

**The Condensed Matter & Complex Systems Seminar**  
**Monday 15 June 2009, Radisson SAS Lillehammer Hotel**

*Organized by  
the Condensed Matter Division of the Norwegian Physical Society (NFS)  
and COMPLEX – a nationally coordinated research network in Norway*

**PROGRAM**

- 11:30 Lunch
- 12:30 **David Rowe** (Cardiff School of Engineering, UK) (invited): Recent advances in thermoelectric power generation and applications
- 13:05 **Johan Taftø** (UiO): An overview of our basic and applied thermoelectric research activity
- 13:20 **Niina Jalarvo** (UiO): Structure of strontium tantalate, a potential fuel cell electrolyte, from neutron powder diffraction and density functional theory calculations
- 13:35 **Vitaliy Yurchenko** (UiO): Application of superconductors to renewable energy conversion and complex phenomena behind it
- 13:50 **Atle Jorstad Qviller** (UiO): Intermittent flux penetration in superconductors
- 14:05 Coffee break
- 14:25 **Denis Weaire** (Trinity College, Ireland) (invited): Foam as a complex system
- 15:00 **Glenn Tørå** (NTNU): A dynamic two-phase network model with film flow
- 15:15 **Joakim Bergli** (UiO): Slow Relaxation and Equilibrium Dynamics in a 2 D Coulomb Glass: Demonstration of Stretched Exponential Energy Correlations
- 15:30 **Geir Helgesen** (IFE): Structure of carbon cones
- 15:45 Coffee break
- 16:05 **Jozef Cernak** (Safarik Univ., Slovak Republic): A transition from multifractal to finite size scaling in self-organized criticality models
- 16:20 **Matti Knaapila** (IFE): Phase behavior of poly(9,9-dialkylfluorene)s as a function of side chain length
- 16:35 **Henning A. Knudsen** (UiO): Snell's Law for Shear Zone Refraction in Granular Materials
- 16:50 **Grunde Løvoll** (UiO): Steady-State Two-Phase Flow in Porous Media: Statistics and Transport Properties
- 17:05 **Kenneth D. Knudsen** (IFE): Gravitationally induced ordering of hectorite nanoplatelets
- 17:20 Finish

## ABSTRACTS OF TALKS

### Invited talk:

### Recent advances in thermoelectric power generation and applications

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#### Abstract

A thermoelectric generator is a solid-state heat engine in which the electron gas serves as the working fluid and converts a flow of heat into electricity. It has no moving components, is silent, scalable and extremely reliable.

Thermoelectric generators were initially developed in the former Soviet Union during the second world war to power wireless communications in remote areas. The availability in the 1950's of radioactive material enabled thermoelectric generators to meet a requirement for long-life sources of electrical power for applications in hostile and inaccessible applications such as the voyager deep space missions.

Following the first oil crises in 1974 attention turned to researching thermoelectrics as an environmentally friendly energy source and In recent years effort has focused on developing thermoelectric generating systems which can harvest waste heat . In this presentation the basic concepts of thermoelectric generation are outlined. An overview is presented of recent advances in the development of high performance thermoelectric materials, modules, and terrestrial applications. Finally, the potential of thermoelectric recovery of waste heat as a renewable energy technology is assessed.

## An overview of our basic and applied thermoelectric research activity

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In our studies of thermoelectric materials [1], we span the range of activity from materials synthesis, through study of their atomic arrangement and electronic structure at the nanoscale, to measurement of their physical properties. A major goal is to develop energy efficient Peltier elements for cooling or heating, or for generating electricity from for example waste heat. This requires materials with low thermal conductivity, high electrical conductivity and large Seebeck coefficients. Strategies for improving known thermoelectric materials are both nanostructuring and doping to increase the Seebeck coefficient and the electrical conductivity, and in particular nanostructuring to scatter phonons, thereby decreasing the thermal conductivity [2]. We study the Zn-Sb system and skutterudites.

We will present experimental results from our study of the ZnSb compound which has a high Seebeck coefficient around room temperature and is thus a potential material for applications in heat-pumps and coolers. We attempt to reduce the thermal conductivity by introducing different types of nanoparticles and by reducing the crystal grain size through ball-milling. The nanostructure is studied by transmission electron microscopy. Furthermore, we measure the Seebeck coefficient, electrical conductivity and thermal conductivity. With a special technique, the Harman technique [3], we measure directly the figure of merit which tells us about the efficiency, without measuring the three involved physical properties separately.

Calculations using density functional theory (DFT), and spectroscopic experimental techniques, in particular electron energy loss spectroscopy (EELS), are used to study the electronic structure of the materials. We present examples from thermoelectric skutterudites [4, 5, 6].

The application part deals with developing and evaluating thermoelectric heat-pumps for heating of houses, thus eliminating compressors and climate gases. In a miniature test, with a difference between in-house and outdoor temperature of 10 degrees, we have achieved a reduction in electricity consumption to less than 40% compared with the use of conventional electrical heaters. We are now scaling up this concept under controlled “outdoor” temperature conditions to test if this is a feasible way of saving energy.

[1] <http://www.fys.uio.no/bate/>

[2] B. Poudel et al., *Science* **320**, 634 (2008)

[3] T. C. Harman, *Journal of Applied Physics*, **29**, 1373 (1958)

[4] O. M. Løvvik and Ø. Prytz, *Physical Review B* **70**, 195119 (2004)

[5] Ø. Prytz, O. M. Løvvik and J. Taftø, *Physical Review B* **74**, 245109 (2006)

[6] Ø. Prytz, R. Sæterli, O. M. Løvvik, and J. Taftø. *Micron* **39**, 685 (2008)

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## Structure of strontium tantalate, a potential fuel cell electrolyte, from neutron powder diffraction and density functional theory calculations

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$\text{Sr}_4(\text{Sr}_2\text{Ta}_2)\text{O}_{11}$  is an end-members of a series of oxygen deficient complex perovskites of general formula  $\text{A}^{\text{II}}_3(\text{B}^{\text{II}}_{1+x}\text{B}^{\text{V}}_{2-x})\text{O}_{9-d}$ . The end-members ( $x=0.50$ ) can be written  $\text{A}^{\text{II}}_3(\text{B}^{\text{II}}_{1.5}\text{B}^{\text{V}}_{1.5})\text{O}_{8.25}$ . However, since they have one oxygen vacancy out of 12 oxide ions, their molecular formulae are more often multiplied by 4/3 and then represented as  $\text{A}^{\text{II}}_4(\text{B}^{\text{II}}_2\text{B}^{\text{V}}_2)\text{O}_{11}$ . This class of perovskites exhibits oxide ion (vacancy) conductivity in dry atmospheres and protonic conductivity in wet atmospheres. In presence of water vapour the perovskite will hydrate into  $\text{Sr}_4(\text{Sr}_2\text{Ta}_2)\text{O}_{11}\times n\text{H}_2\text{O}$  ( $0 \leq n \leq 1$ ). The water incorporation is a critical phenomenon for the proton conducting mechanism. Furthermore, it is assumed that the oxygen vacancy distribution affects strongly the charge carrier mobility. Interestingly, the hydrated oxide may exhibit order-disorder on *three* sublattices as a function of temperature and water content: the B-cation sublattice, the oxide ions and vacancies, and the protons.

In order to shed light into the order-disorder processes we have performed neutron powder diffraction (NPD) studies at E9 spectrometer at BENSC facility (Berlin, Germany) in dry and humid ( $p\text{D}_2\text{O} = 1$  bar) atmospheres between room temperature and 700 °C. Isotopic substitution of H by D allows to detect the D positions in the structure using NPD technique, while presence of H would produce problems in terms of incoherent background. First principles calculations were done to support the structural refinements and to estimate the proton/deuteron positions. The materials electronic structure has been also calculated.

The NPD data analysis has been performed using FullProf software package. For  $\text{Sr}_4(\text{Sr}_2\text{Ta}_2)\text{O}_{11}$  the best refinements were obtained considering a cubic space group  $\text{Fm}\bar{3}\text{m}$ , with  $a = 8.3007$  Å. Compared to an ordinary perovskite structure, this model contains additional “interstitial” oxygen at Wyckoff position 48g. Occupancy of these 48g positions is only about 5%, whereas there is also a slight deficiency at the octahedral oxygen sites. Furthermore, the Fourier maps reveal short-range oxygen disorder to large extent, which can be also seen at the diffraction patterns as diffuse background. Static short range disorder of the O sites complicates the structural picture of dry  $\text{Sr}_4(\text{Sr}_2\text{Ta}_2)\text{O}_{11}$ , and is also most probably responsible for the ionic transport properties of this material.

The structures obtained from the density functional calculations are consistent with the experimental results. Several initial Wyckoff positions were considered in order to span all the possible proton sites. As a result has been found that protons have a tendency to sit along the tantalum octahedral edges. From the electronic structure point of view, the calculations show that the non-hydrated phase has a half-metallic (ferromagnetic) ground state while the hydrated one is a non-magnetic insulator.

## **Application of superconductors to renewable energy conversion and complex phenomena behind it**

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Increasing energy consumption and depletion of conventional fuel resources intensify a search for effective renewable energy solutions. At the moment wind turbines are one of the most mature and the most competitive technologies for green energy conversion, with the greatest potential in off-shore deep water wind parks. Use of superconducting generators may resolve several critical issues specific to deep water wind turbines: besides higher efficiency, it is a substantial weight reduction and improved reliability. The core of the superconducting generators is a superconducting cable. Advances in a technology for the second generation coated conductors are revitalizing an interest to a superconductivity research, which has been given an undeservedly little attention in recent years.

Performance of superconducting applications is up to a great extent determined by a dynamics of a magnetic flux in superconductors. Magnetic field penetrates the so called type-II superconductors, which are most commonly used in practice, in a form of magnetic vortices (or flux lines), each carrying one quantum of the magnetic flux. Being driven by the Lorentz force, moving vortices cause dissipations and may turn superconductors into a normal state. Dynamics of the flux lines is governed basically by two counteracting forces: the driving Lorentz force and a pinning force, i.e. a force due to interaction of the vortices with structural irregularities of material. However, a presence of different types of defects and mutual repulsion between the vortices make flux medium in superconductors a highly complex system with rich variety of dynamic phases.

Real-time magneto-optical imaging is a unique method for non-invasive direct investigations of currents and flux distribution in superconductors. Herewith, we would like to present an overview of our recent results of magneto-optical visualization of flux dynamics in superconductors, including dendritic flux avalanches and intermittent flux propagation in high-temperature superconductors, which are model samples for the coated conductors.

## Intermittent flux penetration in superconductors

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In type-II superconductors, increased applied magnetic fields are associated with a gradual penetration of flux in the form of magnetic vortices. The vortices are pinned to defects in the materials, and the resulting, static flux distribution is known as the critical state model. It is of great interest to understand this phenomenon, as it can severely limit the performance of superconductors in commercial applications. Yttrium barium copper oxide (YBCO) is an important high-temperature superconductor, but it has until recently been hard to manufacture into wires due to superconducting grains misaligning and producing weak links. Recent developments include growing YBCO on textured substrates to align the grains properly.

Magneto-optical imaging has been used to observe the penetration of magnetic flux into thin-films of YBCO grown on tilted substrates. In most samples, the penetration is smooth and critical state-model like, but in some samples, an intermittent penetration of flux bundles is seen. This intermittent penetration is only seen at low temperatures in samples with a high critical current. We suggest how this behavior might arise from the properties of the vortex lattice and its interaction with extended defects in the material.

Invited talk:

## Foam as a complex system

Denis Weaire

*Trinity College Dublin, Ireland*

Disordered foam is a good example of a complex system. It can stand as a prototype for many others (emulsions, grain growth, granular materials,...) depending on the property studied. Of particular interest at present is foam rheology. As often before, two-dimensional foams have been found convenient for both theory and experiment, and have exposed a number of key questions. The most intriguing is: what is the origin of the nonlinearity of the Herschel-Bulkley relation for the dependence of excess stress on shear rate?

## A dynamic two-phase network model with film flow

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(Dated: May 7, 2009)

We present a dynamic network model, based on the governing equations describing two phase flow in porous media. The wetting films in corners of the pore space are incorporated. The model gives rise to the complex interplay of frontal displacements, film swelling and snap-off, which is observed in experiments.

The flow simulations are performed on realistic networks of sandstone. Saturation profiles are compared with experiments for different capillary numbers, and for spontaneous imbibition we find that the penetration length of the wetting saturation front shows a behaviour proportional to the square root of time. We also find that the imbibition rate decrease and the residual oil saturation increase with increasing initial water saturation.

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## Slow Relaxation and Equilibrium Dynamics in a 2 D Coulomb Glass: Demonstration of Stretched Exponential Energy Correlations

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Abstract: We have simulated energy relaxation and equilibrium dynamics in Coulomb Glasses using the random energy lattice model. We show that in a temperature range where the Coulomb Gap is already well developed, ( $T=0.03-0.1$ ) the system still relaxes to an equilibrium behavior within the simulation time scale. For all temperatures  $T$ , the relaxation is slower than exponential. Analyzing the energy correlations of the system at equilibrium  $C(\tau)$ , we find a stretched exponential behavior,  $C(\tau)=e^{-\left(\tau/\tau_0\right)^\gamma}$ . We study the temperature dependence of  $\tau_0$  and  $\gamma$ .  $\tau_0$  is shown to increase faster than exponentially with decreasing  $T$ .  $\gamma$  is proportional to  $T$  at low temperature, and approaches unity for high temperature. We define a time  $\tau_\gamma$  from these stretched exponential correlations, and show that this time corresponds well with the time required to reach equilibrium. From our data it is not possible to determine whether  $\tau_\gamma$  diverges at any finite temperature, indicating a glass transition, or whether this divergence happens at zero temperature. While the time dependence of the system energy can be well fitted by a random walker in a harmonic potential for high temperatures ( $T=10$ ), this simple model fails to describe the long time scales observed at lower temperatures. Instead we present an interpretation of the configuration space as a structure with fractal properties, and the time evolution as a random walk on this fractal-like structure.

## Structure of carbon cones

Geir Helgesen<sup>1,2</sup>, Kenneth D. Knudsen<sup>1,3</sup>, Arnljot Elgsæter<sup>3</sup>, and Stine N. Næss<sup>3</sup>

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Large-scale production of perfect conical carbon nanostructures that are fundamentally different from the other nanocarbon materials, such as buckyballs and nanotubes, can be made using the so-called Kvaerner Carbon Black & Hydrogen Process. This involves pyrolysis of hydrocarbons using a proprietary plasma torch process. The carbon cones (CC) that occur appear in five distinctly different forms. In addition, disk-shaped particles may be produced. The carbon cones consist of curved graphite sheets formed as open cones with one to five carbon pentagons at the tip with successively smaller and discrete cone angles, respectively. The structure and properties of these carbon cones and disks have been relatively little explored until now. We present results from our experimental research on the structure of carbon cones and disks using scanning- and transmission electron microscopy, and X-ray- and electron diffraction. The particles have diameters of 0.5-4  $\mu\text{m}$  and are typically about 20 nm thick, but can have thicknesses up to ~60 nm. The disk particles show 12-fold faceting along the edges, while the flattest cone shows a 10-fold faceting consisting of five pairs of ( $22^\circ$ ,  $38^\circ$ ) for the facet interfacial angles. The thin crystalline cores of these particles are usually coated with amorphous carbon layers. Heat-treatment of the as-produced CC raw material improves the crystalline quality.

## A transition from multifractal to finite size scaling in self-organized criticality models

Jozef Cernak

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I numerically investigated scaling properties of a few self organized criticality models in an effort to know more details about transition from multifractal to finite size scaling. The initial results show that background reasons of the transition are more complex as it was initially thought.

## Phase behavior of poly(9,9-dialkylfluorene)s as a function of side chain length

Matti Knaapila

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We present guidelines on how the phase behavior and solution structure of  $\pi$ -conjugated hairy-rod polyfluorenes are controlled by the side chain length and branching. First, the semi-quantitative mean field theory is formulated to predict the phase behavior of the system as a function of side chain beads ( $N$ ). The phase transition at  $N = N^*$  separates a lyotropic phase with solvent coexistence ( $N < N^*$ ) and a metastable membrane phase ( $N > N^*$ ). The membrane phase transforms into the isotropic phase of dissolved rodlike polymers at the temperature  $T_{mem}^*(N)$  that decreases both with  $N$  and with the degree of side chain branching. This picture is complemented by polymer demixing with the transition temperature  $T_{IN}^*(N)$  that decreases with  $N$ . For  $N < N^*$ , the lyotropic phase turns isotropic with increasing  $T$  at  $T_{IN}^*$ . For  $N > N^*$ , the stable membranes are predicted for  $T_{IN}^* < T < T_{mem}^*$  and metastable membranes with nematic coexistence for  $T < T_{IN}^*$ . Second, in experiment, poly(9,9-dialkylfluorene)s with  $N = 6-10$  were mixed in methylcyclohexane. For  $N = 8$  the side chain branching was controlled by (9,9-dioctylfluorene)/(9,9-bis(2-ethylhexyl)fluorene) (F8/PF2/6) random copolymers. The proportion of F8 to F2/6 repeat units was 100:0, 95:5, 90:10, 50:50, and 0:100. In accord with the theory, the lyotropic, membrane, and isotropic phases with the corresponding phase transitions were observed. The membrane and isotropic phases are present for  $N > N^*$ .  $T_{mem}^*(N)$  decreases from 340 K to 280 K for  $N \geq 8$ . For copolymers, the membrane phase is found when the fraction of F8 units is at least 90%,  $T_{mem}^*$  decreasing with this fraction. The membrane phase contains three material types: Loose sheets of two polymer layers, better packed beta phase and dissolved polymer. For  $N \geq 7$  and  $T < T_{mem}^*$  the tendency for membrane formation becomes stronger with increasing temperature [1].

[1] Knaapila et al. Phys. Rev. E 2008 77 051803

## Snell's Law for Shear Zone Refraction in Granular Materials

Henning A. Knudsen and Joakim Bergli

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Abstract: We present experiments on slow shear flow in a split-bottom linear shear cell, filled with layered granular materials. Shearing through two different materials separated by a flat material boundary is shown to give narrow shear zones, which refract at the material boundary in accordance with Snell's law in optics. The shear zone is the one that minimizes the dissipation rate upon shearing, i.e. a manifestation of the principle of least dissipation. We have prepared the materials as to form a granular lens. Shearing through the lens is shown to give a very broad shear zone, which corresponds to fulfilling Snell's law for a continuous range of paths through the cell.

## Steady-State Two-Phase Flow in Porous Media: Statistics and Transport Properties

Grunde Løvoll<sup>1</sup>, Ken Tore Tallakstad<sup>1</sup>, Henning Arendt Knudsen<sup>1</sup>, Thomas Ramstad<sup>2</sup>,  
Knut Jørgen Måløy<sup>1</sup>, Renaud Toussaint<sup>3</sup> and Eirik Grude Flekkøy<sup>1</sup>

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Abstract: We present results from an experimental study of continuously driven simultaneous two-phase flow in a two-dimensional porous media. The dynamics of the process is dominated by the interplay between the viscous pressure field in the highly viscous wetting fluid and bubble transport of a less viscous, non-wetting fluid. In contrast with more studied invasion processes, steady-state flow is in equilibrium, statistically speaking. The corresponding theoretical simplicity allows us to explain a data collapse in the cluster size distribution as well as the relation  $|\nabla P| \propto \sqrt{Ca}$  between the pressure gradient in the system and the capillary number.

## Gravitationally induced ordering of hectorite nanoplatelets

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### Abstract

Platelet-shaped particles of the synthetic clay sodium-fluorohectorite, suspended in saline solutions with varying salt concentrations, exhibit a rich phase behaviour with up to four phases coexisting in a single sample tube. The use of Small-Angle X-ray Scattering allows us to quantify the anisotropy in the system, and together with x-ray absorption measurements, this provides a precise determination of the phase boundaries, as well as a measure of the orientational ordering of the platelets in the various gel phases. The coexistence of different phases results from a sedimentation-induced vertical gradient in particle fraction. Quantitatively relating the vertical coordinate to the clay particle fraction in these samples allows determination of a phase diagram for these fluorohectorite systems, as a function of the particle volume fraction and salt concentration.