

Physics Institute





CHEMNITZ UNIVERSITY OF TECHNOLOGY

www.tu-chemnitz.de/physik/





Figures on front page from left to right:

Concentration of energy in localized coherent structures studied with methods of nonlinear dynamics and statistical physics · Combined (S)TEM and EELS investigation of Pt atomic segregations at a NiSi₂/ Si(001) interface · Microstructure of human bone imaged with bimodal amplitude modulation scanning force microscopy · Electrochemical deposition of copper crystals on a gold surface (background).

The new physics building inaugurated in spring 2008 provides excellent conditions for experimental and theoretical reasearch.





INTRODUCTION

This brochure provides a short overview of the research activities at the Physics Institute at the Chemnitz University of Technology. It is intended for scientists interested in the work of the department as well as for students choosing an area of specialization for their Bachelor or Master thesis.

The Chemnitz University of Technology is a rather young institution. It has its roots in the former "Königliche Gewerbschule" founded in 1836, which transformed into an engineering college in 1953. It developed into a fullsized Technical College (Technische Hochschule) by 1963. In 1986 it was designated a Technical University.

Until 1989, physics in Chemnitz was primarily dedicated to applied science. In 1990 it was decided to expand the scope of the physics programme to include experimental and theoretical physics, as well as physics teaching covering applied to basic research, and to increase the number of professorships from 7 to 17. The most significant additions were in the areas of numerical methods for disordered and nonlinear dynamical systems, laser based methods for investigations of molecular systems, semiconductor surfaces, soft matter, electronic properties of amorphous systems, and magnetic nanostructures.

The department capacities for research and education have reached an impressive level. The research is financed to a great extent by thirdparty grant money. The level of excellence is maintained through programmes such as Graduate Colleges, cooperations in Collaborative Research Centers (Sonderforschungsbereiche), and a Centre of Excellence (Innovationskolleg). The list of recently started projects includes the DFG Research Group "From local constraints to macroscopic transport" amd German-Chinese International Research and Training Group "Materials and Concepts for Advanced Interconnects"

A new milestone for the Physics Institute was reached this spring when the new physics building was inaugurated. The building contains state-of-the-art laboratories, e.g. cleanroom facilities, and offices that allow a new quality of research. In addition the location of the institute next to the Smart Systems Campus technology park and to two Fraunhofer institutes will have an important impact on further cooperations.

Currently the faculty comprises 13 professors including one junior professor. The reseach interests of the professorships are presented on the following pages.

THE PROFESSORSHIPS

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SURFACE AND INTERFACE PHYSICS Prof. Dr. Manfred Albrecht



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Research fields

- Magnetic nanostructures
- Self-assembly of nanoparticles
- Thin magnetic alloy films and heterostructures
- Magnetic coupling phenomena (i.e., exchange spring effect, exchange bias effect)
- Laser- and lon-induced modifications of thin films and nanostructures

Methods

- Molecular beam epitaxy (MBE) and sputter deposition
- In-situ growth and surface characterization (RHEED, LEED, AES, UHV-STM)
- Magnetic (SQUID, MOKE, XMCD, MFM) and electronic characterization
- Structural characterization (XRD, TEM, SEM)

Equipment

- Deposition tools (MBE-Systems, DC sputter deposition) and processing equipment (Plasma Processor (TePla) and RTA setup)
- VSM-SQUID magnetometer (QUANTUM DESIGN)
- MOKE magnetometer (in-plane, out-of plane)
- 5-Tesla Cryostat (OXFORD INSTRUMENTS) for low-temperature resisitivity measurements
- Scanning Magneto-Resisitive Microscope

Scientific cooperation

- Hitachi Global Storage Technologies, San Jose (USA)
- Oerlikon-Balzers AG, Balzers (Liechtenstein)
- SIMaP CNRS, Grenoble (France)
- University of Sheffield, Department of Engineering Materials (Great Britain)
- H. Niewodniczanski Institute of Nuclear Physics, Polish Academy of Sciences, Kraków (Poland)
- Forschungszentrum Dresden-Rossendorf e.V., Institut für Ionenstrahlphysik und Materialforschung (Germany)



Magnetic data storage projects

Mass data storage on magnetic hard drives in portable products is a new and fast growing market with an estimated turnover of several billion EUR per year. However, continued growth of storage density is limited as a result of the thermal instability of recorded data. To overcome this so called "superparamagnetic effect", the use of discrete media, in which information is stored in single nanostructures, will become mandatory. Therefore, it is likely that magnetic recording media will be the first technology which requires the introduction of nanostructuring by selfassembly processes.

In this regard, it is expected that self-assembly of nanoparticles can be governed and expanded to wafer size scale by pre-patterning the substrate. New material functionality can be introduced by magnetic material deposition onto particle arrays, as illustrated in Fig. 1A. The magnetic Co/ Pd nanostructures formed on top of the particles are in a magnetic single-domain state, as indicated by the dark and bright contrast in magnetic force microscope (MFM) imaging of the particle caps (see Fig. 1B). This nanoscale system is quite distinct from the classical geometries: The Co/Pd multilayer film is extended over a wide region of the sphere and thus shows substantial curvature even for 70-nm-size particles as presented in the dark field transmission electron microscope (TEM) image of Fig. 1C. Moreover, further concepts for recording media such as percolated perpendicular media and exchange spring coupled heterostructures are currently investigated in two EU STREP projects called "MAFIN" (Magnetic Films on Nanospheres) and "TERAMAGSTOR" (TERAbit MAGnetic STOrage technologies).

Fig. 1: A, Schematic drawing showing the nanostructure formation. B, MFM image of a 320 nm particle array after Co/Pd film deposition. C, TEM image of Co/Pd covered 70-nm-size particles (in co-operation with Hitachi GST).



Nanostructuring of thin magnetic films

These investigations include thin films (i.e. FePt, Co/Pd, CoCrPt) with strong perpendicular magnetic anisotropy that are grown on suitable substrates by molecular beam epitaxy or sputter deposition. These films can be structured

by focused ion beam (FIB) as shown in Fig. 2A or laser interference lithography (Fig. 2B), where line and dot structures can be formed by 2-beam and 3-beam interference patterning, respectively.

Fig. 2: A, AFM image of a single row of 80-nm FIB patterned CoCrPt islands. B, Morphology of a Co/Pd multilayer film after exposure to a 3-beam laser interference pattern.

SOLID SURFACE ANALYSIS Prof. Dr. Michael Hietschold



Towards molecular images

Our Group

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Research fields

- Self-Assembling, Organic Molecules, Clusters and Thin Films
- Scanning Probe Microscopies
- Surfaces, Interfaces and Nanostructures

Methods

- Scanning Probe Microscopies and Spectroscopies (STM, STS, AFM, EFM)
- Electron Microscopies (TEM, SEM, EELS, EDX, EBSD, CL)
- Sample Preparation (SAM's, Cross-Sections)

Equipment

- Transmission Electron Microscope CM20 FEG (FEI) with Gatan Imaging Filter
- Scanning Electron Microscope NovaNanoSEM (FEI) with EDX, EBSD, and CL
- Scanning Electron Microscope SEM 515 Philips
- UHV Surface Lab (Omicron with in-Situ Peparation, LEED and VT-STM)
- Digital Optical Microscope Keyence VHX-500
- Ion Milling Systems RES100
- Ambient SPMs (TU Munich, self-made)

Scientific Cooperation

- Germany (LMU Munich, Univ. Kaiserslautern)
- USA (Washington-, Portland State University)
- UK (University Glasgow, Daresbury Laboratory)
- Vietnam (Vinh University, TU Hanoi, NU Ho-Chi-Minh-City)
- France (CNRS Toulouse)
- IRTG "Materials and Concepts for Advanced Interconnects"

Industrial Cooperation

- BalTec AG
- Anfatec AG
- von Ardenne Anlagentechnik
- Innovent Jena





Ultrathin Organic Films

We are interested in the surface structure of ordered monolayers on crystalline substrates and the physical principles governing the appearance of such self-assembled systems. The STM image shows an open mesh-like structure of cyanated phthalocyanine molecules on highly oriented pyrolytic graphite (HOPG). This structure appears due to an interplay between a weak attraction of the molecules to the substrate and an effective repulsion between the CN-groups of adjacent molecules. Small intentional disruptions of such structures get self-repaired. About the corresponding STM experiments see T.G.Gopakumar, Hao Tang, W.R.Thiel, M.Hietschold, J.Phys.Chem. C 112, 7698 (2008)

STM image showing an open mesh-like structure of cyanated phthalocyanine molecules on highly oriented pyrolytic graphite (HOPG).

Silicon-Based Interface Structures

High-resolution TEM on specially prepared cross-sectional samples allows to study the atomic structure at interfaces. The image shows a nickel silicide layer grown epitaxially on Si(001) substrate. These experiments are in collaboration with the SuperSTEM facility at Daresbury National Laboratory, UK. Th.Schaarschmidt, Diploma Thesis, TU Chemnitz 2008

Combined (S)TEM and EELS investigation of Pt atomic segregations at a NiSi $_{\rm z}/{\rm Si}(001)$ interface.

IRTG "Materials and Concepts for Advanced Interconnects"

Within this German-Chinese International Research and Training Group (IRTG), we are contributing

- basic investigations on organic molecular interconnects which can be performed e.g. by stacking of suitable single molecules leading to 1d wires.
- microscopic investigations of technological relevant

EBSD image showing the different crystallographic oreintations of Cu crystals in a PVD Copper film after N $_2$ - annealing at 400°C.

systems as CVD, PVD and electrochemically deposited metal films.

A first paper in terms of this IRTG is B.Graffel, F.Müller, A.-D. Müller, M.Hietschold, Rev.Sci.Instrum. 78, 053706 (2007)

PHYSICS OF THIN FILMS Prof. Dr. Peter Häussler



Cryostat for measuring the thermal conductivity



2D electron density around four atoms resonsable for spherical periodic structural order of disordered systems

Sample holder for in situ resistivity measurments



Sequential flash evaporater for the preparation of ten different alloys

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Research fields

- fundamental research on structure formation at very early stages
- resonance stabilization on different scales, between different subsystems
- general dynamics of phase formation
- amorphous systems (metals, semiconductors, Zintl systems, TM-Al alloys)
- new materials (quasicrystals, Heusler/Half-Heusler alloys, magnetic systems)
- electronic and thermal transport anomalies at various temperatures

Methods

- in-situ preparation of multicomponent thin films by sequential flash evaporation, at low temperature (4 K) and HV or UHV, with high compositional accuracy
- in-situ measuring techniques: electron diffraction, resistivity, thermopower, Hall effect, thermal conductivity
- ex-situ measuring techniques: electron diffraction, Hall effect, EELS, resistivity, profilometry

Equipment

- 6 high vacuum cryostats for in-situ measurements between 1 K and 350 K
 - electron scattering and resistivity
 - thermopower and resistivity
 - Hall coefficient and resistivity at 7 Tesla
 - magnetoresistance at 7 Tesla
 - thermal conductance and resistivity
 - resistivity (for screening measurements of 6 different alloys)
- UHV cryostat for electron scattering and resistivity between 1 K and 750 K
- cryostat for ex-situ Hall effect measurements at 7 Tesla
- UHV chamber for resistivity measurements between 300 K and 1000 K
- glove-box for the handling of highly reactive samples
- white-light profilometer

-Scientific cooperation

- State Key Lab for Materials Modification by Laser, lon and Electron Beams, Dalian University of Technology, China







Structure formation at early stages

Crystal formation is by no means well understood. Bottomup as well as top-down techniques are often applied. On the other hand, any crystalline system has a disordered state (liquid, amorphous) as its precursor, in which medium-range order arises for the first time. Its understanding may once give us a flavour how crystals themselves get formed. Analysing many different disordered systems, as the driving effect we found resonance effects between global subsystems, as there are all the electrons as one and the forming static structure as another one. The resonances can be based on an exchange of momentum as well as angular momentum. By their internal degrees of freedom (via an adjustment of the electron-density and/or particledensity oscillations) the subsystems are able to adjust each other in a way that gaps or pseudogaps are formed at the Fermi energy E_r , decreasing effectively the total energy of the system (Peierls-, Hume-Rothery-like). Subsequently, spherical periodic structural order (SPO) arises in the mean around any atom (Fig. 1), causing band-structure

effects. Different scenarios have been observed: the static structure may adjust to the electronic system, as well as, vice versa, the electronic system to the static structure. Charge transfer as well as hybridization effects have been observed to enhance the global resonance. Since there is a gap or pseudogap involved, the evolvement of the static structure is accompanied by the evolvement of electronic transport properties too (Fig. 3). Therefore, any electronic transport delivers valuable additional information, helping to understand the resonance stabilization and hence structure formation. The model has successfully been applied to amorphous non-magnetic as well as magnetic metals, semiconductors, to amorphous guasicrystals and Zintl systems (the latter showing ionic bonding features), as well as to all the alloys between Aluminum and any 3d-transition element with d-electrons at E,, to Heusler- as well as Half-Heusler alloys, to pure elements, binary as well as ternary alloys (Fig. 2). Presently it gets extended to alloys containing rare earth elements with f-electrons at E.

Dynamic low-T anomalies in disordered systems

The spatially limited SPO-regions cause, due to their limited total mass, anomalies in the dynamic excitations at low energies at wave numbers related to the Fermi wavelength and the resonance-triggered atomic positions. All the electrons, the static structure, as well as the dynamic excitations are resonantly coupled to each other. The dynamic dispersion shows so called phonon rotons a shift of lowlying dynamic states to higher energies. Phonon-rotons states can get occupied thermally as well as by a scattering of other particles. Accordingly, low-temperature anomalies may exist in the electronic and thermal transport. This may also be true for those systems showing extreme resonances, to amorphous semiconductors and insulators.

GAS DISCHARGE AND ION PHYSICS Prof. Dr. Dieter Gerlich



Instruments for astrophysical and -chemical studies

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Research fields

- Ion-molecule reactions, plasma- and astrochemistry
- Ion spectroscopy, laser induced reactions
- Mass spectrometry and analytical chemistry
- Material and nanoparticle science

Methods

- Ion trapping and guiding using inhomogeneous RF fields
- Sub-K cooling of ions using a cold effusive beam
- Laser induced reactions
- Nanoparticle mass spectrometry using AC traps

Equipment

- CEB-22PT: UHV instrument for trapping ultracold ions
- HT-4PT: SRE ion trap for monitoring hot nanoparticles
- Sources for special ions, beams of molecules and atoms
- Lasers: TiSa, Nd:YAG, CO2, IR-diode

Scientific cooperation

- University of Arizona, Department of Chemistry (M. Smith)
- University of Basel, Department of Chemistry (J.P. Maier)
- Charles University Prague, Faculty of Mathematics and Physics (J. Glosik)
- TU Berlin, Institut für Optik und Atomare Physik (O. Dopfer)
- MPI-K Heidelberg, Test Storage Ring (A. Wolf)







Charged particles in rf guides and traps

Most of our research is closely related to the development of innovative experimental instruments which have been applied successfully in many fields of plasma physics and ion chemistry. Examples include the development of the first rf octopole ion guide some decades ago, storage ion sources, ring electrode traps, the temperature variable 22pole ion trap, and innovative nanoparticle traps. Our publications shows the wide range of applications of these tools.

Trajectory of an ion in a 32 pole trap

Laboratory astrophysics and -chemistry

Laboratory astrophysics and -chemistry belongs to an interdisciplinary research area covering the physics and chemistry of molecules, clusters, nanoparticles, and grains under the conditions of interstellar space, ranging from low temperature and low density molecular clouds to hot environments of stars. It is our aim to study the microphysics which control the formation and destruction of interstellar matOutstanding results have been obtained, ranging from precise integral cross sections at low energies, high resolution differential cross sections for ion-molecule reactions, sensitive determination of rate coefficients for radiative association and cluster growth, to ion spectroscopy with an unprecedented sensitivity. The nanoparticle mass spectrometry became an innovative tool in material science.

ter and to use the results for understanding observational facts and for predicting new astrophysical features. These activities have been supported by the DFG via the Forschergruppe Laboratory Astrophysics: Structure, Dynamics and Properties of Molecules and Grains in Space (2000-2006). Present activities include reactions of cold ions with hydrogen atoms and the study of hot nanoparticles.

Special high temperature quadrupole trap for nanoparticles

Ultracold ions for Low Energy Ion beam Facilities

Since 2006, the European Integrated Infrastructure Initiative ITS LEIF offers a platform for interdisciplinary research with high-quality low-energy ion beams. It brings together 17 contractors and 14 user groups from 18 EU member states and associated countries. The main objective of the project is to create a platform for interdisciplinary research based on the use of high-quality low-energy ion beams. Our contribution is the development of an source for ultracold molecular ions, ranging from simple diatomic ions via clusters to biomolecules.

SOLID STATE PHYSICS Prof. Dr. Frank Richter



Group picture from October 2007

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Research fields

- plasma-assisted thin film deposition and surface engineering,
- in-situ characterisation of pulsed plasmas,
- modelling of thin film deposition processes,
- mechanical characterisation and modelling of thin films and surfaces.

Methods

- mechanical and geometrical characterisation (nanoindentation, AFM),
- analytical and finite element modelling of mechanical contacts,
- characterisation of thin film deposition processes by Langmuir probe technique, thermal probe, optical emission, mass spectroscopy, and ion energy analysis.

Equipment

- nanoindentation device UMIS 2000 (CSIRO), resolution of load/displacement 0.7 μN / 0.1 nm,
- universal nanomechanical tester (Asmec) using normal and lateral load,
- advanced development surface profiler (Veeco) with low force and stress module,
- plasma process monitor PPM 422 (Inficon) for positive/negative ions/neutrals up to 500 eV,
- optical UV/VIS spectrometer HR 460S (Jobin Yvon), with LN2 cooled CCD camera,
- various thin film deposition facilities for both PVD and PECVD, up to industrial size.

Scientific co-operation

- Universities of Manchester and Liverpool (Great Britain), Uppsala (Sweden), Oak Ridge and Lawrence Berkely Natl. Labs. (USA),
- Fraunhofer-IST (Braunschweig), IWS, and FEP (both Dresden),
- IRTG "Materials and Concepts for Advanced Interconnects" (Chemnitz, Berlin, Shanghai),
- SFB Transregio PT-PIESA (Chemnitz, Dresden, Erlangen).



In-situ characterisation of pulsed plasmas

(currently supported by DFG and Freistaat Sachsen) Pulsed middle-frequency (25 - 250 kHz) magnetron discharges are increasingly important for instance for the high-rate large-area deposition of insulating thin films. However, this process is quite complex and not well understood. Our research interests are the deposition parameters on the atomic scale as described by the fluxes of neutral

Spatial distribution of the plasma potential, $V_{\rho \prime}$ in front of a magnetron sputter source measured at the end of the "on"-phase of the pulse (0.4 Pa Argon, frequency 100 kHz, discharge power 100 W)

particles and ions, their physical nature (mass, charge state, excitation) as well as kinetic energies. These parameters are measured spatially and temporally resolved and provide a basis for an adequate description of the process which eventually enables its optimisation and up-scaling.

IRTG "Materials and Concepts for Advanced Interconnects"







(supported by DFG)

The International (German-Chinese) Research Training Group is focussed on links between preparation of materials, their characterisation on the nanoscale as well as their application to microelectronic devices. The Solid State Physics group provides unique experimental and theoretical methods for mechanical characterisation of thin films and bulk materials. Current highlights are the determination of Young's modulus and yield strength of thin films down to a thickness of 10 - 100 nm as well as the development of methods for the locally resolved measurement of intrinsic stresses in solids by nanoindentation.

Collaborative Research Centre / Transregio "PT-PIESA"

(supported by DFG)

This research is aimed at scientific fundamentals for an efficient production of active structural components. The contribution of the Solid State Physics group is the investigation and development of a thin film system which provides electrical insulation between the piezoelectric sensor/actuator and the metallic support but has at the same time desired mechanical properties. The film has to be grown with sufficient homogeneity at a surface as well as within trenches.

Scanning electron micrograph of a thin film grown within a trench. The arrows visualise the different ion fluxes at the wall and bottom of the trench causing different surface morphology.

SEMICONDUCTOR PHYSICS Prof. Dr. Dr. h. c. Dietrich R. T. Zahn



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Research fields

- Organic semiconductors
- Organic/inorganic interfaces
- Low dimensional semiconductor structures
- Electronic and optoelectronic devices

Methods

- Optical spectroscopies (Raman, IR, spectroscopic ellipsometry, reflectance anisotropy)
- Electron spectroscopies (photoemission, NEXAFS, inverse photoemission)
- Electrical characterisation methods (IV, CV, DLTS, admittance)

Equipment

- Dilor XY 800 triple monochromator with Ar⁺, Kr⁺, HeCd lasers for *ex situ* micro-Raman investigations and *in situ* Raman monitoring (UHV chamber for (organic) molecular beam deposition)
- Variable angle spectroscopic ellipsometer, J. A. Woollam, (240nm-1700nm) FTIR spectrometer Bruker IFS 66 / Vertex 80v
- UHV chambers for *in situ* I-V / C-V measurements and electron spectroscopies (ARUPS, IPES)
- Deposition chamber for *in situ* ellipsometry and reflection anisotropy spectroscopy

Scientific cooperation

- Institute of Semiconductor Physics, 630090 Novosibirsk, Russia
- ISAS Berlin and BESSY
- IRTG "Materials and Concepts for Advanced Interconnects"

Industrial cooperation

- Infineon
- Aixtron

Service

- Metrology of thin films by optical spectroscopies





Organic/inorganic interfaces

The research work of Semiconductor Physics group focuses on the detailed understanding of organic/inorganic interfaces phenomena, their electronic and chemical as well as geometrical and electrical properties. Ultra-thin organic molecular semi-conducting layers are prepared by molecular beam deposition in UHV on inorganic substrates and

Combined VB-PES and IPES measurements of the perylene derivative PTCDI with the charge density contours of the HOMO and LUMO on top of the figure.

IRTG "Materials and Concepts for Advanced Interconnects"

The main objective of the Chinese-German IRTG is highlighting links between fundamental materials properties, their characteristics on the nanoscale, technological aspects of materials and their applications to microelectronic devices. The Semiconductor Physics group provides expertise in optical characterisation of thin films and porous materials. investigated *in situ*. Experimental techniques include high resolution angle resolved photoemission spectroscopy, inverse photoemission spectroscopy and several optical characterisation methods, *e. g.* Raman spectroscopy and reflection anisotropy spectroscopy.

The group has access to a worldwide unique ellipsometer working from the visible to the VUV-XUV range (photon energies 2 - 30 eV) at the synchrotron radiation light source BESSY. The short wavelengths in the VUV-XUV range match to the smallness of device structures and ensure sensitivity at the sub-nanometer thickness level.



Synthesis and optical investigation of novel semiconductor self-assembled quantum dot structures

Quantum dots are attractive systems for new electronic, photonic, or opto-electronic devices. Accurate control of the size, shape, and position of the dots together with a deeper understanding of their influence on final device properties is, however, crucial for the exploitation of these nanostructures in quantum devices. In this research field the Semiconductor Physics group has long term collaboration with the Institute of Semiconductor Physics in Novosibirsk. In the Russian institute high quality quantum dot structures are prepared. These structures are optically characterised in Chemnitz, *e. g.* by means of Raman spectroscopy. The high yield of joint research activities is displayed in more than 50 papers.

InAs QDs embedded in GaAs

CHEMICAL PHYSICS Prof. Dr. Robert Magerle



Microstructure of a cylinder forming block copolymer. Nanotomography volume image reconstructed from a series of tapping-mode scanning force microscopy phase images. From: R. Magerle, Phys. Rev. Lett. 85, 2749 (2000); © 2000 American Physical Society

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Research fields

- Structure and properties of polymeric materials on the nanometer scale. Our current research focus is on block copolymers, semicrystalline polymers, and biological materials

Methods

- Scanning force microscopy,
- Nanotomography: volume imaging based on scanning probe microscopy,
- Scientific image processing.

Equipment

- 4 scanning probe microscopes (JPK NanoWizard I and II, Veeco MultiMode) with accessories for imaging in liquids, at elevated temperatures (up to 240°C), and automated Nanotomography imaging.
- 2 optical microscopes with digital imaging.
- 1 rotary microtome (Leica RM2265) with freezing attachment for cutting at low temperatures (-150°C).
- Thin film preparation laboratory including snow jet for substrate cleaning, spincoater, and ovens.
- Setup for annealing in solvent vapor.







Semicrystalline polymers

Semicrystalline polymers, like polyethylene and polypropylene, are widely used polymeric materials. Their properties can be controlled through synthesis and processing conditions. The material's microstructure is an important parameter and can be imaged with Nanotomography. An example is the structure of a screw dislocation in a crystalline lamella (see figure). Before volume imaging, the formation of the dislocation has been observed with in-situ scanning force microscopy (SFM). With a micro-tensile test setup we track with SFM the deformations of individual crystals during deformation of the material. The data provide a detailed view on the micromechanics of the material on the scale of 10 - 1000 nm. The data are expected to provide a better understanding of the mechanical properties of semicrystalline polymers.

Screw dislocation in a crystalline lamella of elastomeric polypropylene. From: M. Franke, N. Rehse, Macromolecules 41, 163 (2008); © 2008 American Chemical Society.

Mesoscale dynamics of block copolymers

With in-situ tapping mode scanning force microscopy we observe how microdomain patterns rearrange at the surface of a fluid block copolymer film. We study the processes during long-range ordering, terrace formation, and formation of surface reconstructions. Our scanning force microscopy time-laps movies show with 10 nm spatial resolution the mesoscale dynamics and fluctuations during structural phase transitions and phase boundaries between differently ordered phases. Computer simulations based on dynamic density functional theory (MesoDyn) capture the experimental observations in stunning detail.

Nucleation and growth of a perforated lamella phase. Snapshots from an scanning force microscopy movie. From: A. Knoll et al., Nature Materials 3, 886 (2004).,

Biological materials

Biological materials have a complex hierarchical structure ranging from the molecular scale over the nano- and micrometer scale up to the macroscopic length scale. From the materials science point of view, bone can be considered as a composite material of inorganic hydroxyl apatite particles embedded in an organic collagen matrix. We study the structure of human bone and aim establishing routine imaging of native human bone based on Nanotomography. The imaging of mechanical properties with scanning force microscopy is of particular interest for understanding the structure property relationship of bone. For this purpose we develop suitable preparation, etching, and imaging techniques based on scanning probe microscopy.

Microstructure of human bone imaged with bimodal amplitude modulation scanning force microscopy.

X-RAY AND NEUTRON DIFFRACTION Prof. Dr. Walter Hoyer





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X-ray diffractometer SEIFERT XRD-3000PTS

Research fields

- Atomic structure of molten metals and alloys
- Thermophysical properties of molten metals and alloys
- Structural properties of thin solid films and crystalline materials

Methods

- X-ray and neutron diffraction methods
- X-ray absorption techniques
- Computer modelling using the reverse Monte Carlo method
- Tensiometric methods and sessile drop technique
- Viscosity measurements with the oscillating cup technique

Equipment

- SEIFERT-FPM XRD7 two-circle X-ray diffractometer with Eulerian cradle and x-y-moving sample holder
- SEIFERT XRD-3000PTS four-circle X-ray diffractometer equipped with Eulerian cradle, various monochromators and a multilayer mirror
- FPM HZG-4 two-circle diffractometer
- Theta-theta diffractometer for liquid and amorphous samples with secondary monochromator
- Oscillating-cup viscometer for temperatures up to 1400°C
- Tensiometer for measurement of surface and interfacial tension up to 1200°C
- Differential scanning calorimeter NETZSCH DSC-404
- Sessile drop surface tension measurement

Scientific cooperation

- DLR Köln, Institute of Materials Physics in Space, Prof. I. Egry and Prof. L. Ratke
- Paul Verlaine University Metz, Institute of Physics, Prof. J.-G. Gasser
- Ivan Franko National University Lviv, Institute of Physics, Dr. Yu. Plevachuk
- Scientific Research Comp. CARAT Lviv, Prof. 0, Shpotyuk
- Univ. of Chemical Technology and Metallurgy Sofia, Dept. of Physics; Prof. P. Petkov
- CNRS-CEMHTI Orleans, Dr. Louis Hennet
- University of Vienna, Materials Chemistry, Prof. A. Mikula, Dr. S. Knott







Heterogeneous nucleation in the liquid-liquid demixing process in monotectic alloys

Al-based alloys containing soft metals like Bi, In or Pb are considered as very promising candidates to be used as self-lubricating bearings. The main problem putting obstacles in the way of practical application of these alloys (called as monotectic alloys) is their demixing. As an example, $(AI_{0.345}Bi_{0.655})_{90}Sn_{10}$ alloy solidified in graphite crucible is shown in the Figure.

The aim of the project is to investigate how materials like

Cross section of a demixed sample in a graphite crucible

TiB₂, TiC and Circonia (so called grain finer which are acting as heterogeneous nuclei) influence the kinetics of demixing. In this way an important step is the determination of wetting angles between melt and grain finer ceramics. This enables to calculate the catalytic factor of the heterogeneous nucleation rate in theoretical models.

(Supported by DFG, in co-operation with DLR Köln, Institute of Materials Physics in Space, Prof. L. Ratke)

Atomic structure and dynamic viscosity of liquid Al-Ni-Si alloys

Multi-component aluminium-based alloys gain further importance as lightweight materials with high mechanical strength. Their industrial application usually involves casting processes which are governed mainly by the dynamic viscosity. Investigation of both, the dynamic viscosity as a function of temperature and composition using a hightemperature oscillating-cup viscometer developed in our group, as well as the atomic structure in the liquid state by X-ray and neutron diffraction techniques is therefore important for the optimization of the properties of the final material as well as manufacturing processes. (Supported by DFG, in co-operation with DLR Köln, Institute of Materials Physics in Space, Prof. I. Egry)

Cup and sample container of the high-temperature oscillating-cup viscometer

The dynamic viscosity of phase-change materials for data storage applications

Phase-change data storage, as for instance employed in CD- and DVD-media, relies on a distinct difference in the optical or electrical properties in the crystalline and amorphous state of a material. The data rate to be gained in such a storage device is governed by the kinetics of solidification (liquid to glass transition) and crystal growth, and thus, by mass transport properties described by the dynamic viscosity in the liquid and under-cooled liquid state. This research project aims to measure the dynamic viscosity of liquid Ag-Sb-Te alloys, which seem to have promising properties. The experiments are carried out using an high-temperature oscillating cup viscometer and will be supported by model calculations applying suitable thermophysical models. (Supported by DFG)

Cross section of a sample after viscosity measurement

OPTICAL SPECTROSCOPY AND MOLECULAR PHYSICS Prof. Dr. Christian von Borczyskowski



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Research fields

- Optical Spectroscopy and Microscopy on Molecular and Complex Materials:

Soft Matter Physics

- Molecular Dynamics at Interfaces
- Photochemistry of Organic Materials
- Self-Aggregation Processes

Quantum Confined Systems

- Optical Properties of Semiconductors
- Photoluminescence Dynamics
- Electron-Phonon Interaction

Nanolithographie

- Generation of Nanostructures
- Functionalisation of Nano-Devices

Laser Induced Plasma

- Plasma Dynamics
- Plasmagenerated Materials

Methods

- (Time resolved) Optical Spectroscopy
- Single Quantum System Detection
- Nano-Optical Microscopy
- AFM- Microscopy
- Laser Interferometrie

Scientific cooperation

- DFG Research Group "From local constraints to macroscopic transport"; Institute of Astrophysics, Jena; National Academy of Science, Minsk; University Lyon; University of Buenos Aires; Department of Materials Engineering Science, Osaka; Institute of Applied Physics, Gießen; Institute of Physical Chemistry and Electrochemistry, Hannover;IZM Fraunhofer Institute; Berlin, Chemnitz; Moscow Institute for Physics and Technology; 3D- Micromac AG, Chemnitz







Single Molecule Probes in Soft Matter

Individual fluorescent dye molecules are used as probes for nanoscale structure and dynamics in various soft materials, such as liquids, polymers or liquid crystals. Typical single molecule observables, such as mobility, excited state lifetime, luminescence polarization or intensity fluctuations are used by us as reporters on the spatial and temporal heterogeneity in this class of materials. Since many properties of soft materials are closely related to thermal fluctuations and heterogeneities we are able to contribute to central questions in the field.

Distribution of diffusion constants for single molecules in thin films

Diffusion tracks of single molecules

Manipulation and Analytics of Surfaces and Interfaces

Self-assembled monolayers covalently linked on silicon and silicon oxide are used for adjustment of surface properties as hydrophobicity or selective anchoring sites. The properties are investigated by water contact angle measurement, atomic force microscopy and by optical methods. Structuring on the nanometer scale by atomic force microscope followed by selective binding e.g. by electrostatic interactions of optical active materials opens the way to functional nanostructures. Spatial, spectral and time-resolved optical methods are used for characterization of the prepared nanostructures.

AFM lithographie of silicon oxide

AFM lithographie

Interferometrie on Laser induced Plasma

Picosecond laser pulses at the wavelength of 1064 nm have been focused onto copper cathodes in coincidence with electric fields to produce laser-induced breakdown in vacuum. At high power densities formation of local regions with high pressures and temperatures have been investigated in cathode micro-volumes. As a result of an intensive energy deposition in a small volume a strongly coupled cathode micro-plasma was formed, of which the properties varied during non-stationary processes of heating and hydrodynamic motion over a wide range of the phase diagram : from a Fermi-like to an ideal plasma. org. ML SiOx

Spatial distribution of pressure for t = 2.075 ns



Laser induced plasma bullets

Calculation of metal plasma for a cathode micro-plasma

COMPLEX SYSTEMS AND NONLINEAR DYNAMICS Prof. Dr. Günter Radons



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Research fields

- Lyapunov instabilities of extended dynamical systems
- Anomalous diffusion processes
- Dynamical systems with hysteresis
- Systems with varying delay
- Formation of localized modes and coherent structures
- Time series analysis of complex systems

Methods

- Smart brain-work
- Analysis of complex systems and problem solving
- Numerical and analytical tools of nonlinear dynamics and disordered systems
- Time-series and data analysis
- Parallel and high-perfomance computing

Equipment

- Compute cluster with 48 Opteron Dual Core processors
- Compute cluster with 96 Opteron Dual Core processors (Theoretical Physics)
- CHiC (Chemnitz University of Technology)
- JUGENE (Forschungszentrum Jülich)
- Jump cluster (Forschungszentrum Jülich)

Scientific cooperations

- Max Planck Institute for the Physics of Complex Systems, Dresden
- Queen Mary, University of London, School of Mathematical Sciences
- Sächs. Forschergruppe 877 (From Local Constraints to Macroscopic Transport)
- Max Planck Institute for Plasmaphysics, Garching
- Technical University of Lublin, Department of Applied Mechanics
- CEA-Saclay, France
- Fraunhofer Institutes (IPA, IWU, EMI)

Industrial cooperations

- Robert Bosch AG, Stuttgart
- Airbus Deutschland GmbH, Hamburg









Lyapunov instabilities of extended dynamical systems

The modern theory of nonlinear dynamics is of great importance for the understanding of the fundamentals of statistical mechanics. We are mainly interested in the Lyapunov instabilities of extended dynamical systems and possible implications for their macroscopic behavior. The systems we deal with include coupled map lattices, Hamiltonian lattice models, partial differential equation (PDE) systems and glass formers.

Lyapunov spectral gap

Dynamical systems with hysteresis

Many systems ranging from magnetic materials to shape memory alloys, or fluids in porous structures, and certain friction models show complex hysteretic behavior in the sense that besides major loops, subloops and non-local memory effects are observed. The most prominent phe-

Return map for tent map under hysteresis

Systems with varying delay

Delay differential equation with constant delay are nowadays well understood. In real applications, ranging from machining operations such as turning or milling to the evolution of biological systems, the delay is actually time- or

Turning process

Anomalous diffusion processes

Recently it has been recognized that many transport processes do not show standard or normal diffusion, but behave anomalously. Our research on anomalous diffusion processes is motivated by stability considerations in plasma

Two-layer diffusion process

nomenological model to account for such effects is the so-called Preisach model. Our main interest lies in the investigation of general properties of dynamical systems with hysteresis.

state-dependent. Such systems are much less understood. Our research aims at a deeper understanding especially of stabilty issues in dependence on the delay characteristics.

physics, by the experimental observation of molecular diffusion in thin fluid layers at solid surfaces, and more generally, by questions of transport in disordered environments.

THEORY OF DISORDERED SYSTEMS Prof. Dr. Michael Schreiber



Group members and research collaborators



Ensemble of disordered icecream containers (long term study)

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Research fields

- Disordered quantum systems (Anderson localization, Coulomb glass)
- Quantum and molecular dynamics
- Quasicrystals
- Formation of correlations and structure
- Nanostructures and interfaces

Methods

- Solution of large-scale eigenvalue problems especially for sparse matrices
- Analysis of eigenvalue spectra and wave functions (multifractal analysis, participation ratio, etc.)
- Random matrix theory (level spacing distribution)
- Quantum master equations for density matrices (molecular wires)
- Density functional methods (molecules, molecular crystals, inorganic semiconductors)
- Empirical tight-binding approach (inorganic semiconductors, nanotubes, metal-nonmetal interfaces)

Equipment

- Compute Cluster with 86 Opteron Dual Core processors
- Compute Cluster with 96 Opteron Quad Core processors, InfiniBand interconnect, 816 GB total memory and 24TB external raid storage

Scientific cooperation

- Research center Forschungszentrum Dresden-Rossendorf e.V.
- Jacobs University Bremen
- Leibniz Institute for Solid State and Materials Research Dresden
- Max-Planck-Institute for Physics of Complex Systems, Dresden
- Technical University Munich
- University of Tartu (Estonia)
- University of Warwick (England)







Disordered quantum systems

The transition between metallic and insulating phase (MIT) of a solid exhibits a variety of interesting phenomena. Fundamentally, the MIT can be well described by a variation of disorder in the sample or/and of interactions between charge carriers. We study a purely disorder driven MIT using the Anderson model of localization discretized on a lattice, where disorder is contained as potential disorder on the sites and as topological disorder in the links between sites. In a disordered potential exceptional statistical fluctuations lead to so-called anomalously localized states that appear in the metallic phase and also at the MIT. We find that these states can influence the behaviour of the critical properties. Topological disorder is investigated for quasicrystalline structures and samples with sites connected according to a small-world network. The MIT is located numerically and characterized by its critical parameters.

Anomalously localized state for a system with size 120³. The probabilities are proportional to the volume of the colored boxes.

Semiconductor spectroscopy

The spectroscopic properties of inorganic and organic materials are investigated with complementary microscopic approaches. For molecules and molecular materials, the coupling between electronic excitations and internal vibrations plays a key role. Therefore, microscopic models for the optical response have to account for the coupling between excitons and internal vibrations.

Highest occupied molecular orbital of Si₁₇H₃₆ (B3LYP/double-zeta)

Interacting Fermi- and Bosegases

Near Feshbach resonances it is possible to tune the interaction in ultra-cold Fermi and Bose gases. One can therefore vary the interaction in a Bose-Einstein condensate (BEC) or drive a Fermi gas through a transition from Cooper pairs in a BCS state to two-particle bound states which can also form a BEC. The main interest of the group lies on the conditions for the formation of bound states, Cooper pairs or a We have recently investigated the photoluminescence (PL) of H-passivated tetrahedral silicon nanocrystals up to a diameter of 2.5 nm by using a time-dependent DFT method. From a comparison of our calculations with measured PL bands obtained on clusters with known size distribution, we find an agreement of the PL energies within better than 0.2 eV.

BEC. Especially the dependence of these conditions on the interaction is investigated. Calculations are done mainly analytically with a many-body Green functions technique for idealized potentials. Therefore also medium effects such as Bose enhancement and Pauli repulsion can be included. Furthermore the deformations of surfaces of superconductors caused by vertex motion are investigated.

Phase diagram for bound states (BS) of an interacting Bose gas.

THEORETICAL AND COMPUTATIONAL PHYSICS Prof. Dr. Karl Heinz Hoffmann



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Research fields

- Dynamics of Complex Systems
- Spin Glasses
- Energy Landscapes
- Irreversible Thermodynamics
- Quantum Thermodynamics
- Anomalous Diffusion
- Phase Transitions and Thermodynamic State Equations
- Stochastic Optimization

Methods

- Mathematical Analysis
- Algebraic Computing
- High Performance Computing
- Parallel Computing

Equipment

- Super-Scalar-Cluster (44 CPU Intel Opteron, 192 GB RAM)
- Hochleistungs-Linux-Cluster CHiC (Nutzung)

Scientific cooperation

- San Diego State University, USA, Complex Systems, Optimization
- University of Western Ontario, Canada, Mathematics, Fractals
- University of Southern Denmark, Denmark, Spin Glasses
- University of Copenhagen, Denmark, Thermodynamics
- Jadavpur University, India, Complex Systems, Fractals
- University of Chicago, USA, Thermodynamics, Energy Landscapes
- MPI Festkörperforschung Stuttgart, Complex Systems

Industrial cooperation

- BASF AG, Ludwigshafen, Thermodynamics







Complex Systems

An often-used picture for complex systems is that of a mountainous landscape, where the heights of the mountains represent the energy, which depends on the state in all the degrees of freedom. Typical examples of such complex systems are spin glasses, cluster of molecules with their thermal relaxation behavior, or proteins with their folding dynamics. Studying the dynamics of complex

An example for complex systems: Amorphous carbons

Irreversible Thermodynamics

Usually, results of simple thermodynamics are obtained from the study of reversible processes. However, this contradicts the dynamics of the world we are living in. Existing heat engines, for example, never attain more than a fraction of the reversible Carnot efficiency. A number of approaches - Finite-Time Thermodynamics and Endoreverssystems means to overcome the problem of the enormous number of states. This number can be reduced considerably by coarse graining the state space. Often the resulting structure has a tree topology. The result is that Marcov processes on tree structures are good modelling tools for the thermal relaxation of complex systems.

ible Thermodynamics - have been developed to overcome that shortcoming and to provide better limits and bounds. Innovative theoretical techniques have been developed to model the performance of for instance automobile engines, refrigerators, heat pumps, solar cells, and chemical distillation processes.

A distillation column

Stochastic Optimization

Stochastic optimization procedures try to provide solutions to optimization problems which have many local minima in their objective function. For these optimization problems the usual steepest descent algorithms fail as they get easily caught in local minima. Therefore, we investigate controlled optimization dynamics using tools based on theoretical physics concepts. Stochastic optimization procedures and especially simulated annealing have been used with growing success, to provide at least "good" solutions which are not too "far" apart from the desired global minimum. A typical field of application is the travelling salesman problem.

The "travelling salesman" problem

ORGANIC SEMICONDUCTORS JProf. Dr. Georgeta Salvan





Group picture from February 2008



Magneto-optical Kerr effect spectrometer

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Research fields

- Heterostructures of organic semiconductors and magnetic metals
- Organic semiconductors
- Metal-organic complexes

Methods

- magneto-optical Kerr effect (MOKE) spectroscopy
- optical spectroscopies (in cooperation with the Semiconductor Physics group)

Equipment

- home-built MOKE spectrometer (1.5 eV 5 eV)
- electromagnet (up to 1 T) for magneto-optical investigations (Schüler Magnetik)
- spin-coater

Scientific cooperation

- Babes-Bolyai University Cluj-Napoca, Romania
- University of Florence
- Princeton University

Service

- MOKE spectroscopic characterization



Metal-organic complexes

Molecule based magnetic materials are of potential interest for a new generation of magneto-optical data storage elements. Transition metal complexes are promising candidates due to the many possibilities of varying their structure and thereby influencing their physical and chemical properties, e. g.: transition metals, heteroatoms (0, N, S), bridging ligands, central bridge, nuclearity. Technological applications of magnetic molecules such as magneto-strictive sensors, spintronic components, and magneto-optical data processing units may arise when thin films, multi-layers or nanostructures with well defined physical properties can be produced in a controlled way. In collaboration with the department of chemistry we synthesize such compounds and deposit them in form of thin films and perform electron paramagnetic resonance (EPR), magnetic susceptibility, and magneto-optic Kerr effect (MOKE) investigations.

Polarization microscopy images of a tri-nuclear Cu complex on Si(111)/SiO2 using unpolarized (a)/(c) and polarized light (b)/(d), respectively, for a film produced by dipping into a solution (a)/(b) and a sample spin coated with 1000 rpm (c)/(d).

Heterostructures of organic semiconductors and magnetic metals

Organic materials have great application potential in the field of spintronic devices, since pure organic layers or organic layers doped with magnetic nanoparticles can be used to mediate or control a spin-polarized signal. One research direction of the Organic Semiconductors group is the investigation of the formation of transition metal nanoparticles in organic matrices and their structural and magnetic properties. Another research focus lies in the understanding the role played by the properties of an organic film on the growth and magnetic properties of a top transition metal electrode in structures similar to those met in vertical spin valves.

Tuning of the MOKE signal of a metal/organic heterostructure by changing the organic film thickness

Magneto-optical properties of organic semiconductors

Organic molecules are known since decades to change the polarization state of the light transmitted through a solution or a film under applied magnetic field. In the view of possible applications in the emerging field of organicbased spintronic devices, however, the magneto-optical activity of molecular thin films in reflection mode when deposited on opaque substrates is of higher interest. The Organic Semiconductors group showed that molecules Spectra of the magneto-optical constant (Voigt) of CuPc for three groups of thin films having different molecular orientation.

from the class of phthalocyanines exhibit a significant MOKE signal at room temperature, only two to three orders of magnitude lower than that of ferromagnetic systems. The MOKE spectra in the visible to near ultraviolet spectral range can be exploited to determine the magneto-optical material constant and subsequently the orientation of the molecules with respect to the substrate in the thin films.





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