoms desorb as ions from the surface, are separated by a mass analyzer and detected by a position sensitive detector. With the reconstruction of each atomic species and position in the needle shaped specimen volume valuable information about the materials chemical microstructure can be gained. The materials investigated in this project are thin carbide films. The expression “thin” refers to the nanometer range. The term “carbides” refers to any kind of material with the chemical formula EC where E is an element with less electronegativity than carbon. It is distinguished between ionic, covalent and metallic carbides. In this work, the microstructure of two novel metallic carbides, CrMnGaC and amorphous CrBC is investigated. Both materials were synthesized by magnetron sputtering, a physical vapor deposition (PVD) method. CrMnGaC is interesting in terms of novel predicted magnetic properties with possible application in spintronics. Amorphous CrBC is investigated in terms of phase composition. APT shows interesting Both materials are investigated in terms of phase composition and microstructure.

P7 Investigation of X750 Ni-Alloy

Silvia Tuzi, TF

Nuclear power is a big energy source, which has low carbon emissions. However, the storage of nuclear waste is expensive and difficult. The Ni-based alloy X750 is used for components in the fuel assembly. Understanding the corrosion of this alloy, it is possible to extend the working time of devices used in the plants and contribute to improved economy and safety. Different Fe contents in the alloy are suggested to give different corrosion processes. We have investigated the oxide morphology and the constitution of the oxide of different samples by using SEM and FIB/SEM.

P8 Metalion-exchange in small-pore zeolites for catalytic emission control applications

Anna Clemens, TF

In order to reduce the release of toxic exhaust gases, catalytic emission control is essential for every vehicle. For the treatment of nitrogen oxide (NO$_x$) exhaust gases, metal-exchanged zeolites have shown high activities, stabilities and selectivities as catalysts. Zeolites are crystalline aluminosilicates with a three-dimensional pore system that can vary in the pore diameter. Metal cations can be inserted in the porous structure by ion-exchange. In my PhD project, I investigate the effect of different metal cations
in a small-pore zeolite on the catalytic activity, stability and selectivity of the reaction of NO$_x$ to the environmentally harmless N$_2$.

**P9 Characterisation of polycrystalline cubic boron nitride tool materials**

*Kristina Lindgren, TF*

Cubic boron nitride is the second hardest material known. In this project the reactions that occur during sintering of polycrystalline cubic boron nitride (PCBN) composite tool materials have been mapped. Their dependence on starting powder composition have been investigated and the microstructure of the materials have been characterized. The starting powder mixtures of the PCBN composites consist of cBN, Ti(C,O,N), Al, and debris from the milling bodies used in the process. Two different types of milling bodies were used, WC-Co and cermet ((Ti,W)(C,N) grains in a Co binder phase). The PCBN materials were investigated before sintering, after pre sintering (900 °C) and after high pressure high temperature (HPHT) sintering (1400°C) in order to understand the processes taking place during densification. Methods used were XRD, SEM/XEDS and TEM/XEDS. The WC-Co milled and the cermet milled materials behave differently during pre sintering at 900°C. The WC-Co milled materials start to sinter. Phases detected in the HPHT sintered WC-Co milled materials include cBN, (Ti,W)(C,O,N), AlN, TiB$_2$, WC, Al$_2$O$_3$ and W$_2$CoB$_2$. W-rich areas between the larger Ti(C,O,N) grains were observed in the SEM. Phases containing Al were found close to cBN grains and between Ti(C,O,N) grains. In the HPHT sintered cermet milled materials Co-rich or Al-rich areas were found between the (Ti,W)(C,O,N) grains. In this case cBN, (Ti,W)(C,O,N) and two unidentified phases were found using XRD. The amount of W in the (Ti,W)(C,O,N) varied locally. The phase composition is, hence, dependent on the raw material composition. The amounts of Al, W and Co affect both the pre sintered and the HPHT sintered phase compositions. Especially the cermet milled materials show a wide diversity in local structure and composition.

**P10 The capability of ESEM in-situ techniques in evaluation of the initial corrosion stages of stainless steels at 450°C**

*Nooshin Mortazavi, TF*

The oxidation behavior of stainless steels is principally affected by the very initial stages of the oxidation process. In the present study, the early stages of oxidation of some selected stainless steels are investigated by means of ESEM in-situ exposures in the presence of KCl(s) on the surface at 450°C for 1 hour and in laboratory air. The ESEM in-situ experiment is used to monitor the oxide growth at temperature “live”, as it occurred. The influence of KCl on the corrosive behavior and the probability of the formation of a protective oxide scale on the exposed samples are also analyzed through post-exposure SEM/EDX and FIB. Standard tube furnace experiments are also performed to produce reference samples in order to examine the effect of the presence of electron beam and the lower pressure in the ESEM on the corrosion behaviour. A comparison between the microstructure of the oxide scales of
samples exposed in ESEM and that of the furnace exposures exhibited a reasonable conformity. In general, the corrosion attack at this relatively low temperature was mainly located around KCl particles, where large oxide structures grew from the salt/metal contact regions.

P11 The effect of surface treatment on the corrosion behavior of Ni-based alloys studied by high-resolution techniques

Haiping Lai, TF

The resistance of alloys operating at elevated temperatures relies on the formation of a protective oxide scale. The ability of the material to form such a scale depends on several factors including material composition, microstructure and surface treatment. However, while the influence of the two first mentioned factors is well recognized, the importance of surface finish has not yet been addressed to the same extent. The investigation showed that, under the applied conditions, SCA425+ material is able to form a protective continuous alumina layer on the ground sample but that an extensive internal oxidation is observed on the polished sample. For the two different surface treatments of IN792 material, the observed mass gains and the structure of the outer layer of the oxide scale are on the other hand, very similar. However, since the different surface finish causes different degree of surface deformation, it will create different size of the recrystallized grains close to the oxide-metal interface. Thus, some difference is observed in the oxidation of the metal grain boundaries in the two conditions of IN792. The details concerning structure and chemistry of the scales formed during the exposures will be presented and discussed.

P12 Interactions and mechanisms for surface sizing polymer particles

Frida Iselau, KB

Surface size polymers are used for hydrophobization of paper grades. They are widely used but little is known about the basic underlying chemical and physical principles that are important for efficient surface sizing. In this project the interactions between the different components in the surface size system will be studied and model systems will be used to study the adsorption of the surface size polymers onto the paper surface, their penetration into the porous material, their film-forming properties as well as the nature of the hydrophobic film on the paper surface.

P13 Catalysts for ammonia production - fundamental studies towards passive SCR systems

Emma Adams, KB

Selective catalytic reduction of NOx with ammonia (NH3-SCR) is a well-established technique for abatement of emissions in heavy-duty vehicles. However, handling ammonia on-board vehicles is problematic. Passive SCR is a newly developing area that may contribute to solving some of these
problems. The concept of this technique is to generate NH₃ on-board the vehicle by utilizing the NOₓ that is readily available in the exhaust stream whilst the engine undergoes rich operation (high fuel/low O₂). The formed NH₃ can then be stored on an SCR catalyst down-stream and used to reduce slipped NOₓ when the engine is set back to operate under lean conditions. In the present study we have investigated different catalyst formulations that enable formation of ammonia from NO and hydrogen. Also, we have studied whether or not water as a source for hydrogen via water-gas-shift reaction, \((\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2)\) can be used to produce significant amounts of hydrogen to enable ammonia production. The results show that significant amounts of ammonia can be formed over alumina and titania supported platinum or palladium catalysts. Specifically, the results show that both the noble metal and the metal oxide support are crucial for the NH₃ formation.

**P14 Characterization and evaluation of surface functionalized silica nanoparticles**
_Sanna Björkegren, KB_

Colloidal particles can spontaneously accumulate at the interface of two immiscible liquids and thereby stabilize disperse systems such as emulsions and foams. Properly designed particles can adsorb irreversibly at the interface of an emulsion droplet, providing an unusually high stability of the system. In emulsion and foam applications surface modified silica nanoparticles with controlled hydrophobicity and surface activity have great potential. The control of the surface chemistry of the particles opens up to interesting opportunities. In this work, colloidal silica provided by AkzoNobel Pulp and Performance Chemicals is functionalized through attaching both hydrophobic moieties, creating particles with an amphiphilic character. Particles functionalized with only hydrophilic silane have also been prepared. The particles are evaluated and characterized to obtain a deeper knowledge of how they behave not only in emulsion and dispersion systems, but also in terms of stability of the modification and steric stabilization effects. NMR diffusometry can be used to evaluate the surface modification and is an essential tool in the characterization of the surface.

**P15 Structural investigation of cellulose using solid-state NMR spectroscopy**
_Alexander Idström, KB_

Cellulose is the most abundant polymer in nature. Even though cellulose at first sight looks rather simple, being an un-substituted glucan chain, a lot about its structure is still debated. Cellulose contributes to a very complex structure on a variety of length scales, from the crystalline parts in the elementary fibrils, to the tree or flower. Prior to the use of solid-state NMR the structure of native cellulose was debated. A proposed crystal structure consisting of just one crystal form, cellulose I, was most widely acknowledged. However, with the use of solid-state NMR the crystal structure of cellulose was explained as a combination of two allomorphs, named cellulose Iα and Iβ.
In addition to native cellulose, a number of other crystalline structures such as cellulose II, III, IV etc., can be formed when treating cellulose to solvents, heat or other treatments. With the use of solid-state NMR spectroscopy, a lot of information can be acquired, when studying cellulose. A large benefit of NMR is that two nuclei with different electron environment can be distinguished in the NMR spectrum. By doing the measurements in solid form, it is possible to distinguish between different kinds of crystalline forms. Each cluster of peaks can be attributed to a specific carbon in the anhydroglucose unit (AGU) of cellulose. Additional information can be apprehended from the spectra by looking closer to the different carbon regions. The C-4 signals between 92 and 80 ppm are often quite resolved and are widely considered to hold most information. For processing of solid-state NMR spectra, overlapping signals could be separated by applying spectral deconvolution. Using the deconvolution of the C-4 region, information about crystallinity index, fibril size, elementary fibril size and relative allomorph amount can be apprehended.

P16 Developing a biomimetic water desalination device using mesoporous supported lipid bilayers with aquaporins
Simon Isaksson, KB

The growing population in areas where fresh water supplies are scarce is resulting in difficulties satisfying the demands for drinking water. Pollution and environmental changes are increasing the demands further. Improvements in water treatment processes are therefore needed, an achievement we suggest to fulfil by constructing a device that desalinate water using a biomimetic approach. The idea is to desalinate sea water to drinking water using a membrane that resembles the membrane of living cells, by reconstituting aquaporins in a lipid bilayer. Lipid bilayers are suitable as separation membranes since transmembrane transporter proteins, such as aquaporins, can readily be reconstituted to add selectivity, whereas a general characteristic of lipid bilayers is that they are inert and impermeable to most substances. The proposed device has to overcome the osmotic pressure that arises, due to for example differences in salt concentration, by applying an external pressure to the membrane. The pressure is suggested to force the water molecules to penetrate the membrane through the aquaporins. The lipid bilayer is by itself not rigid enough to withstand such pressures, which urges the use of a support that is able to stabilise the bilayer. Lipid bilayers are commonly constructed as an aperture spanning membrane or as a bilayer deposited on a solid support. We have previously shown that it is possible to take advantage of the best from each of these designs using cubic mesoporous silica as a support for the lipid bilayer, where the walls of the pores provide stability to the bilayer and the pore spanning part of the bilayer provides a suitable environment for aquaporins. In this project we aim to use a mesoporous supported lipid bilayer with reconstituted aquaporins to evaluate the possibility of water treatment by applying an external pressure to the system.
P17 Zeolite SSZ-13 as NH3-SCR catalyst
Alexander Shishkin, KB

P18 Atmospheric corrosion behavior of Mg-Al alloys in high pressure die cast and semi-solid casting forms
Mohsen Esmaily, KB

Magnesium-aluminum (MgAl) alloys are the lightest engineering structural materials, being extensively employed in the automotive and many other engineering sectors owing to their high specific strength and good castability. However, the more widespread use of MgAl alloys is limited by their low corrosion resistance and poor high temperature mechanical properties [4-6]. The corrosion properties of MgAl alloys have therefore attracted scientific attention. In this study, the influence of the microstructure on the atmospheric corrosion of Mg-Al alloy AM50 produced by rheo-casting (RC) and high pressure die casting (HPDC) is investigated. The RC AM50 alloy showed better corrosion resistance than HPDC AM50. The superior atmospheric corrosion behavior of RC AM50 compared to HPDC AM50 is carefully discussed in relation to differences in the as-cast microstructures.

P19 Nano-coated ferritic steel foils for SOFC interconnect applications
Hannes Falk Windisch, KB

Solid Oxide Fuel Cells (SOFCs) is one of the most promising candidates able to provide electricity in a sustainable way to a modern society. In SOFC the electrolyte is a ceramic oxygen conductor hence high operating temperatures (600-900°C) are necessary. One of the main advantages in comparison to other fuel cell types is that SOFC can operate not only on hydrogen but also on fuels such as natural- or biogas as well as diesel. Today, the main obstacles for commercialization are limited lifetimes combined with high production costs. To increase the life time of a SOFC two important degradation mechanisms which are directly related to the metallic interconnects has to be understood and reduced. The interconnect is made out of a ferritic stain less steel, which connects the single cells to a SOFC stack. At high temperatures volatile chromium oxides are formed causing degradation due to poisoning of the cathode. The other important lifetime limiting factor related to the metallic interconnect is the ability to form a thin protective oxide. Both issues have been addressed by the use of nano-coatings that have been applied to typical interconnect steel grades in order to minimize Cr evaporation and increase corrosion resistance. The samples are analyzed using SEM, TEM/EDX and XRD and the volatilization of Cr is measured using an in house developed denuder technique.
Austenitic stainless steels (ASS) are among the most used engineering materials, particularly suitable for applications where high corrosion and oxidation resistance is required: e.g. chemical, pharmaceutical and food industry but also kitchenware. ASS have a face centered cubic crystalline structure, with substitutional alloying elements being chromium and nickel, are responsible for the anticorrosion properties: chromium forms a protective passive layer of Cr$_2$O$_3$ and nickel is austenite stabilizer allowing higher working temperatures. However, its outstanding chemical stability is not matched by other properties such as surface hardness and wear resistance, which can greatly hinder the lifetime of components where surface stresses are present. ASS are not hardenable by conventional heat treatments, on contrary, at high temperatures (>500°C) sensitization might occur due to precipitation of Cr at the grain boundaries, creating Cr depleted areas which can easily become source of corrosion. One possible improvement is given by low temperature carburizing/nitriding techniques (e.g. plasma), which triggers the formation a supersaturated interstitial solid solution case structure called S-phase, or expanded austenite. S-phase is characterized by the same corrosion resistance as the base material, but surface hardness up to five times higher and substantially higher wear properties. However, mechanisms of formation and stability, along with internal residual stresses and other structural characteristics are not fully understood. This topic is of great industrial interest due to the possible implications for improving materials properties both on a performance and economical point of view.

Materials used in wheels and rails are exposed to a complex combination of mechanical and thermal loadings. Understanding the behavior is essential for materials selection for different environments, for design of railway components as well as for tuning of traction and braking systems. The stress state in rolling contact loading is not readily simulated under laboratory conditions, but in this project an attempt to examine material properties under realistic conditions will be made by use of a bi-axial servo-hydraulic test frame equipped with a temperature chamber (-70°C – 350°C). Means to prevent buckling under compressive loads will be taken by specimen design, inherent test frame stiffness and/or a fixture. Also uni-axial tests at higher temperatures and with alternating thermal and mechanical loads (thermo-mechanical fatigue) will be done. Both the virgin material and the anisotropic surface layer will be investigated with the aim to give a better understanding of material behavior in service and enable implementation and calibration of realistic material models describing the behavior.
Needle punching of cellulose fibre structures was studied, in order to explore the possibility for a new method for bonding to be used in the paperboard industry. The interest in such subject was based on the need for stronger fibre-to-fibre bonding in the thickness direction of paperboard. The studied samples were prepared with a laboratory handsheet former, and the sheets were then couched to a three-ply paperboard. The middle layers were needled with and high (60 stitches/cm$^2$) and low (40 stitches/cm$^2$) needle stitch density at different needling depths, the different needling depths enabled the use of 0 to 3 barbs of the needle. The needling performed changed both the fibre orientation and the density of the fibre structure locally, i.e. close to the needled holes. For samples needled with two barbs, there were also some fibres tilted in the thickness direction. The local density was estimated to increase around 25% compared to the surrounding regions. Due to the needling, the peak bending moment was found to increase 8% and the peak bending angle increased 19%, measured on three-ply paperboard samples having a middle layer needled with two barbs and the higher stitch density. The bending stiffness and the tensile and compression strength in the thickness direction were also measured, indicating no significant changes by the needling of the middle layer.

Microfibrillar cellulose has in principle good specific mechanical properties which make them interesting as reinforcing agents in composite materials. There are however problems associated with the hydrophobicity of common polymer matrices and the stress transfer between the fibrils. A possible route to avoid problems of this kind is to produce composite fibres to be used in structural components. The work has the aim of making these kind of composite fibres

A recyclable plastics waste stream of electrical and electronic equipment has previously been found to contain acrylonitrile-butadiene-styrene copolymer (ABS, ~40 wt%), high impact polystyrene (HIPS, ~40 wt%), polypropylene (PP, ~10 wt%) and a rest fraction consisting mainly of other styrene-based thermoplastics. In this work, one virgin and one recycled ternary blend consisting of these three components were melt-blended in an extruder to study the influence of processing conditions on the mechanical and thermal properties. Favourable processing conditions with respect to tensile properties of the virgin blend were found at intermediate screw rotations (40-80 rpm) and relatively low barrel temperatures (170-220°C). The recycled blend and recycled ABS, HIPS and PP showed higher stiffness and yield stress, but
lower elongation at break than the corresponding virgin materials. The stiffness and yield stress of the blends were found mainly to follow the rule of mixtures of their components while the elongation at break exhibited adverse characteristics indicating incompatibility between ABS, HIPS and PP. A comparison between single screw extrusion and twin screw extrusion is interesting since it is two of the most common melt-processing options for thermoplastics. It was found that the difference in stiffness and yield strength of the recycled and virgin blend were insignificant, while a higher elongation at break could be seen for twin screw extrusion for all the blends.

P25 Delubrication of Powder Metallurgy Steels
Seshendra Karamchedu, MoT

Powder metallurgy (PM) is a manufacturing route wherein powders are used as the starting material which is processed into useful components. The typical processing steps for PM steels consist of compaction at room temperature, where the final shape of the component is achieved, followed by a temperature assisted sintering process which imparts sufficient strength to the compact through the formation of metallurgical bonds between the particles. The powders are mixed with lubricants prior to the compaction stage since they reduce the friction between the powder particles and between the particles and the die-wall, thereby promoting compaction homogeneity and decreasing die-wear. However, these lubricants have to be removed after the compaction stage since they hinder the sintering process. Lubricants commonly used for processing of PM steels are based on ethylene bis-stearamide and lubricant removal is achieved through thermolysis in the initial zone of the sintering furnaces. Improper delubrication can lead to defects in parts such as micro-cracking and sooting and can also lead to deposition of delubrication products on the furnace components and compacts. This results in a decrease in productivity and increase in maintenance costs. Hence an industrially feasible method for monitoring delubrication process would be valuable. In the present work, a methodology for monitoring the delubrication process has been proposed based on analyzing the processing atmosphere through sensors (dew-point, CO₂ and O₂) commonly used in the industry (see Figure 1-a). Through the experiments performed using the laboratory set-up, it has been shown that the O₂ sensor is useful in monitoring the initial stages of delubrication and the CO₂ sensor can be used to monitor the later stages (see Figure 1-b). Using the proposed methodology a systematic study of the effect of various process parameters- heating rate, temperature, effect of graphite addition, composition and purity of the process atmosphere on delubrication has been performed. Based on the results it has been suggested that delubrication has to be performed at 450°C in dry N₂ atmosphere at a slow heating rate with flow sufficient enough to provide dynamic conditions around the component surfaces.