



# DIVISION OF X-RAY PHYSICS ANNUAL REPORT 2006



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# ANNUAL REPORT 2006

*Division of X-ray Physics  
Department of Physical Sciences  
University of Helsinki*

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EDITED BY KAISA KISKO

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# 1 Preface

*The main areas of research within the division are hard and soft condensed matter physics, biophysics and applied research including imaging. The research emphasis is on experimental and computational studies of radiation-matter interaction processes. X-ray based characterization techniques are used to explain the macroscopic properties of novel materials from fundamental principles. In addition to the versatile X-ray instrumentation in our laboratory, the synchrotron radiation based experiments play a vital role in our research activities.*

It is becoming obvious that knowledge of *static structures* of materials is not enough but *dynamics* and *functions* play progressively crucial role in novel materials science. This is obvious for biomaterials including the study of human body and functions as well as for modern electronics materials, for example. The development of multi-technique in-situ experiments shows up strongly also in our research profile. For example in 2006 is the PhD thesis of Liisa Porra on Lung Structure and Function Studied by Synchrotron Radiation. This work addressed the basic functions of breathing process as well as stages of asthma by utilizing high-brightness synchrotron radiation. Another example is the PhD work of Matti-Paavo Sarén on the structure of wood that required a combination of various experimental techniques in materials characterization. The structural information obtainable with x-rays plays a key role in understanding the macroscopic properties of wood, economically important matter. The third PhD thesis from our division during 2006 by Manuel Fernández on imaging of breast cancer tissue with synchrotron radiation also represents applied materials science where the importance and impact of the research are evident.

The success in the aforementioned and other multidisciplinary research projects is based on the fundamental understanding of various x-ray techniques and electronic structure whose study forms the backbone of our research activities. In more fundamental projects significant advances were made on the computational characterization of electronic structure via various x-rays scattering techniques while openings were also made to new materials including many complex engineered polymers. At the same time the structure of simple ordinary water still remained as a strong research field. For all research the synchrotron radiation based experimental activities continued on a large breadth. Our division continued to be the most active unit from Finland at the European Synchrotron Radiation Facility (ESRF, Grenoble, France) while we also utilized synchrotron radiation sources in Germany (HASYLAB), Japan (SPring-8) and Sweden (MAX).

May 3, 2007

Keijo Hämäläinen  
head of the division



## 2 Personnel

### Head of the division



**Hämäläinen, Keijo**

professor, ext. 50640  
experimental solid state physics, x-ray scattering  
and spectroscopy, synchrotron radiation

### Professors



**Annala, Arto**

professor, ext. 50629  
biophysics, protein structure determination, small-  
angle scattering, NMR spectroscopy



**Manninen, Seppo**

professor (acting), lecturer (on leave), ext. 50634  
x-ray scattering and spectroscopy, synchrotron ra-  
diation



**Serimaa, Ritva**

professor, ext. 50630  
weakly ordered materials, computational x-ray  
physics

### Emeritus professors



**Paakkari, Timo**

professor emeritus, ext. 50633  
powder diffraction, weakly ordered materials



**Suortti, Pekka**

professor emeritus, ext. 50633  
synchrotron radiation, medical applications

### Postdoctoral research scientists



**Hakala, Mikko**

Dr.Tech., research scientist, ext. 50625  
computational condensed matter and x-ray physics



**Soininen, Aleksis**

Ph.D., doctoral assistant, ext. 50631  
computational condensed matter and x-ray physics



**Torkkeli, Mika**

Ph.D., university lecturer, ext. 50643  
structure of materials, small-angle scattering

## Technical staff



**Blomberg, Merja**

Doc., senior laboratory manager, ext. 50635  
low-temperature crystallography, materials science



**Arar, Leith**

B.Eng., laboratory technician (1.1. – 11.5.)

## Graduate students



**Andersson, Seppo**

Lic.Phil., amanuensis, ext. 50655  
weakly ordered materials, structure of wood cells



**Fernández, Manuel**

M.Sc., PhD thesis in June 2006  
small-angle x-ray scattering, medical imaging



**Galambosi, Szabolcs**

M.Sc., assistant, ext. 50631  
x-ray scattering and spectroscopy



**Ikonen, Teemu**

M.Sc., research assistant (graduate school)  
nanoscale structures in biology



**Kisko, Kaisa**

M.Sc., research assistant (graduate school), ext. 50627  
structure of biomaterials



**Louhivuori, Martti**

M.Sc., research assistant, ext. 50727  
biophysics



**Mattila, Aleksi**

M.Sc., research assistant (graduate school), ext. 50625  
x-ray scattering and spectroscopy



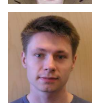
**Nygård, Kim**

M.Sc., research assistant, ext. 50632  
x-ray scattering and spectroscopy



**Peura, Marko**

M.Sc., assistant, ext. 50628  
weakly ordered materials



**Pirkkalainen, Kari**

M.Sc., research assistant, ext. 50638  
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**Porra, Liisa**

M.Sc., PhD thesis in April 2006, ext. 50628  
medical imaging

## Graduate students (continued)



**Pylkkänen, Tuomas** M.Sc., research assistant, ext. 50632  
x-ray scattering and spectroscopy



**Sakko, Arto** M.Sc., research assistant, ext. 50641  
x-ray scattering and spectroscopy



**Suhonen, Heikki** M.Sc., research assistant, ext. 50727  
scattering simulation, medical imaging



**Vainio, Ulla** M.Sc., research assistant (graduate school), ext. 50627  
small angle x-ray scattering, polymers

## Undergraduate students



**Leppänen, Kirsi** research assistant, ext. 50638  
structure of biomaterials



**Ruokola, Päivi** research assistant, ext. 50638  
biophysics



**Ruotsalainen, Kari** research assistant, ext. 50638  
x-ray scattering and spectroscopy

### 3 Research activities

#### 3.1 Hard condensed matter

#### Experimental local density of electronic states in diamond

S. Galambosi, J. A. Soininen, K. Nygård, S. Huotari<sup>1</sup> and K. Hämäläinen

We have exploited the  $q$ -dependence of the IXS spectrum to study the electronic angular momentum projected unoccupied local density of states ( $\ell$ DOS) in diamond. We measured the IXS spectrum using three  $q$ -values with  $\omega$  close to the carbon 1s electron binding energy. The experiments were carried out on the beamline ID16 at the European Synchrotron Radiation Facility, Grenoble, France.

The  $q$ -dependent IXS spectra together with the theoretically calculated transition matrix elements were used following a recently proposed scheme\* to find the final state  $\ell$ DOS. The experimental  $s$ - and  $p$ DOS of diamond were obtained over an energy range of 30 eV above the 1s absorption threshold.

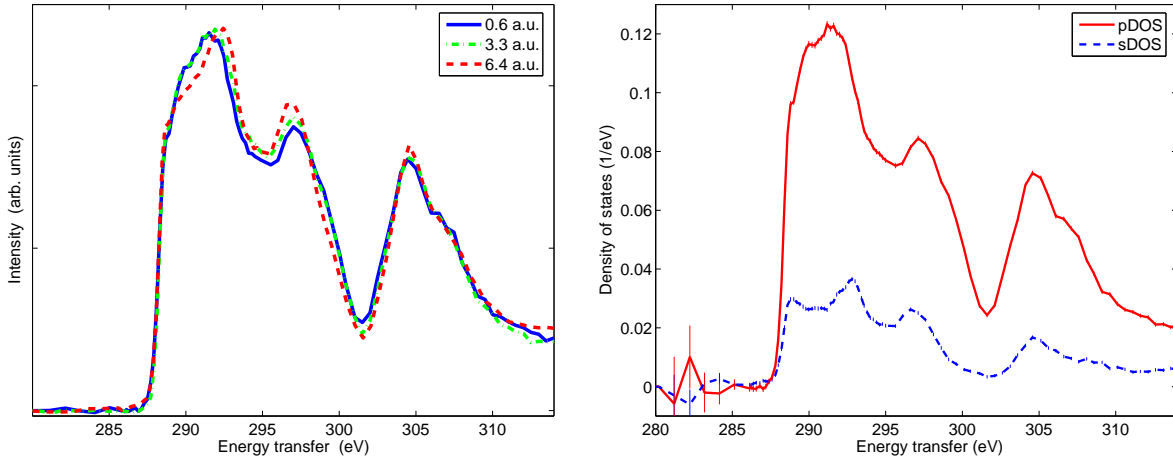


Fig. 1. The momentum transfer dependence of the IXS spectrum (left) is used to extract the angular momentum projected unoccupied local density of states (right).

We analyzed in detail the stability of this angular momentum projected decomposition scheme against some experimental factors. The effect of the finite statistical accuracy of the experimental data on the resulting  $\ell$ DOS was derived. We also studied how various ways to normalize the data affect the results.

\* J. A. Soininen *et al.*, *J. Phys.: Condens. Matter* **18** (2006), 7327.

<sup>1</sup> ESRF, Grenoble, France

## Valence electron momentum density studies with the PAW method

I. Makkonen<sup>1</sup>, M. Hakala, K. Hämäläinen, S. Manninen and M. J. Puska<sup>1</sup>

Calculations for valence electron momentum densities within the supercell approach\* have been continued. Density-functional theory, plane-wave basis and projector-augmented wave (PAW) method are employed using the VASP code. Extension to calculate momentum distributions of annihilating positron-electron pairs in solids has been accomplished<sup>†,‡</sup>.

\* I. Makkonen, M. Hakala, and M. J. Puska, *J. Phys. Chem. Solids* **66** (2005), 1128.

† I. Makkonen, M. Hakala, and M. J. Puska, *Phys. Rev. B* **73** (2006), 035103.

‡ I. Makkonen, M. Hakala, and M. J. Puska, *Physica B* **376-377** (2006), 971.

<sup>1</sup> Helsinki University of Technology

## Form factor for molecular systems from density functional theory

A. Sakko, M. Hakala and K. Hämäläinen

We have developed a new program for calculating the form factor for atom clusters and molecules. Our program uses Gaussian type orbitals and the electronic structure is solved with an all-electron density functional theory code STOBE-DEMON\*. The program can be used to calculate the molecular form factors for systems up to about 200 light atoms. The program is currently used in the study of the structure of water at the University of Stockholm. The method can also be utilized in the diffraction studies of polymers and molecular materials.

\* K. Hermann *et al.*, *StoBe-deMon version 2.1.*, StoBe Software (2005).

## A computational study of X-ray Raman scattering from aromatic molecules and polyfluorene

A. Sakko, M. Hakala, J. A. Soininen and K. Hämäläinen

We have used our recently developed computational method for studying X-ray Raman scattering (XRS) from several aromatic hydrocarbon molecules and aligned polyfluorene. The method is based on the transition potential approximation within density functional theory\*. We found that our calculated results are in a good agreement with the previously published<sup>†,‡</sup> experimental spectra. With the use of our results we were able to study the orientation and the symmetry properties of the unoccupied electronic states, which play an important role in determining the electrical properties of condensed matter. This analysis shows that the method is well suited for studying XRS from several molecular systems. We plan to apply our method for new systems, such as other organic molecules and liquids, in the future.

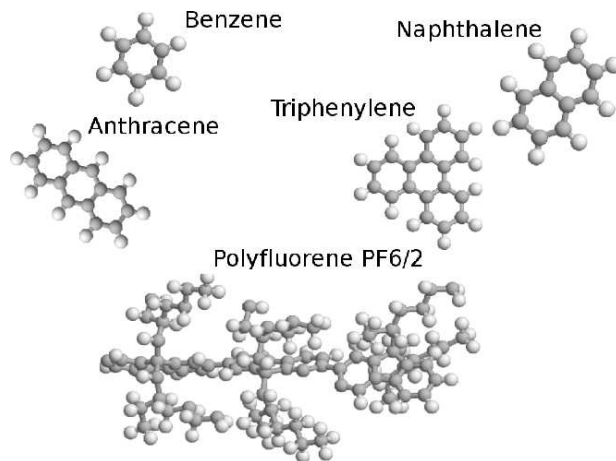


Fig. 2. We have performed a computational study of X-ray Raman scattering from a set of organic molecules and a polymer.

\* K. Hermann *et al.*, *StoBe-deMon version 2.1.*, StoBe Software (2005).

† M. L. Gordon *et al.*, *J. Phys. Chem. A* **107** (2003), 8512.

‡ S. Galambosi *et al.*, *Macromolecules* **39** (2006), 9261.

## Background Proportional Enhancement of the Extended Fine Structure in Nonresonant Inelastic X-ray Scattering

T. T. Fister<sup>1</sup>, G. T. Seidler<sup>1</sup>, C. Hamner<sup>1</sup>, J. O. Cross<sup>2</sup>, J. A. Soininen and J. J. Rehr<sup>1</sup>

The early works of non-resonant x-ray Raman scattering (XRS) were done at low momentum transfer limit i.e. probing only the dipole type final states. The great success of these works was that they were able to show the equivalence of XRS studies with extended x-ray absorption fine structure (EXAFS) studies. This suggests that the XRS could be used as an alternative to EXAFS. However, the x-ray Raman scattering is a relative weak process meaning the weak fine structures high above the edge are experimentally arduous to observe. In the recent work\* we were able to show that by increasing the momentum transfer in XRS we can enhance the fine structure in the extended energy range. This makes the initial weak EXAFS oscillations readily observable in XRS. This observation was also confirmed by theoretical calculations based on our earlier work†.

\* T. T. Fister *et al.*, *Phys. Rev. B* **74** (2006), 214117.

† J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, *Phys. Rev. B.* **72** (2005), 045136.

<sup>1</sup> Department of Physics, University of Washington, USA

<sup>2</sup> Argonne National Laboratory, USA

## Inelastic X-ray scattering studies of methane and tetrahydrofuran hydrate

C. Sternemann<sup>1</sup>, F. Lehmkuhler<sup>1</sup>, **A. Sakko**, **M. Hakala**, S. Huotari<sup>2</sup>, M. Paulus<sup>1</sup>, M. Volmer<sup>1</sup>, C. Gutt<sup>1</sup>, T. Buslaps<sup>2</sup>, N. Hiraoka<sup>2</sup>, D. D. Klug<sup>3</sup>, **K. Hämäläinen**, M. Tolan<sup>1</sup> and J. S. Tse<sup>4</sup>

Clathrate hydrates are crystalline structures in which gaseous guest atoms or molecules are trapped in a water cage-like structures at low temperatures and high pressures. These structures have appeared to be widespread in the nature, thus attracting scientific interest. They are important also from a technological point of view, because of their potential use as sources of energy warrants\*. Although the formation of the water cage is very important for the applications, the physical process is a somewhat unknown subject. Recently we have completed our Compton scattering study of methane hydrate<sup>†</sup>. It was shown that the guest-host interaction as well as the formation of the water cage influences the Compton profile. We have begun the Compton and X-ray Raman scattering studies of tetrahydrofuran (THF) hydrate. Combining experimental and computational studies, our aim is to elucidate the electronic properties of this compound and obtain information of its formation.

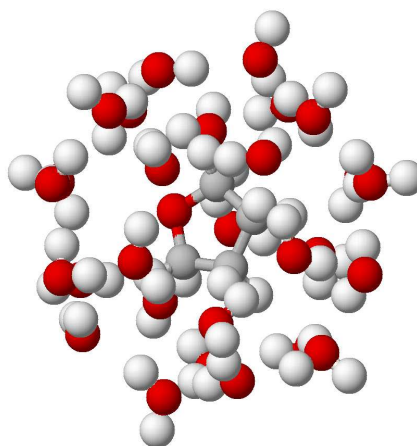


Fig. 3. At low temperature and high pressure, a tetrahydrofuran (THF) molecule can be trapped in a water cage structure and a crystalline molecular compound, THF hydrate, is formed.

<sup>1</sup> Department of Physics/DELTA, University of Dortmund, Germany

<sup>2</sup> European Synchrotron Radiation Facility, Grenoble, France

<sup>3</sup> Stacie Institute of Molecular Science, National Research Council of Canada, Ottawa, Canada

<sup>4</sup> Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, Canada

\* W. L. Mao and H.-K. Mao, *Proc. Natl. Acad. Sci. U.S.A.* **101** (708), 2004.

† C. Sternemann *et al.*, *Phys. Rev. B* **73** (195104), 2006.

## Symmetries of the final state density matrix

**J. A. Soininen**, T. T. Fister<sup>1</sup>, G. T. Seidler<sup>1</sup>, J. J. Rehr<sup>1</sup> and **K. Hämäläinen**

Following the recently proposed scheme\* we have determined the final state angular momentum projected local density of states ( $\ell$ DOS) at the boron site in MgB<sub>2</sub>.<sup>†</sup> This scheme relies on the close connection between the final state density matrix  $\rho_{LL'}(E)$  and the x-ray Raman scattering (XRS) spectrum. From the momentum transfer dependence of experimental XRS spectra we are able to extract  $\rho_{LL'}(E)$  and use it to determine  $\ell$ DOS.

An important approximation we made in our previous work<sup>†</sup> was that we assumed the density matrix to be diagonal, i.e.  $\rho_{LL'}(E) \approx \rho_{LL}(E)\delta_{LL'}$ . However, this approximation is exact only in randomly oriented systems such as powders and liquids. In highly oriented system like single-crystals this is only approximately true. We have developed a symmetry analysis that enables us to determine all the independent and non-zero elements of  $\rho_{LL'}(E)$  once the symmetry operations of the system are known. In the future this method will be important by reducing the number of independent parameters when trying to determine the non-diagonal components of  $\rho_{LL'}(E)$ .

\* J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, *Phys. Rev. B* **72** (2005), 045136.

† J. A. Soininen, J. J. Rehr, S. Galambosi, A. Mattila, and K. Hämäläinen, *J. Phys: Condens. Matter* **16** (2006), 7327.

<sup>1</sup> Department of Physics, University of Washington, USA

## Modeling RIXS with real-space multiple scattering

**J. A. Soininen**, J. J. Rehr<sup>1</sup> and **K. Hämäläinen**

In resonant inelastic x-ray scattering (RIXS) the electronic structure of a sample is studied by tuning the incident energy close to the absorption edge of the sample and observing the emitted photon. RIXS has become increasingly more popular in recent years due to its versatility. Besides obviously being element specific, RIXS can also be used to obtain additional information through the site and spin selectivity of the scattering process.

We have started a long term development project to apply real-space multiple scattering theory (RSMS) to modeling of RIXS. The work is based on the FEFF code which in the past has been successfully applied to modeling e.g. x-ray absorption, x-ray emission and non-resonant inelastic x-ray scattering.\*<sup>†</sup> The strength of RSMS approach is that it is applicable to aperiodic and periodic systems alike. In practice this means that it can be applied to systems ranging from biological samples to different kinds of solids. When completed this approach will give a valuable and practical tool for modeling RIXS.

\* A. L. Ankudinov *et al.*, *Phys. Rev. B* **58** (1998), 7565.

† J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, *Phys. Rev. B* **72** (2005), 045136.

<sup>1</sup> Department of Physics, University of Washington, USA

## Crystal spectrometers for Compton scattering studies

P. Suortti, T. Buslaps<sup>1</sup>, V. Honkimäki<sup>1</sup>, N. Hiraoka<sup>2</sup> and U. Lienert<sup>3</sup>

The design and performance of focusing crystal spectrometers for Compton scattering studies are reviewed. In the modern spectrometers large perfect crystal analyzers and efficient detectors are used. The reflectivity and energy resolution of the analyzer can be tailored to the needs of the experiment by the asymmetric cut, thickness and bending radius of the crystal, and the response function of the spectrometer can be calculated precisely. The latest developments at the ESRF and Spring-8 synchrotron radiation laboratories include spectrometers that operate in the 100 keV range, and count rates are enhanced by wide energy bands and dispersion compensation. Results obtained by a scanning reflection-type spectrometer installed at a rotating-anode X-ray generator demonstrate that accurate Compton profiles of light-element compounds can be determined even with a laboratory instrument. A map of the reciprocal form factor of silicon is constructed from 10 directional Compton profiles, and the map reveals details of chemical bonding.\*

\* P. Suortti *et al.*, *Z. Phys. Chem.* **220** (2006), 831-847.

<sup>1</sup> ESRF, Grenoble, France

<sup>2</sup> SPring-8, Hyogo, Japan

<sup>3</sup> APS, Argonne, USA

## 3.2 Soft condensed matter

### Self-assembled films of hydrophobin protein HFBIII

K. Kisko, G. R. Szilvay<sup>1</sup>, E. Vuorimaa<sup>2</sup>, H. Lemmetyinen<sup>2</sup>, M. B. Linder<sup>1</sup>, M. Torkkeli and R. Serimaa

Hydrophobins are a group of very surface active proteins. They have an amphiphilic structure and self-assemble on air/water interface. Hydrophobins contain typically eight cysteine residues, making four disulfide bridges. A new hydrophobin, HFBIII from *Trichoderma reesei*, has one extra cysteine, giving the protein a naturally reactive site.

Self-assembled films of HFBIII were studied on an air/water interface (ESRF, ID10B) and a silicon substrate (HasyLab, W1) using grazing-incidence x-ray diffraction and reflectivity. The hydrophobins form hexagonally ordered films with similar lattice constants on both cases. The film on air/water interface is a monolayer and on silicon a few monolayers thick.\*

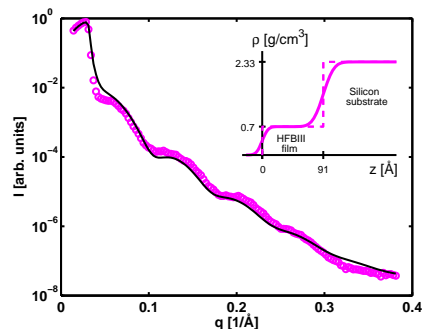


Fig. 4. Reflectivity curve of HFBIII on silicon substrate, showing the film thickness of 90 Å, and the fit using a box model (insert).

\* K. Kisko *et al.*, *J. Appl. Cryst.*, in press.

<sup>1</sup> VTT Biotechnology, Espoo, Finland

<sup>2</sup> Department of Materials Chemistry, Tampere University of Technology, Finland

### Structural studies of aqueous lignosulfonate solutions

U. Vainio, R. A. Lauten<sup>1</sup> and R. Serimaa

Lignosulfonate is a negatively charged colloidal polyelectrolyte that is formed from lignin during sulfite pulping of wood. Lignin is a complex branched polymer that holds the wood fibres together and is an important component of the wood cell wall.

Interactions between fractionated lignosulfonate particles (polydispersity 2.1) were studied in water and in 0.2 M NaCl aqueous solution using small-angle x-ray scattering and rheology. The studied concentrations of the polyelectrolyte ranged from semidilute to concentrated.

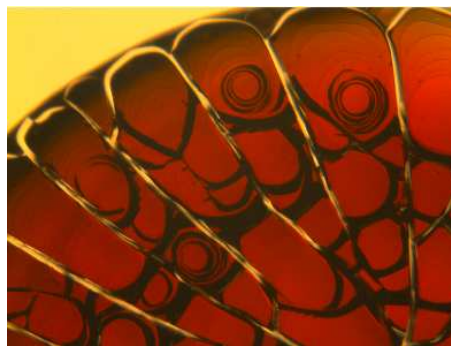


Fig. 5. A microscope image of dried lignosulfonate solution.

<sup>1</sup> Borregaard Lingotech, Norway

## Structure of cobalt nanoparticles in microcrystalline cellulose matrix using EXAFS and WAXS

K. Leppänen, K. Pirkkalainen, U. Vainio, N. Kotelnikova<sup>1</sup> and R. Serimaa

Cobalt nanoparticles synthesized into a microcrystalline cellulose matrix were examined using wide angle x-ray scattering (WAXS) and extended x-ray absorption fine structure (EXAFS) measurements. Particles were manufactured by using two different kinds of reducers,  $\text{NaH}_2\text{PO}_2$  and  $\text{NaBH}_4$ . The EXAFS measurements were analyzed by the standard data procedures using VIPER\* computer program and theoretical calculations using FEFF-code. The k-space fitting procedure was then made by VIPER.

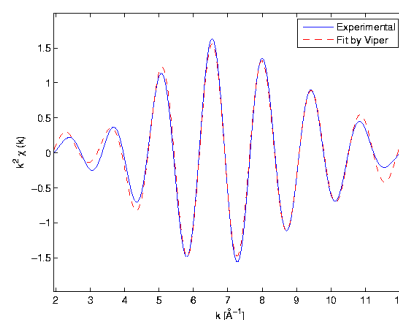


Fig. 6. A first two shells fit of EXAFS oscillations from sample reduced with  $\text{NaH}_2\text{PO}_2$ .

The crystallinity of the MCC matrix is not affected by the synthesis of cobalt particles according to the x-ray diffraction measurements. The cobalt in the samples reduced with  $\text{NaH}_2\text{PO}_2$  is in hcp form on the basis of the positions of the diffraction peaks. EXAFS-analysis indicated reduced coordination numbers for these particles. X-ray diffraction measurements did not reveal any well-defined diffraction maxima for the cobalt samples which were reduced using  $\text{NaBH}_4$ . X-ray absorption measurements indicated oxidation of these particles and reduced coordination numbers compared to bulk material.

\* K. V. Klementiev, *J. Phys. D: Appl. Phys.* **34** (2001), 209-17.

<sup>1</sup> Institute of Macromolecular Compounds, Russian Academy of Sciences, Russia

## Novel measurement setup for monitoring the rigidity and the crystallisation of a polymer suspension *in situ* during solvent evaporation

Marko Peura, Timo Karppinen<sup>1</sup>, Edward Haeggström<sup>1,2</sup>, Maija Tenkanen<sup>3</sup> and Ritva Serimaa

Polymer films are very important for numerous industrial and scientific end-uses. In order to understand the relationship between the mechanical properties and the structure of such films during formation, a measurement setup was developed that allowed to concurrently monitor the temporal development of the rigidity of a polymer suspension *in situ* with the crystallisation of the suspension. The crystallisation was determined by x-ray diffraction (XRD) and the rigidity by measuring the shear modulus of the suspension by ultrasonic reflection.

As a test of the measurement scheme, five parallel samples of a xylan suspension (distilled water, 10 g/L xylan, 4 g/L glycerol) were studied at  $24 (\pm 2) ^\circ\text{C}$ ,  $37 (\pm 5) \% \text{RH}$ .

In these conditions, the suspensions formed 73 - 87 ( $\pm 2$ )  $\mu\text{m}$  thick solid films via water evaporation.

The crystallisation and the temporal development of the shear modulus of the xylan suspension samples were successfully monitored. Both processes occurred in three stages as a function of time and exhibited an active period between two nearly idle periods. The crystallisation occurred in 80 - 110 minutes after an idle period of 80 - 125 minutes, while the increase in the shear modulus took place in 25 - 30 minutes after an idle period of 150 - 215 minutes. The maximum value of the shear modulus was 0.1 - 0.5 GPa. The difference in the duration of the second stage between crystallisation and the increase in the shear modulus is likely due to the effect of water content of the film on the shear modulus and possibly also due to the effect of entanglement and cross-linking of the polymer chains on the shear modulus. XRD measurements performed *ex situ* on dry samples showed that the crystallinity of the films was 15 - 19 ( $\pm 5$ ) % and that there was a fairly isotropic orientation of the crystallites in the surface plane.

<sup>1</sup> Department of Physical Sciences, University of Helsinki

<sup>2</sup> Helsinki Institute of Physics, University of Helsinki

<sup>3</sup> Division of General Chemistry, Department of Applied Chemistry and Microbiology, University of Helsinki

## Structure of transition metal nanoparticles in microcrystalline cellulose matrix

**K. Pirkkalainen, U. Vainio, N. E. Kotelnikova<sup>1</sup> and R. Serimaa**

Nanosized transition metal particles were manufactured by chemical reduction within a microcrystalline cellulose matrix. The porous cellulose matrix was introduced to act as a nanoreactor for nanoparticle formation, as a deterrent for spontaneous oxidation and irreversible aggregation of particles. Different chemical reduction agents were used, and so-formed nanoparticles were characterized with x-ray diffraction, anomalous small-angle x-ray scattering, x-ray absorption spectroscopy, scanning electron microscopy and vibrating sample magnetometer. These experimental techniques were used to gain insight into the effect of different synthesis routes on nanoparticle size distribution, shape, oxidation state and magnetic behavior. Transition metals used to manufacture the particles in our study include copper<sup>\*</sup>, nickel<sup>†</sup> and cobalt.

As an example, our latest results on the nickel nanoparticles are presented. Nickel nanoparticles were manufactured by adding aqueous nickel salt into microcrystalline cellulose matrix, in which the Ni-ions were chemically reduced with sodium borohydride,  $\text{NaBH}_4$ , or potassium hypophosphite,  $\text{KH}_2\text{PO}_2$ , in water or aqueous ammonium medium. The so-manufactured nanoparticles were mostly in nanocrystalline or amorphous metallic phase, but heating the samples revealed several coexisting crystalline phases, such as fcc Ni, hcp Ni, NiO,  $\text{Ni}_3\text{P}$ , and others, which are possibly metastable phases of Ni-P. Measurements on magnetic properties showed that the samples were paramagnetic or ferromagnetic depending on the synthesis route. The synthesis had

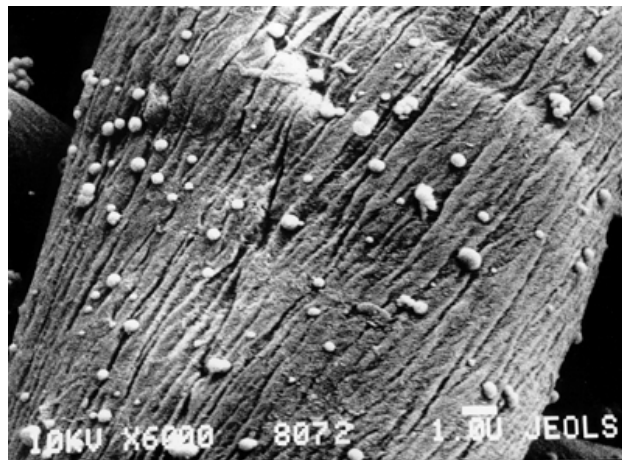


Fig. 7. The  $\mu\text{m}$ -scale structure from one of the nickel samples obtained by scanning electron microscopy. The small white spheres contain nickel and the structure at the background is the fibrous cellulose matrix. The scale bar is  $1\ \mu\text{m}$  in length.

no distinct effect on the structure of the cellulose matrix.

\* U. Vainio *et al.*, *Eur. Phys. J. D*, in press.

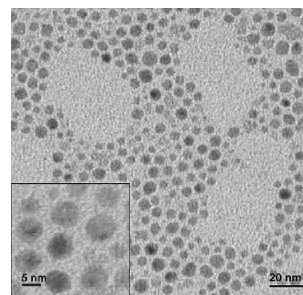
† K. Pirkkalainen *et al.*, *J. Appl. Cryst.*, in press.

<sup>1</sup> Institute of Macromolecular Compounds, Russian Academy of Sciences, Russia

## Characterization of CoAg-nanoparticles with a proposed core-shell morphology

K. Pirkkalainen, T. Laaksonen<sup>1</sup> and R. Serimaa

Chemically manufactured CoAg-nanoparticles were characterized with wide-angle x-ray scattering, anomalous small-angle x-ray scattering, x-ray absorption spectroscopy and transmission electron microscopy (figure to the right). The motivation for the study was to show the existence of a core-shell structure, in which the noble metal silver would form a protective thin layer around a spherical cobalt core. In the case of a perfect silver coverage, the cobalt core should retain its metallic phase. Imperfect coverage should result in oxidized cobalt particles.



Preliminary studies with aforementioned experimental methods implied that at least four different morphology models could be applied for the studied particles (Fig. 8): a) complete silver layer around the cobalt core, b) incomplete silver layer around the cobalt core, c) aggregation of cobalt on the surface of silver particles, d) separate phases of silver and cobalt particles. A thorough analysis of the accumulated data indicated that the most probable morphologies for the studied CoAg-particles are alternatives c) and/or d). The distinction between these two morphologies could not be made using the currently collected experimental data. In any case, the proposed core-shell morphology, in which the cobalt stays protected from oxidation and other chemical

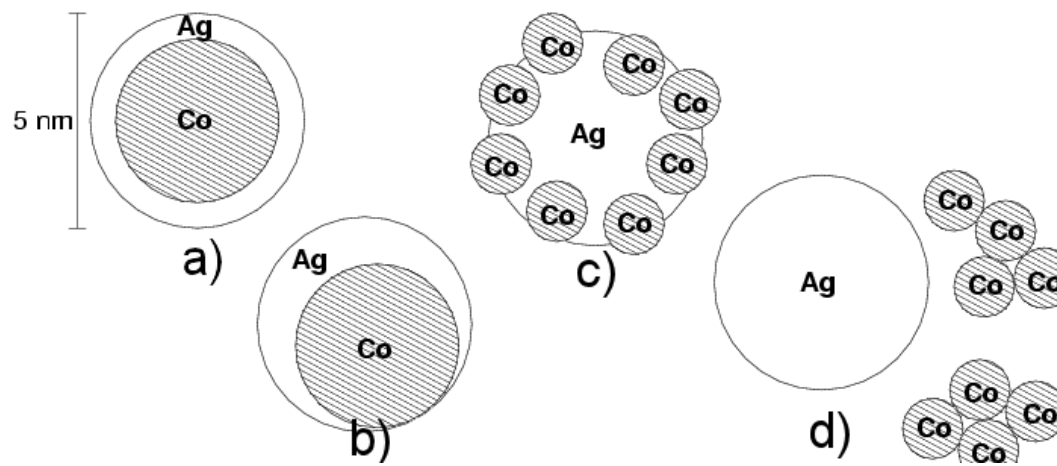


Fig. 8. Possible morphologies for the studied nanoparticles.

reactions, seems a highly unlikely alternative.

<sup>1</sup> Laboratory of Physical Chemistry and Electrochemistry, Helsinki University of Technology

### 3.3 Atomic and molecular physics

#### Prediction of new cyanide and dicarbide compounds

M. Hakala, P. Zaleski-Ejgierd<sup>1</sup> and P. Pyykkö<sup>1</sup>

Cyanides  $MCN$ ,  $M=Cu, Ag, Au$ , have experimentally a structure with hexagonally packed, infinite  $-M-CN-M-CN-$  chains. The valence isoelectronic systems  $MC_2$ ,  $M=Mg-Ba$ , are also known to exist in chain structures. We have predicted that solid gold cyanide  $AuCN$  could have an alternative planar crystal structure, of almost the same energy as the known one\*. Following this work, we have predicted the existence of new planar structures for cyanides involving group 11 coinage metals and dicarbides involving group 2 and 12 metals<sup>†</sup>. For some new structures the densities of states suggests small band gaps and even metallic character. When available, the experimental geometries agree well with the calculated ones for both cyanides and dicarbides. Density-functional theory, plane-wave basis and projector-augmented wave (PAW) method are employed using the VASP code.

\* M.O. Hakala and P. Pyykkö, *Chem. Comm.* (2006), 2890.

† M. Hakala, P. Zaleski-Ejgierd and P. Pyykkö, *Phys. Rev. B*, submitted.

<sup>1</sup> Laboratory for Instruction in Swedish, Department of Chemistry, University of Helsinki

#### Local structure of molecular liquids by Compton scattering

K. Nygård, M. Hakala, T. Pylkkänen, S. Manninen, T. Buslaps<sup>1</sup>, M. Itou<sup>2</sup>, A. Andrejczuk<sup>2</sup>, Y. Sakurai<sup>2</sup>, M. Odelius<sup>3</sup> and K. Hämäläinen

The project on structural studies of molecular liquids by Compton scattering was continued. The experimental work concentrated on liquid water, with studies on the isotope quantum effects being carried out. Moreover, a Compton scattering study on the high-pressure effects in water was also performed. The computational analysis based on the density-functional theory was refined by inclusion of *ab initio* Car-Parrinello molecular-dynamics configurations. The project will be extended to simple alcohols and their aqueous solutions in the near future.

Compton scattering is sensitive to both the intra- and intermolecular structure of water\*. By comparing normal ( $H_2O$ ) and heavy ( $D_2O$ ) water Compton profiles, the technique is found to primarily provide intramolecular structural information on the isotope quantum effects in water. Moreover, the distinctly different temperature evolution of the  $H_2O$  and  $D_2O$  Compton profiles is interpreted as predominantly reflecting intramolecular structural effects. The temperature-induced changes in the Compton profile of  $D_2O$  can be qualitatively reproduced by a Car-Parrinello molecular-dynamics approach, the quantitative disagreement possibly implying a necessity of including nuclear quantum effects. The high-pressure Compton-scattering experiment on water clearly demonstrated the demerits of diamond-anvil cells for such experiments; hence, a refined experiment using a large-volume cell will be carried out shortly.

\* See, e.g., M. Hakala *et al.*, *Phys. Rev. B* **73** (2006), 035432.

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<sup>2</sup> SPring-8, Hyogo, Japan

<sup>3</sup> Department of Physics, Stockholm University, Sweden

## Modeling the size-selected growth of nanosized clusters with reaction kinetics

K. Pirkkalainen and I. T. Koponen<sup>1</sup>

The size-selection of nanoclusters during growth stage was studied by computer simulations. The reaction kinetic model\* (RKM) and classic Becker-Döring (BD) kinetics<sup>†</sup> were used to study the time evolution of size distributions with a pre-deposited adatom concentration. In both models, the nanocluster growth was described only by adatom attachment and detachment processes. These processes were governed by self-consistent reaction rates, which fulfill the condition of detailed balance\*.

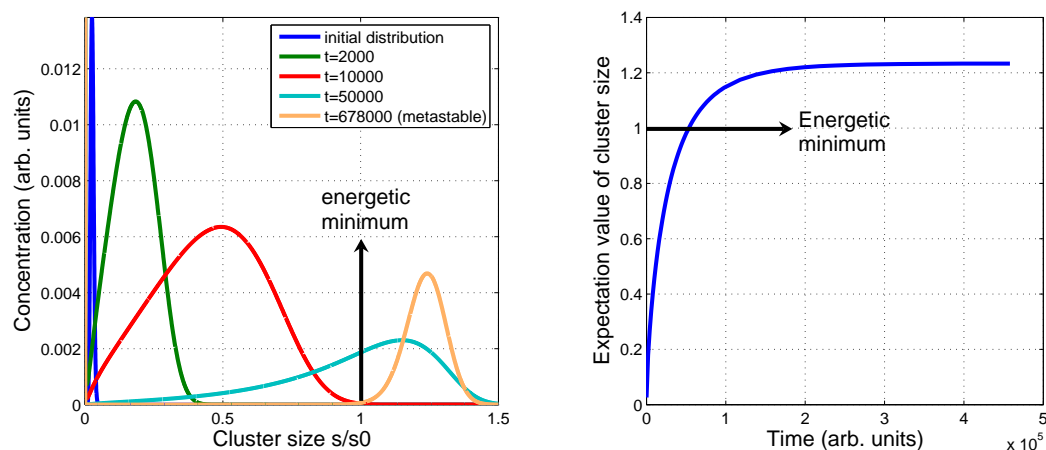


Fig. 9. Time evolution of cluster sizes according to the BD model. Cluster sizes  $s$  are normalized according to the energetic minimum cluster size  $s_0$ .

The motivation for the study was to develop a fast and efficient way to calculate the discrete set of equations which corresponds to the RKM and BD models. We applied a discretization scheme proposed by Grima *et al.*<sup>‡</sup>, in which the rate constants of attachment and detachment of a single size cell are governed only by the “hopping” rates from nearest neighbor sites. The method is often referred as the Master Equation Discretization (MED) scheme, and it allows better numerical efficiency without the loss of accuracy. The MED scheme typically allows spatial grid scales between two and four times larger than any traditional discretization schemes. Our future plans include the use of these “coarsed-grain” simulations to complement the experimental results on the growth of metallic nanoclusters and polymer aggregates.

\* K. A. Nevalainen, M. Rusanen and I. T. Koponen, *Phys. Rev. B*, submitted.

<sup>†</sup> J. J. L. Velázquez, *J. Stat. Phys.* **92** (1998), 195-236.

<sup>‡</sup> R. Grima and T. J. Newman, *Phys. Rev. E* **70** (2004), 70-79.

<sup>1</sup> Department of Physical Sciences, University of Helsinki

## 3.4 Medical and biophysics

### Analyzer Based Imaging (ABI) of Breast Tissue

**M. Fernández**<sup>1</sup>, J. Keyriläinen<sup>1</sup>, **H. Suhonen**, A. Bravin<sup>1</sup>, S. Fiedler<sup>2</sup>, M.-L. Karjalainen-Lindsberg<sup>3</sup>, M. Tenhunen<sup>4</sup>, M. Leidenius<sup>5</sup>, K. von Smitten<sup>5</sup>, **M. Torkkeli**, **R. Serimaa**, T. H. Weiss<sup>1</sup> and **P. Suortti**<sup>1</sup>

Analyzer based imaging (ABI) utilizes refraction and scattering of x-rays to get better contrast for soft tissues. This is especially important in diagnosis of breast cancer, as the density differences involved are small. Refraction signal is sensitive to interfaces of different tissue types. Scattering signal gives indication of nanoscale structural changes, reflecting often the progression of some pathology.

In dedicated SAXS experiments from thin in vitro samples, the changes in the scattering patterns are easy to observe\*. In imaging however, the thick sample gives rise to much scattering from different tissues and small changes in the scattering patterns are difficult to observe. Simulation studies of scattering in realistic imaging situations have been done.

A model based on pseudo-Voigtian (pV) functions has been developed, based on beam interactions within the sample and at the analyzer crystal. The observed beam is divided into scattered and directly transmitted components and both of these are represented by a pV. The intensity ratio of the compounds gives information about the total amount of scattering, and the width of the scattering pV curve indicates structural changes on the molecular level.

\* M. Fernández *et al.*, *Phys. Med. Biol.* **50** (2005), 2991-3006.

<sup>1</sup> ESRF, Grenoble, France

<sup>2</sup> EMBL, Hamburg, Germany

<sup>3</sup> Department of Pathology, HUCH, Finland

<sup>4</sup> Department of Physics, HUCH, Finland

<sup>5</sup> Breast Surgery Unit, Maria Hospital, HUCH, Finland

### Functional Lung Imaging with Synchrotron Radiation

**Liisa Porra**<sup>1</sup>, **Satu Strengell**, **Heikki Suhonen**, **Pekka Suortti**, Sam Bayat<sup>2</sup>, Tibor Janosi<sup>3</sup>, Ferenc Petak<sup>3</sup>, Walid Habre<sup>3</sup> and Anssi Sovijärvi<sup>4</sup>

Functional lung imaging uses xenon K-absorption edge subtraction (KES) imaging to obtain the absolute gas content distribution within lungs. High spatial resolution (0.1 mm<sup>3</sup>) and good time resolution (1 s / CT slice) allow quantification of dynamical effects at high level of detail\*. Current application of the method is in studying the basic lung physiology.

A new long term proposal (LTP) was accepted at the ESRF, which gives the possibility for several experimental runs during the next two years. Project entered a new phase by adopting a sensitized animal model for better understanding of lung diseases. First

experiments with the sensitized animals were carried out in December 2006.

New collaboration was started with a team from Geneva to measure lung mechanics parameters accurately during imaging. A forced oscillation (FO) setup was used to measure lung resistance and elastic properties. The first results indicate that the FO measurements have good correspondence with the values calculated from the images.

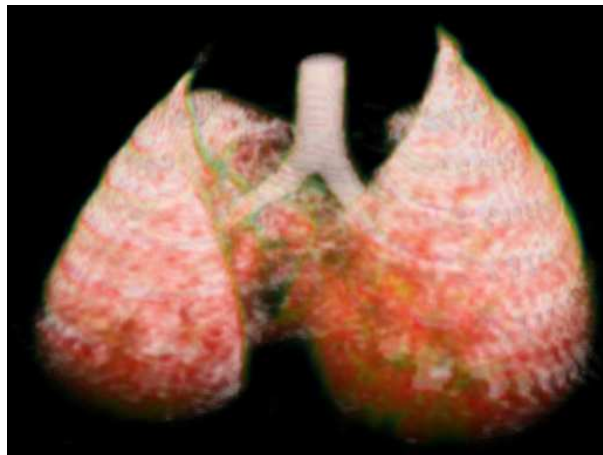


Fig. 10. The gas content in a healthy rabbit lung.

\* S. Bayat *et al.*, *J. Appl. Physiol.* **100** (2006), 1964-1973.

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<sup>2</sup> CHU Nord, Amiens, France

<sup>3</sup> University Hospital of Geneva, Geneva, Switzerland

<sup>4</sup> Helsinki University Central Hospital

## Evidence of molecular alignment fluctuations in aqueous dilute liquid crystalline media

M. Louhivuori, R. Otten<sup>1</sup>, K. Lindorff-Larsen<sup>2</sup>, T. Salminen and A. Annala

NMR measurements of biomolecules in dilute liquid crystal media are routinely done in order to obtain scalar and dipolar couplings, that give structural information of the molecule. The measured signal is a combination of all the individual signals from each of the horde of molecules present in the sample. All the molecules in a sample are undergoing various internal and external motions, from bond librations to translational diffusion. Liquid state NMR measurements report on these motions as an average over the molecules in a sample.

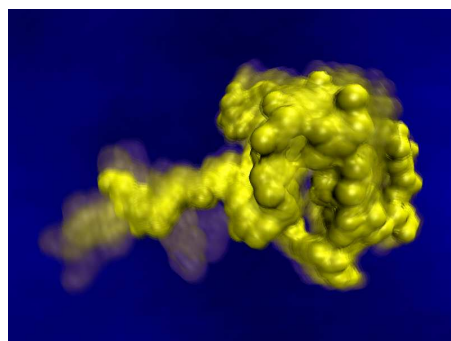


Fig. 11. Human ubiquitin protein undergoing structural fluctuations due to internal motions.

Each and every conformation has its own unique effective alignment, i.e. an effective orientation relative to the magnetic field. This is essentially what is captured by the measured signal. Because the effective alignment of the various conformations of a stable, folded protein are nearly the same, it has been assumed that the alignment fluctuations do not influence the interpretation of RDC data significantly. We have recently shown\* that this is not universally so.

*Novel* nanosecond–microsecond internal motions have been recently inferred† from RDC data. The hypothesis for these large-scale correlated secondary-structure motions is partly inspired by recent RDC based evidence of lower than expected order parameters. Alas, in these studies the effects of dynamics modulated alignment (DMA) are neglected. We have looked for evidence of dynamics modulated alignment from experimental data and have concluded‡ that the lower order parameters are explained at least in part by DMA.

\* M. Louhivuori, R. Otten, K. Lindorff-Larsen and A. Annala, *J. Am. Chem. Soc.* **128** (2006), 4371–4376.

† N. A. Lakomek, C. Farés, S. Becker, T. Carlomagno, J. Meiler and C. Griesinger, *Angew. Chem. Int. Ed.* **44** (2005), 7776–7778.

‡ R. Otten, M. Louhivuori, T. Salminen and A. Annala, *J. Biomol. NMR*, submitted.

<sup>1</sup> GBB, University of Groningen, Netherlands

<sup>2</sup> Institute of Molecular Biology and Physiology, University of Copenhagen, Denmark

## Natural Statistics of Open Systems

V. Sharma<sup>1</sup> and A. Annala

The theory of evolution by natural selection provides an overall picture of Life and a unifying description of biodiversity on Earth. Charles Darwin's insight has stood the test of time remarkably well, even strengthened by the wealth of data from recent genome sequencing projects. The theory, despite its central role in biology, has remained without a firm mathematical formulation in terms of physics. Consequently our understanding of complex nature has remained obscure and imprecise.

Recently we succeeded in formulating statistics for open systems\*. We find that evolution is a natural process, i.e. a course of events where matter moves towards more probable states via chemical reactions. Consequences of increasing entropy under an influx of external energy are easy to demonstrate and to analyze using simulations. The principle of increasing entropy can be applied at all scales hence the natural statistics is valid for large and complicated systems as well. We find entropy of an open system to increase in processes that identify with proliferation, differentiation, expansion, energy intake and adaptation. To reach high-entropy states of metastable diversity, matter organizes spontaneously in functional structures. We identify the rate of entropy production as the fitness criterion of natural selection. Biological mechanisms, functions and structures have no meaning as such but their existence is only warranted by their ability to reach and maintain high-entropy states. This break through in theoretical understanding sheds light on the primordial emergence of life, fundamental laws gov-

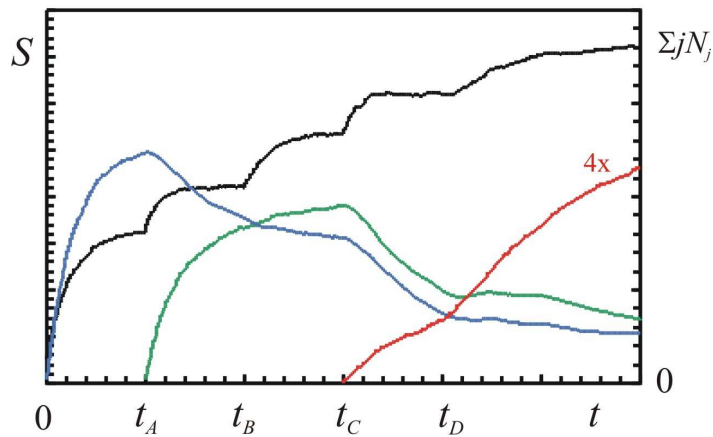


Fig. 12. Entropy of an open system obtained from a simulation. Initially the system contains only basic constituents  $j = 1$  in numbers  $N_1$ . At time  $t = 0$  reaction pathways open and  $S$  increases rapidly when various compounds  $j > 1$  proliferate (blue). The approaching steady state is perturbed anew at  $t_A$  when a new set of faster reaction pathways open (green). A growth in  $S$  follows from this diversification. A subsequent growth bursts at  $t_B$  when the system couples more external energy in various transitions. A rapid growth initiates again at  $t_C$  when a new set of autocatalytic pathways open (red). The catalytic powers are assigned progressively to compounds  $j > 1$ . The final increase in  $S$  begins at  $t_D$  when autocatalytic pathways are modeled to draw more matter to the system. Eventually the state of maturity is reached when no more ways to increase entropy appear. The amount of matter ( $\Sigma j N_j$ ) is divided among the three pathways, original (blue), fast (green) and autocatalytic (red) as function of time.

erning today's ecosystems as well as on our existence in the future.

\* V. Sharma and A. Annala, *Biophys. Chem.*, in press.

<sup>1</sup> Institute of Biotechnology, University of Helsinki

## 4 Publications

### Articles in peer-reviewed journals

1. S. Bayat, **L. Porra**, **H. Suhonen**, C. Nemoz, **P. Suortti** and A.R.A. Sovijärvi, Differences in the time course of proximal and distal airway response to inhaled histamine studied by synchrotron radiation CT, *J. Appl. Physiol.* **100** (2006) 1964-1973.
2. T.S. Chernaya, S.S. Kazantsev, V.N. Molchanov, I.A. Verin, **M.K. Blomberg**, B.A. Maksimov and V.I. Simonov, Crystal structure of  $\text{La}_3\text{Nb}_{0.5}\text{Ga}_{5.5}\text{O}_{14}$  at 20 K, *Crystallogr. Rep* **51** (2006) 23-28.
3. R. Diamant, S. Huotari, **K. Hämäläinen**, R. Sharon, C.C. Kao and M. Deutsch, The evolution of inner-shell multielectronic X-ray spectra from threshold to saturation for low- to high-Z atoms, *Radiation Physics and Chemistry* **75** (2006) 1434-1446.
4. T.T. Fister, G.T. Seidler, C. Hamner, J.O. Cross, **J.A. Soininen** and J.J. Rehr, Background proportional enhancement of the extended fine structure in nonresonant inelastic x-ray scattering, *Phys. Rev. B* **74** (2006) 214117.
5. **S. Galambosi**, M. Knaapila, **J.A. Soininen**, **K. Nygård**, S. Huotari, F. Galbrecht, U. Scherf, A.P. Monkman and **K. Hämäläinen**, X-ray Raman scattering study of aligned polyfluorene, *Macromolecules* **39** (2006) 9261-9266.
6. **M. Hakala**, **K. Nygård**, **S. Manninen**, L.G.M. Pettersson and **K. Hämäläinen**, Intra- and intermolecular effects in the Compton profile of water, *Phys. Rev. B* **73** (2006) 035432.
7. **M. Hakala**, **K. Nygård**, **S. Manninen**, S. Huotari, T. Buslaps, A. Nilsson, L.G.M. Pettersson and **K. Hämäläinen**, Correlation of hydrogen bond lengths and angles in liquid water based on Compton scattering, *J. Chem. Phys.* **125** (2006) 084504.
8. **M.O. Hakala** and P. Pyykkö, Gold as intermolecular glue: a predicted planar triauritriazine,  $\text{C}_3\text{Au}_3\text{N}_3$ , isomer of gold cyanide, *Chem. Commun.* **27** (2006) 2890-2892.
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- and its oxides using hydrazine dihydrochloride as reductant, *Russ. J. Appl. Chem.* **79** (2006) 1902-1906.
12. **M. Louhivuori**, R. Otten, K. Lindorff-Larsen and **A. Annila**, Conformational fluctuations affect protein alignment in dilute liquid crystal media, *J. Am. Chem. Soc.* **138** (2006) 4371-4376.
  13. I. Makkonen, **M. Hakala** and M.J. Puska, First-principles calculation of positron states and annihilation at defects in semiconductors, *Physica B* **376-377** (2006) 971-974.
  14. I. Makkonen, **M. Hakala** and M.J. Puska, Modeling the momentum distributions of annihilating electron-positron pairs in solids, *Phys. Rev. B* **73** (2006) 035103.
  15. **K. Nygård**, **M. Hakala**, **S. Manninen**, **K. Hämäläinen**, M. Itou, A. Andrejczuk and Y. Sakurai, Ion hydration studied by x-ray Compton scattering, *Phys. Rev. B* **73** (2006) 24208.
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  17. L. von Ossowski, H. Tossavainen, I. von Ossowski, Chunlin Cai, O. Aitio, K. Fredriksson, P. Permi, **A. Annila** and K. Keinänen, Peptide binding and NMR analysis of the interaction between SAP97 PDZ2 and GluR-A: Potential involvement of a disulfide bond, *Biochemistry* **45** (2006) 5567-5575.
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  19. J. Psencik, J.B. Arellano, **T.P. Ikonen**, C.M. Borrego, P.A. Laurinmäki, S.J. Butcher, **R.E. Serimaa** and R. Tuma, Internal structure of chlorosomes from Brown-colored Chlorobium species and the role of carotenoids in their assembly, *Biophys. J* **91** (2006) 1433-1440.
  20. M.-P. Sarén, **R. Serimaa** and Y. Tolonen, Determination of fiber orientation in Norway spruce using X-ray diffraction and laser scattering, *Holz als Roh- und Werkstoff* **64** (2006) 183-188.
  21. M.-P. Sarén and **R. Serimaa**, Determination of microfibril angle distribution by X-ray diffraction, *Wood Science and Technology* **40** (2006) 445-460.
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  23. **J.A. Soininen**, **A. Mattila**, J.J. Rehr, **S. Galambosi** and **K. Hämäläinen**, Experimental determination of the core-excited electron density of states, *J. Phys.: Condens. Matter* **18** (2006) 7327-7336.

24. C. Sternemann, S. Huotari, **M. Hakala**, M. Paulus, M. Volmer, C. Gutt, T. Buslaps, N. Hiraoka, D.D. Klug, **K. Hämäläinen**, M. Tolan and J.S. Tse, Electronic structure of methane hydrate studied by Compton scattering, *Phys. Rev. B* **73** (2006) 195104.
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26. **P. Suortti**, T. Buslaps, V. Honkimäki, N. Hiraoka and U. Lienert, Crystal spectrometers for Compton scattering studies, *Z. Phys. Chem.* **220** (2006) 831-847.
27. M. Tiitu, J. Laine, **R. Serimaa** and O. Ikkala, Ionically self-assembled carboxymethyl cellulose/surfactant complexes for antistatic paper coatings, *J. Colloid. Interf. Sci.* **301** (2006) 92-97.
28. **U. Vainio**, **R. Serimaa** and J. Gravitis, X-ray scattering methods in the study of soft materials, *Latvian Journal of Physics and Technical Sciences* **4** (2006) 14-24.
29. G. Vankó, J.-P. Rueff, **A. Mattila**, Z. Németh and A. Shukla, Temperature- and pressure-induced spin-state transitions in LaCoO<sub>3</sub>, *Phys. Rev. B* **73** (2006) 024424.
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## Articles in Books

- **M. Peura**, **R. Serimaa**, **M.-P. Sarén**, P. Saranpää and M. Müller, The orientation of cellulose microfibrils in single tracheids and solid wood samples as measured by x-ray diffraction. In U. Schmitt, P. Ander, J. Barnett, A. Emons, G. Jeronimidis, P. Saranpää and S. Tschegg, *Wood Fiber Cell Walls, Methods to Study their Formation, Structure and Properties* ISBN **91-5766803-5** (2006) 141-150.

## Editorial Activity

- **S. Manninen**, *Nordsync Annual Report 2005* (2005, 23 pages).

## Articles in other journals

- **K. Hämäläinen**, Preface, *Proceedings of the XL Annual Meeting of the Finnish Physical Society* **Tampereen Teknillinen Yliopisto, Fysiikan laitos** (2006) 1.
- **K. Hämäläinen**, Kansainvälinen fysiikan vuosi 2005 / World Year of Physics 2005, *Suomen Unesco-toimikunnan toimintakertomus 2005* **Yliopistopaino, Helsinki** (2006) 15–16.
- **K. Hämäläinen**, EPS:n Councilin vuosikokous, *Arkhimedes* **2** (2006) 9.
- **K. Hämäläinen**, Vuoden 2005 viksuin lukiolaisfyysikko palkittiin, *Arkhimedes* **3** (2006) 15–16.

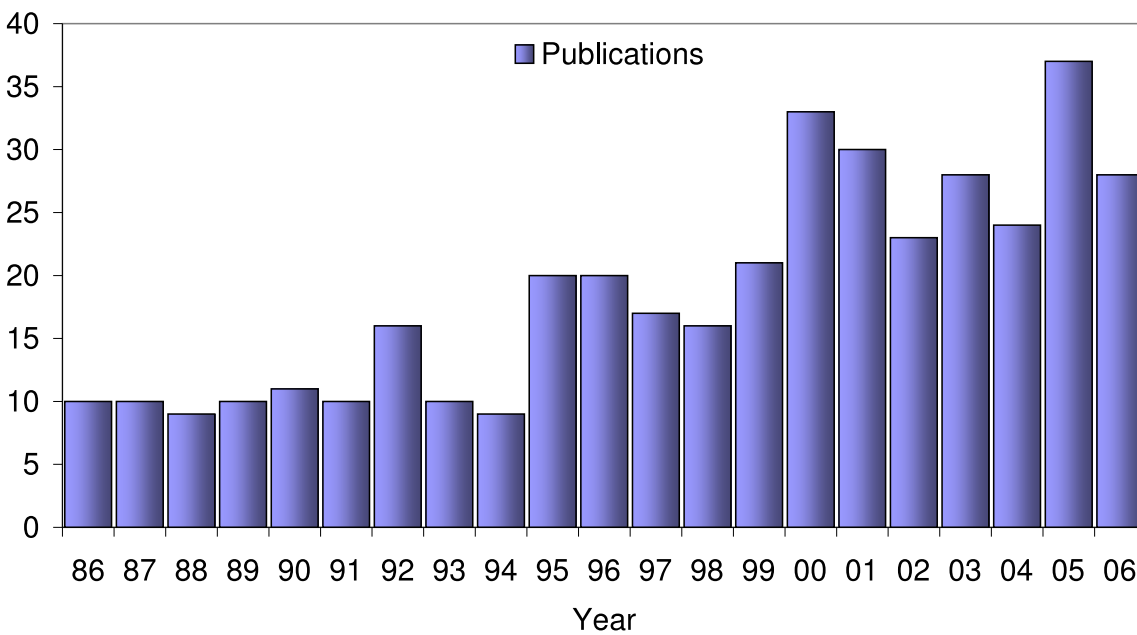


Table 1. Annual number of publications in peer-reviewed journals from 1986 to 2006.

## Ph.D. theses

- **L. Porra**, Lung structure and function studied by synchrotron radiation (Suortti).
- **M.-P. Sarén**, Characterisation of properties of coniferous wood tracheids by x-ray diffraction, laser scattering and microscopy (Serimaa).
- **M. Fernández**, X-ray scattering and diffraction enhanced imaging studies of in vitro breast tissues (Suortti).

## M.Sc. theses

- **T. Pykkänen**, Veden rakenteen tutkimus Compton-sironnalla (Hämäläinen / Hämäläinen, Manninen).
- **A. Sakko**, Atomiryypäistä tapahtuvan Röntgen-Raman-sironnan mallintaminen (Soininen, Hakala / Hämäläinen, Kajantie).
- **J. Seitsonen**, Coxsackieviruksen A9 ja parechoviruksen 1 rakenteet kryoelektronimikroskopian ja rekonstruktio menetelmän avulla (Butcher / Annala, Manninen).
- **K. Pirkkalainen**, Metallinanopartikkelien tutkimus anomaalisella pienkulmasironnalla (Serimaa / Serimaa, Manninen).

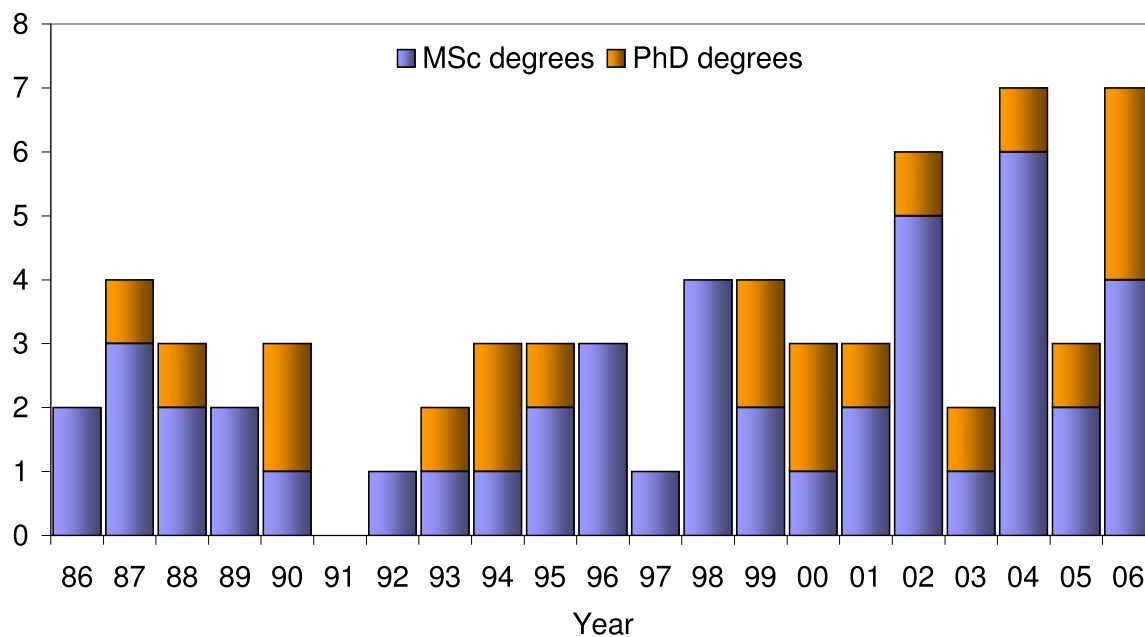


Table 1. Annual numbers of the Msc and PhD degrees from 1986 to 2006.

## Invited conference presentations

- **Stockholm Discussion Meeting**, 14.6. – 16.6., Stockholm, Sweden
  - **M. Hakala**. X-ray Compton Scattering as a probe of hydrogen bonds and local coordination in water.
- **Sagamore XV Conference**, 13.8. – 18.8., University of Warwick, UK
  - **M. Hakala**. Hydrogen Bonds in Water and Aqueous Systems Studied by Compton Scattering and DFT Calculations.

## Conferences

- **XL Annual Meeting of the Finnish Physical Society**, 9.3. – 11.3., Tampere, Finland
  - **K. Pirkkalainen**, **U. Vainio**, **K. Kisko**, N. Kotelnikova and **R. Serimaa**. Structure of Ni nanoparticles in microcrystalline cellulose matrix using ASAXS. Abstract 01-28.
  - **M. Hakala**, **K. Nygård**, **S. Manninen**, L.G.M. Pettersson and **K. Hämäläinen**. X-ray Compton scattering as a probe of hydrogen bonds in liquid water. Abstract 02-7.
  - **A. Sakko**, **M. Hakala**, **J.A. Soininen** and **K. Hämäläinen**. A new program for calculating X-ray Raman scattering cross sections of atom clusters. Abstract 02-30.
  - **K. Nygård**, **M. Hakala**, **S. Manninen**, M. Itou, A. Andrejczuk, Y. Sakurai and **K. Hämäläinen**. Ion hydration studied by X-ray Compton scattering. Abstract 02-31.
  - **T. Pylkkänen**, **K. Nygård**, **M. Hakala**, **S. Manninen** and **K. Hämäläinen**. The H/D isotope effect in the Compton profile of water. Abstract 02-32.
  - A. Salmi, E. Hægström, T. Karppinen, P. Saranpää and **R. Serimaa**. Comparing ultrasonic and bending estimates of wood-elasticity. Abstract 04-23.
  - **K. Kisko**, G. Szilvay, **U. Vainio**, **M. Torkkeli**, M. Linder and **R. Serimaa**. Self-assembled films of hydrophobin proteins. Abstract 06-3.
  - **U. Vainio**, T. Laitinen, **R. Serimaa** and O. Ikkala. Structural studies of DNA-surfactant self-assemblies. Abstract 06-23.
  - T. Ruotsalainen, J. Turku, **U. Vainio**, **R. Serimaa**, J. Ruokolainen, A. Harlin and O. Ikkala. Self-assembly of comb-coil block copolymer -amphiphile complexes in electrospun fibers vs. in bulk. Abstract 06-48.
  - **A. Mattila**, J.-P. Rueff, J. Badro, G. Vanko and **K. Hämäläinen**. Transition metal oxides at high pressure: a multiplet approach to magnetic collapse. Abstract 08-14.

- **J.A. Soininen, A. Mattila, S. Galambosi** and **K. Hämäläinen**. Extraction of the local density of states from X-ray Raman scattering data. Abstract 08-15.
- **S. Galambosi**, M. Knaapila, **J.A. Soininen** and **K. Hämäläinen**. X-ray Raman scattering studies on poly[9,9-bis(2-ethylhexyl)-fluorene-2,7-diyl]. Abstract 08-21.
- **H. Suhonen, L. Porra**, S. Bayat, A.R.A. Sovijärvi and **P. Suortti**. Combining K-edge subtraction and temporal subtraction for simultaneous measurement of ventilation and perfusion. Abstract 10-4.
- **L. Porra, H. Suhonen**, S. Bayat, **P. Suortti** and A.R.A. Sovijärvi. In vivo imaging of regional ventilation before and after histamine provocation using synchrotron radiation CT. Abstract 10.5.
- **M. Peura, U. Vainio**, M.-P. Sarén, M. Müller, P. Saranpää and **R. Serimaa**. The orientation of cellulose microfibrils in Norway spruce tracheids: Structural and mechanical implications. Abstract 10-17.
- **H. Suhonen, M. Fernández**, A. Bravin, J. Keyriläinen and **P. Suortti**. X-ray scattering in diffraction enhanced imaging. Abstract 10-20.
- **M. Louhivuori**, R. Otten and **A. Annala**. Conformational fluctuations affect protein alignment and create a bias in residual dipolar coupling data. Abstract 10-24.
- **Biophysical Society Annual Meeting**, 18.2. – 22.2., Salt Lake City, USA
  - **T. Ikonen**. Effect of Carotenoid Biosynthesis on the Lamellar Pigment Arrangement in Chlorosomes from Green Sulfur Bacteria.
- **XIII International Conference on Small-angle Scattering SAS2006**, 9.7. – 13.7., Kyoto, Japan
  - **K. Kisko**, G. Szilvay, E. Vuorimaa, H. Lemmetyinen, M. Linder, **M. Torkkeli** and **R. Serimaa**. Self-assembled films of hydrophobin protein HFBIII from *Trichoderma reesei*.
  - **K. Pirkkalainen, U. Vainio, K. Kisko**, N. E. Kotelnikova and **R. Serimaa**. Structure of Ni nanoparticles in microcrystalline cellulose matrix using SAXS.
- **XAFS 13 Conference**, 9.7. – 14.7., University of Stanford, USA
  - **J. A. Soininen**. Recent developments in the analysis of X-ray Raman scattering.
- **Sagamore XV Conference**, 13.8. – 18.8., University of Warwick, UK
  - **K. Nygård, M. Hakala, S. Manninen**, L.G.M. Pettersson and **K. Hämäläinen**. Structural studies of water by Compton scattering.
- **XXII International Conference on Magnetic Resonance in Biological Systems**, 20.8. – 25.8., Göttingen, Germany
  - **M. Louhivuori**. Conformational fluctuations affect protein alignment.

## Seminars, symposia and workshops

- **Kasvifysiologian päivä**, 9.1., Turku, Finland
  - **R. Serimaa**. The effect of hemicellulose-lignin matrix on elastic properties of wood cell wall.
- **CMS Unit of Excellence seminar**, 10.1.-12.1, Stockholm, Sweden
  - **M. Hakala**. Simulations and inelastic x-ray scattering of solids and liquids.
- **3rd Scandinavian Workshop on Scattering from Soft Matter**, 2.2. – 3.2, Uppsala, Sweden
  - **K. Kisko**. GIXD Studies on Hydrophobin Protein Monolayers on Air/Water Interface
- **Multidisciplinary Post-Graduate Course "Nanotechnology In Drug Research And Development"**, 8.2., Helsinki, Finland
  - **R. Serimaa**. X-ray scattering methods: SAXS, SANS
- **Polymeerikemian esitelmäsarja**, 24.2., Helsinki, Finland
  - **R. Serimaa**. The effect of tension on the nanostructure of native and kraft cooked wood.
- **Joint Meeting of ESWM and COST Actions E35**, 14.5. – 17.5., Florence, Italy
  - A. Salmi, E. Hægström, T. Karppinen, P. Saranpää and **R. Serimaa**. Comparing ultrasonic and static bending test estimates of elasticity of Norway spruce.
- **Workshop Molecular-, nano-, composite- level research and biological re-engineering of plant cell wall composition - challenges moving towards new biorefineries**, 22.5. – 24.5., Riga, Latvia
  - **R. Serimaa**. Studies on nanostructures of natural polymers using x-rays and synchrotron radiation.
- **Time Dependent Density Functional Theory: Prospects and Applications, 2nd International Workshop and School**, 27.8. – 11.9, Bidasoa center for science, Spain
  - **A. Sakko, M. Hakala, J. A. Soininen** and **K. Hämäläinen**. Simulation of X-ray Raman scattering from molecules using density functional theory.
- **Seminar series of Laboratory of Physical Chemistry, Univ. Helsinki**, 28.9., Helsinki, Finland
  - **K. Hämäläinen**. Novel x-ray spectroscopy using synchrotron radiation.

- **CMS Unit of Excellence seminar**, 10.10., Helsinki, Finland
  - **M. Hakala**. Prediction of new chemical species and x-ray properties of molecular systems.
- **MAX Laboratory**, 19.10., Lund, Sweden
  - **K. Hämäläinen**. Novel hard x-ray spectroscopy.
- **COST E-50 CEMARE Conference Cell Wall Macromolecules and Reaction Wood, COST Action E50 International Conference**, 19.10. – 22.10., Warsaw, Poland
  - P. Saranpää, A. Salmi, V. Kananen, E. Hæggström, T. Karppinen and **R. Serimaa**. Spiral compression wood in *Pinus sylvestris*.
- **University of Dortmund**, Dortmund, Germany
  - **A. Sakko**. Simulation of X-ray Raman scattering using density functional theory.
- **COST Action E50 Workgroup 1 Meeting**, 18.12. – 21.12., Wageningen, Netherlands
  - **M. Peura**. X-ray analysis of cellulose
- **ESRF**, 20.12., Grenoble, France
  - **J. A. Soininen**. Recent Developments in Analysis of Inelastic X-ray Scattering.

## Summer schools

- **Future trends in synchrotron radiation based research in materials physics and chemistry**, 4.6. – 7.6., Käringsundby in Åland, Finland
  - **Teaching**
    - **K. Hämäläinen**. Novel x-ray spectroscopy techniques in the study of advanced materials.
    - **S. Manninen**. Opening of the Summer School.
    - **R. Serimaa**. Soft condensed matter studies at the University of Helsinki.
  - **Students**
    - **K. Kisko**. Grazing-incidence x-ray diffraction studies of self-assembled films of hydrophobin proteins.
    - **K. Nygård** and **K. Hämäläinen**. Local structure of water studied by x-ray Compton scattering.
    - **K. Pirkkalainen**. Anomalous X-ray scattering study on metal nanoparticles in cellulose matrix.

- **T. Pykkänen.** Short introduction to water science.
- **A. Sakko.** Simulation of x-ray Raman scattering using density functional theory.
- **H. Suhonen.** Functional lung imaging using synchrotron radiation.
  
- **NENA training course / summer school of ESPOM graduate school,** 22.8., Stockholm, Sweden
  - **R. Serimaa.** Application of X-ray and synchrotron radiation based methods in fuel cell research.
  
- **Joint Graduate School Seminar. Physics and Chemistry of Materials: Towards Nano,** 8.12. – 9.12., Hanasaari, Espoo, Finland
  - **Teaching**
    - **K. Hämäläinen.** Large scale research infrastructures for materials science and nanotechnology
  - **Students**
    - **K. Kisko.** Self-assembly of hydrophobin proteins.
    - **A. Mattila.** Transition metal oxides at high pressure: A multiplet approach to magnetic collapse.
    - **K. Nygård.** Local structure of water studied by x-ray Compton scattering.

## 5 International collaboration

### Research abroad

#### Annala

|                   |  |                                  |
|-------------------|--|----------------------------------|
| <b>Blomberg</b>   | Leuven, Belgium                            | 6.8. – 11.8.                     |
| <b>Galambosi</b>  | ESRF, France                               | 25.4. – 3.5.<br>27.6. – 4.7.     |
| <b>Hakala</b>     | Stockholm, Sweden                          | 10.1. – 12.1.                    |
| <b>Hämäläinen</b> | EU ESFRI expert meeting, Belgium           | 19.1. – 20.1.<br>21.2.<br>23.3.  |
|                   | ESRF Annual Meeting, France                | 6.2. – 8.2.                      |
|                   | ESRF evaluation panel & scientific council | 15.5. – 19.5.                    |
|                   | ESRF scientific board meeting, France      | 7.11. – 11.11.                   |
|                   | ESRF, France                               | 12.6. – 16.6.<br>21.11. – 25.11. |
|                   | SPring-8, Japan                            | 20.5. – 27.5.                    |
|                   | EPS council meeting, France                | 24.3. – 25.3.                    |
|                   | EPS board meeting, France                  | 22.6. – 25.6.<br>27.10. – 29.10. |
|                   | University of Warwick, UK                  | 13.8. – 18.8.                    |
|                   | Estonian Physical Society, Estonia         | 10.5                             |
|                   | MAX-IV scientific evaluation, Sweden       | 18.10 – 19.10                    |
|                   | SOLEIL evaluation panel meeting, France    | 12.12 – 14.12                    |
|                   | EU Young Scientist Competition, Sweden     | 23.9. – 25.9.                    |
| <b>Ikonen</b>     | Diamond Synchrotron, Great-Britain         | 28.1. – 2.2.                     |
|                   | Salt Lake City, USA                        | 18.2. – 22.2.                    |
| <b>Kisko</b>      | Uppsala, Sweden                            | 2.2. – 3.2.                      |
|                   | EMBL, HASYLAB, Germany                     | 29.6. – 1.7.                     |
|                   | Kyoto, Japan                               | 9.7. – 13.7.                     |
| <b>Louhivuori</b> | Vancouver, Canada                          | 14.7. – 24.7.                    |
|                   | Göttingen, Germany                         | 20.8. – 25.8.                    |
| <b>Leppänen</b>   | MAX-lab, Sweden                            | 13.12. – 17.12.                  |
| <b>Manninen</b>   | University of Warwick, UK                  | 13.8. – 18.8                     |
|                   | Nordsync board meeting, Trondheim Norway   | 7.10.                            |
|                   | ESRF council meeting, France               | 27.11. – 18.11.                  |
| <b>Mattila</b>    | ESRF, France                               | 27.6. – 4.7.<br>6.11. – 14.11.   |

|                     |  |                                  |
|---------------------|--|----------------------------------|
| <b>Nygård</b>       | ESRF, France                                 | 25.4. – 2.5.                     |
|                     | SPring-8, Japan                              | 12.6. – 23.6.<br>18.5. – 27.5.   |
| <b>Peura</b>        | Wageningen, Netherlands                      | 18.12. – 21.12.                  |
| <b>Pirkkalainen</b> | Hasylab, Germany                             | 6.7 – 10.7                       |
| <b>Pykkänen</b>     | DESY, Germany                                | 28.2. – 3.3.                     |
|                     | ESRF, France                                 | 12.6. – 18.6.                    |
|                     |  | 27.6. – 4.7.                     |
|                     |  | 1.10. – 15.10.<br>6.11. – 12.11. |
| <b>Sakko</b>        | DESY, Germany                                | 28.2. – 3.3.                     |
|                     | University of Dortmund, Germany              | 29.5. – 2.6.                     |
|                     | Benasque center for science, Spain           | 10.12. – 15.12.<br>27.8. – 11.9. |
| <b>Serimaa</b>      | EMBL Priorities Committee meeting, Germany   | 27.1. – 29.1.                    |
|                     | Uppsala, Sweden                              | 2.2. – 3.2.                      |
|                     | Riga, Latvia                                 | 22.5. – 24.5.                    |
|                     | Stockholm, Sweden                            | 22.8.                            |
| <b>Soininen</b>     | University of Dortmund, Germany              | 25.5. – 2.6.                     |
|                     | University of Washington, USA                | 1.9. – 30.11.                    |
|                     | ESRF, France                                 | 19.12 – 21.12.                   |
| <b>Suhonen</b>      | ESRF, France                                 | 27.6. – 7.7.                     |
|                     |  | 4.12. – 13.12.                   |
| <b>Suortti</b>      | ESRF, France                                 | 23.1. – 8.2.                     |
|                     | Australian Synchrotron Laboratory, Australia | 11.2. – 22.2                     |
|                     | Daresbury, Warwick Oxford, Great-Britain     | 13.8 – 27.8.                     |
| <b>Torkkeli</b>     | HASYLAB, Germany                             | 19.2. – 27.2.                    |
|                     | MAX-lab, Sweden                              | 19.11 – 25.11<br>13.12 – 17.12.  |
| <b>Vainio</b>       | EMBL, HASYLABL, Germany                      | 29.6. – 1.7.                     |
|                     | Kyoto, Japan                                 | 9.7. – 13.7.                     |

**Visitors**

|                           |  |
|---------------------------|--|
| <b>Dr L. Almasy</b>       | 17.3. – 1.4.<br>Research Institute for Solid State Physics and Optics, Hungary       |
| <b>PhD C.J. Hall</b>      | 29.6. – 1.7.<br>Daresbury Laboratory, Great-Britain                                  |
| <b>PhD N. Kotelnikova</b> | 11.12. – 14.12.<br>Institute of Macromolecular Compounds, Russia                     |
| <b>MSc C Krywka</b>       | 24.8. – 28.2.<br>University of Dortmund, Germany                                     |
| <b>PhD C. Sternemann</b>  | 23.8. – 26.8.<br>University of Dortmund, Germany                                     |
| <b>MSc H Sternemann</b>   | 21.2. – 23.2.<br>21.8. – 22.8.<br>16.11. – 17.11.<br>University of Dortmund, Germany |
| <b>Prof B. Thomlinson</b> | 19.12. – 20.12.<br>Canadian Light Source, Canada                                     |

## 6 Teaching

### Lectures

|                     |   |        |
|---------------------|---|--------|
| <b>Annala</b>       | Aaltoliikeopin perusteet                    | SPRING |
|                     | Biomolekyylien NMR-spektroskopia            | SPRING |
|                     | Molekulaarinen biofysiikka                  | FALL   |
| <b>Blomberg</b>     | Säteilysuojelun perusteista ja käytännöstä  | FALL   |
| <b>Hakala</b>       | Kumpula Computational Chemistry and Physics | FALL   |
| <b>Hämäläinen</b>   | Arkipäivän fysiikkaa                        | SPRING |
|                     | Fysiikan laudatur-seminaari                 | SPRING |
|                     | Fysikaalisten tieteiden esittely            | FALL   |
|                     | Röntgenfysiikan tutkijaseminaari            | FALL   |
| <b>Manninen</b>     | Kiinteän olomuodon fysiikka I               | SPRING |
|                     | Mekaniikan perusteet                        | FALL   |
| <b>Serimaa</b>      | Pehmeän tiiviin aineen fysiikka I & II      | SPRING |
|                     | Tieteellisen laskennan peruskurssi I & II   | FALL   |
| <b>Soininen</b>     | Tiiviin aineen teoria                       | SPRING |
| <b>Suhonen</b>      | Tvt-ajokortti                               | FALL   |
| <b>Torkkeli</b>     | Sivuaineapprobatur II                       | SPRING |
| <b>Exercises</b>    |   |        |
| <b>Hakala</b>       | Tiiviin aineen teoria                       | SPRING |
| <b>Louhivuori</b>   | Aaltoliikkeen perusteet                     | SPRING |
|                     | Molekulaarinen biofysiikka                  | FALL   |
| <b>Nygård</b>       | Kiinteän olomuodon fysiikka I               | SPRING |
| <b>Pirkkalainen</b> | Pehmeän tiiviin aineen fysiikka I & II      | SPRING |
| <b>Pykkänen</b>     | Arkipäivän fysiikkaa                        | SPRING |
|                     | Mekaniikan perusteet                        | FALL   |
| <b>Sakko</b>        | Mekaniikan perusteet                        | FALL   |

**Laboratory excercises**

|                     |                               |               |
|---------------------|-------------------------------|---------------|
| <b>Galambosi</b>    | Aaltoliikkeen perusteet       | SPRING        |
|                     | Mekaniikan perusteet          | FALL          |
|                     | Sähkömagnetismin perusteet    | SPRING        |
| <b>Kisko</b>        | Approbatur I                  | FALL          |
|                     | Approbatur II                 | SPRING        |
| <b>Mattila</b>      | Aaltoliikkeen perusteet       | SPRING        |
|                     | Mekaniikan perusteet          | FALL          |
|                     | Sähkömagnetismin perusteet    | SPRING        |
| <b>Peura</b>        | Cum laude (Laboratoriotyöt I) | SPRING & FALL |
| <b>Pirkkalainen</b> | Mekaniikan perusteet          | FALL          |
| <b>Torkkeli</b>     | Approbatur I                  | FALL          |
| <b>Vainio</b>       | Approbatur I                  | FALL          |
|                     | Approbatur II                 | SPRING        |

## 7 Experimental facilities

### Small-angle x-ray scattering setup

- Siemens K710H x-ray generator, Cu-anode x-ray tube
- Incoatec Montel 2D parallel beam multilayer optics
- Linkam TP93 hot stage with liquid nitrogen pump for sample temperature control (-150 – +350 °C)
- Bruker AXS HI-STAR area detector system
- Braun OED-50M position sensitive proportional counter with metal wire

### Rotating anode x-ray system

- Rigaku UltraX18S generator (18 kW)
- Cu or Mo anode
- two beamlines: small-angle scattering and spectroscopy
- *mar345* image plate detector

### Powder diffractometer I

- complete Seifert XRD 3000 TT system with measurement control and data analysis software
- Cu- or Mo-anode x-ray tube
- vertical  $\theta$ - $\theta$  goniometer
- secondary graphite or LiF monochromator, NaI(Tl) scintillation detector
- Anton-Paar temperature attachment (-190 – +450 °C)

### Powder diffractometer II

- Seifert ID 3003 x-ray generator, Cu-anode x-ray tube
- primary Johansson-type quartz monochromator
- optional goniometer systems:
  1. Huber 414 2-circle goniometer
  2. Huber Guinier diffractometer with
    - a) a model 642 goniometer for flat powdered specimens, Seemann-Bohlin focusing principle, symmetric/asymmetric transmission/back-reflection geometry, or
    - b) a model 653 goniometer including a model 656 texture device for solid specimens coated with a thin film or material different from the substrate, reflection geometry under grazing incidence of the primary x-ray beam
- NaI(Tl) scintillation detector
- PC-based motion control (Oregon Micro Systems PC48-4) and data acquisition systems (Keithley Metrabyte CTM-10), both controlled with `spec` software
- Laue camera with Polaroid XR-7 Land Diffraction Cassette or Molecular Dynamics image plate

## Powder diffractometer III

- for texture studies of weakly ordered materials and powder diffraction
- Seifert ID 3003 x-ray generator, Cu-anode x-ray tube
- primary germanium monochromator
- Huber 420/511 4-circle goniometer, reflection or transmission geometry, various specimen holders
- versatile beam size control either by slits or by pinhole collimators
- NaI(Tl) scintillation detector
- PC-based motion control and data acquisition with `spec` software

## Four-circle diffractometer

- for collection of three-dimensional x-ray diffraction data at 10-300 K
- Siemens K710H x-ray generator
- Mo- or Ag-anode x-ray tube, graphite monochromator
- Huber 5042 4-circle goniometer
- PC-based motion control (Galil DMC-1040) and data acquisition systems (National Instruments PC-TIO-10) controlled with `spec` software
- sample cooling system based on a closed-cycle two-stage helium cryostat (Displex CSW-202A), a specially designed refrigerator mount functioning as a goniometer head, and a control unit for temperature measurement and adjustment (LakeShore DRC-93CA)

## W $K\alpha_1$ spectrometer

- for inelastic scattering, diffraction and fluorescence analysis
- 160 kV x-ray generator (Philips MG163), W-anode x-ray tube
- focusing Ge (400) monochromator to produce 59.32 keV W  $K\alpha_1$  radiation, continuous spectrum can be used for energy dispersive diffraction experiments
- Ge solid state detector, Tennelec PUR-amplifier, Nucleus MCA-card
- thermoelectrically cooled x-ray detector (Amptek XR-100T Si-PIN photodiode with power supply PX2T)
- motorized X-Z stage for sample positioning
- PC-based motion control and data acquisition with `spec` software

## Two-crystal spectrometer

- for reflectivity curve measurements with 10 nanorad angular resolution
- Siemens K710H x-ray generator, Mo  $K\alpha_1$  radiation
- PC-based motion control and data acquisition with `spec` software

## Soft x-ray chamber

- placed in a clean room (class 10000)
- Ti-anode miniature x-ray tube, 50 kV HV generator
- x-ray energy range 0.1 - 50 keV depending on the detector
- chamber volume approximately 100 litres, diameter 63 cm, height 30 cm
- final pressure  $\approx 1$  mbar in less than 10 minutes
- motorized X-Z and theta stages inside the chamber
- PC-based 4-channel motion control and counter system, `spec` software

## X-ray fluorescence demonstration apparatus

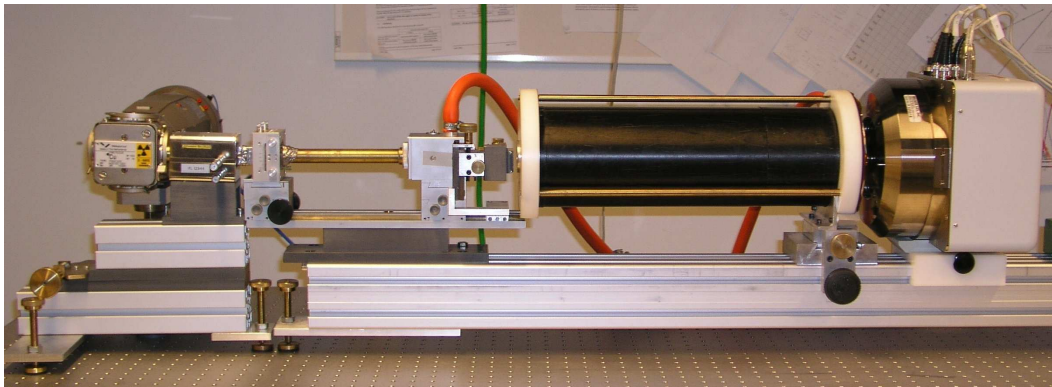
- Americium-241 sealed source
- lead shielded measurement chamber
- thermoelectrically cooled x-ray detector (Amptek)
- PC-based sample-changer control, data acquisition and data analysis

## Image plate detector system

- Molecular Dynamics PhosphorImager 445 SI
- A4 cassette, resolution 88/176  $\mu\text{m}$ , scanning time 7 min
- image display software

## Materials testing device

- Tinius Olsen H5kT
- tensile tests, compression tests, cyclic tests
- compression plates, pneumatic sample grips



Small-angle x-ray scattering setup