## Institute of Physics

of the University of Rostock

# **Research Report**

# 2004 - 2006

University of Rostock

2007

Editor:

Institute of Physics University of Rostock

The Institute of Physics was known as the Department of Physics until Nov. 15, 2004 when the Faculty of Mathematics and Natural Sciences decided in favor of the new name.

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## Preface

The Institute of Physics at the University of Rostock herewith presents its Research Report for the time span 2004 - 2006. This preface briefly introduces the reader to the city and the university, and their historical development.

### City of Rostock: On the Shores of the Baltic

The city of Rostock is located on the shores of the Baltic Sea in the North-East of Germany, between Hamburg (150 km to the southwest), Berlin (160 km to the south), Copenhagen (170 km to the North), and Sczeczin (160 km to the East). Over 700 years ago, Rostock was one of the founding members of the Hanseatic League, an alliance of trading guilds which held a trade monopoly over most of

Northern Europe from the 13<sup>th</sup> to the 17<sup>th</sup> century. During this time Rostock prospered through international commerce. After a long history of ups and downs, the city now has 200 000 inhabitants and is by far the largest town in the state of Mecklenburg-Vorpommern. Rostock is the cultural and commercial hub in one of the most favored holiday regions in Germany.



#### A view of Rostock

One of Germany's major ports is found here; busy ferry lines serve Denmark, Sweden, Finland, and the Baltic States. The city is home to shipbuilding, wind turbine, and other industries. At the same time, there are wide sandy beaches; the waters are clean and invite swimming, yachting, and fishing. The hinterland is a large expanse of lakes and forests, and the climate gives Rostock more annual sunshine hours than in most of the rest of Germany. The charming, beautifully restored inner city features quite a few authentic half-a-millennium-old houses and impressive churches. Take the brick gothic St. Mary's church: The astronomical clock on display there keeps using many of its original parts and has been ticking away basically without interruption for more than half a millenium, which is quite unique. Rostock has achieved a couple of technological "firsts": the first German propeller-driven all-steel ship was built here in 1842, and the world's first jet engine airplane, The Heinkel He 178, took off in 1939. Today, this town has a lot to offer both for guests and residents, of which 14 000 are students of this university.

#### The University of Rostock: Tradition and Innovation



Rostock University

The University of Rostock was founded in 1419 – three decades after Heidelberg and one decade after Leipzig. This makes it the oldest university in the realm of the Baltic Sea (Scandinavia and North-East Europe). The original faculties were Law, Medicine, and Arts; the latter back then was understood to encompass Rhetoric, Grammar, Dialectics, Geometry, Astronomy, Arithmetics and Music. 13 years later, a faculty of Theology was added.

A famous student during the early years was Tycho Brahe, later in life an eminent astronomer who provided the observational data which prompted Johannes Kepler to overturn our concept of Earth's role in space.

As universities here and elsewhere diversified, a first chair of physics was created in 1874 for Ludwig Matthiessen. Since then,

several scientists with well-known names in the world of physics have been professors here, like Otto Stern, Pascal Jordan, Walter Schottky, and Friedrich Hund. Today Rostock University is a place where time-honored tradition meets rapid innovation; hence the university's motto:

#### Traditio et Innovatio

Presently the university comprises nine faculties; among them, the Faculty of Mathematics and Natural Sciences is the home of the Institutes for Mathematics, Physics, Chemistry, and Biology. The Institute of Physics consists of 15 groups, each headed by a professor; between them they cover the field of physics in its breadth both in teaching and in research. Two external research institutions are closely linked to the Institute of Physics: The Baltic Sea Research Institute in Rostock and the Leibniz Institute of Atmospheric Physics in Kühlungsborn, a short drive out of town.

After the turmoil of German unification, this university underwent a complete reorganization. Meanwhile that pays off nicely: Our institute prides itself for having fully competitive equipment ranging from electron microscopes to tunnel microscopes, from high-power lasers to femtosecond lasers, from state-of-the-art computing infrastructure to an all-new first-rate library, and so on. And besides, our student's restaurant has repeatedly been ranked one of Germany's best (or actually the best)...

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### 2004-2006: The Period of This Report

The Institute of Physics focuses its research on the following topics:

- Optics and laser physics
- Nanostructured materials
- Particles and fields
- Physics of the atmosphere and the oceans

There is also a group devoted to the Didactics of Physics. The traditional study program leads to the degree of  $Physik-Diplom^1$ . There are also programs for teachers of all types of schools, and an International Master's Program. Those who remain in research after their first degree can proceed towards a doctoral degree, and beyond that in the German system there is a second doctoral degree, the *Habilitation*.

The period of this report saw the expiry of a *Graduiertenkolleq* (research training group) which successfully helped our students reach their PhD in a structured, cooperative atmosphere. Also during the period, a Sonderforschungsbereich (Collaborative Research Center) on 'Kinetics of Partially Ionized Plasmas' (in cooperation with the University of Greifswald) expired after the theoretical maximum funding period of 12 years. However, our proposal of a new Collaborative Research Center on 'Strong correlations and cooperative effects in radiation fields: Coulomb systems, clusters, and particles' was positively assessed and granted, and took up its work in 2005. We also offer an International Postgraduate Program on 'Physics, Chemistry, and Technology of New Materials'.



The Institute of Physics

In the following, this report provides statistical information about the institute, gives a short summary for each of the research groups including Didactics of Physics and the associated institutes, and presents a full bibliography for the report period.

Prof. Dr. Fedor Mitschke Managing Director, Institute of Physics

<sup>&</sup>lt;sup>1</sup>Beginning 2007, this is phased out in favor of a Bachelor's / Master's program.

## 1 Overview of the Institute

## 1.1 Scientific Staff

Members	2004	2005	2006
C4 professors	9	9	8
C3 professors	6	5	5
Other Sci. Teachers (Privatdozent)	7	8	6

In 2006 the Institute of Physics had 52 PhD scientists and 45 PhD students.

## 1.2 Research Projects Supported by External Sources

The research projects of the Institute of Physics are supported by various organisations such as Deutsche Forschungsgemeinschaft (DFG), Bundesministerium für Bildung und Forschung (BMBF), and European Union (EU), by programs within the scope of the Hochschulbauförderungsgesetz (HBFG), and by the Volkswagen-Stiftung. The major part of both salaries and operational expenses was financed by these external financial sources.

The budget from external sources exceeded 3 Mio  $\in$  in 2006.

## **1.3** Academic Qualifications

Type of Qualification	2004	2005	2006
Habilitation /Postdoctoral Lecture Qualification	1	1	1
Doctor's Degree / PhD	13	19	6

Authors and Titles of Postdoctoral Theses (Date of Conferment):

Rapp, Markus	On the Physics of Polar Mesosphere Summer Echoes (03.05.2004)
Reinholz, Heidi	Dielectric and Optical Properties of Dense Plasmas (27.06.2005)
Achatz, Ulrich	Gravity-Wave Breakdown in a Rotating Boussinesq Fluid: Linear and Nonlinear Dynamics (06.11.2006)

## Authors and Titles of PhD Theses:

## 2004

2004	
Behnke, Danilo	Conformal Cosmology Approach to the Problem of Dark Energy
Döppner, Tilo	Aufladungsdynamik von Metallclustern nach Anregung mit intensiven Femtosekunden-Laserpulsen
Fricke-Begemann, Cord	Lidar Investigations of the Mesopause Region: Temperature Structure and Variability
Gehre, Matthias	Entwicklung moderner Methoden zur Analytik stabiler Umwelt- isotope
Körnich, Heiner	Variabilitätsmuster der atmosphärischen Zirkulation in Abhängigkeit von der Orographie und der Land-Meer-Verteilung
Lakshmi Narayanan, Kamatchi	Nanostructure of Silica in Biological Systems
Millat, Thomas	Absorption und dynamische Stoßfrequenz in nichtidealen Plasmen
Müllemann, Arno	Temperaturen, Winde und Turbulenz in der polaren Sommer- mesosphäre
Neißner, Christian	Quantenstatistische Beschreibung des Bindungsverhaltens der Elektronen in dichten COULOMB-Systemen
Pernack, Robert	J/ $\psi$ - und $\psi$ '-Produktion bei HERA-B
Sändig, Beate	Die Mischung passiver Tracer in Troposphäre und Stratosphäre in ihrer Abhängigkeit zur Anregung planetarer Wellen
Stir, Manuela Elena	Structure and dynamics of amorphous and nanostructured materials
Teuber, Silvio	Wechselwirkung von Metallclustern mit intensiven Laserfeldern
<b>2005</b> Adelswärd, Anicka	Laser-driven quantum motion of small molecules
Aguilera, Deborah Nancy	Color superconducting quark matter in a two flavor nonlocal chiral model under compact star constraints
Fennel, Thomas	Semiklassische Vlasov-Simulationen zur Beschreibung der Ioni- sationsdynamik von Metallclustern in intensiven Laserfeldern
Ivanov, Dennis	Feedback Control of Trapped Atoms
Jonas, Karl-Ludwig	Tunnelmikroskopie und -spektroskopie an Silberclustern und -inseln
Juranek, Hauke	Zustandsgleichung von Wasserstoff bei hohen Drücken im Mbar-Bereich
Klähn, Thomas	Einfluß der Elektron-Phonon-Wechselwirkung auf das Absorptionsverhalten von polaren Halbleitern

Klein, Torsten	Austauschgekoppelte magnetische Schichten: Variation der Kopplung durch Magnetfelder
Kuligk, Angelika	Stoßionisation und Hochfeldtransport in GaAs, GaN und ZnS
Mattiello, Stefano	Dreiquarkkorrelationen in heißer und dichter Quarkmaterie
Methling, Ralf-Peter	Erzeugung und Untersuchung von Nanoteilchen aus der Clusterquelle ACIS
Radcliffe, Paul	The Ionization Dynamics of Silver Clusters after Exposure to Strong Laser Pulses
Remer, Ralf	Theorie und Simulation von Zeitreihen mit Anwendungen auf die Aktienkursdynamik
Roth, Thomas	Development and Applications of the Nuclear Lighthouse Effect at high energies and at grazing incidence
Seemann, Matthias	Characterisation of optically excited semiconductors by phase- resolved pump-probe spectroscopy
Seifert, Birger	Phasensensitive Charakterisierung von klassischem und nicht- klassischem Licht
Soliman, Ragab M.	Early Stages of Polymer Crystallisation studied by Dielectric Spectroscopy
Stratmann, Martin	Moleküle aus Solitonen in Glasphasern
Voigt, Tom-Michael	Zur Dynamik von Erbium-Faserlasern: Vom Einmodenbetrieb bis zu Pulsstrukturen
2006	
Kleibert, Armin	Massengefilterte Eisennanopartikel auf ultradünnen Kobaltfil- men — eine in situ Studie mit weicher Röntgenstrahlung
Meinke, Frithjof	Einfluß der räumlichen Dispersion auf die exzitonische Lumi- neszenz direkter Halbleiter
Schreckenberg, Martin	Messungen unelastischer Röntgenstreuung an Silizium
Schwedt, Daniel	Räumlich und spektral hochaufgelöste Spektroskopie der Resonanzfluoreszenz an Exzitonen in ungeordneten Halbleiterquantenfilmen
Serafimovich, Andrei	Investigation of gravity waves with VHF radar measurements
Wong, Stefanie Yi Chuin	Variability-Lifetime Relation of Atmospheric Tracers Based on Aircraft Measurements during the INDOEX and STREAM 98 Campaigns

## 1.4 Scientific Colloquia

The Scientific Colloquium of the Department has a long tradition. It is an attractive forum where reputable scientists, both domestic and international, present the latest research and discuss hot topics.

The speakers and their subjects were:

08.01.04	Prof. Dr. R. Zimmermann (Humboldt-Universität Berlin)	Excitonen in dimensionsreduzierten Halb- leiterstrukturen
08.01.04	Daniel Mandelik (Weizmann Institute of Science, Rehovot, Israel)	Solitons in Waveguide Arrays
22.01.04	Prof. Dr. W. Hofmann (Max-Planck-Institut für Kernphysik Heidelberg)	Elementarteilchen aus dem Kosmos
29.01.04	Jochen Lehmann (FH Stralsund)	Hydrogen as an energy carrier — technical and political aspects
13.04.04	H. Wang (Eugene/Oregon, USA)	Controlling photons with spin coherences in semiconductors
15.04.04	Ch. Minx, D. Penski, P. Hartmann (Schüler des Goethe-Gymna- siums Rostock)	Projektarbeit im Leistungskurs Physik: Hauptmaschinenanlage des MS Georg Büchner
15.04.04	Prof. Dr. H. Schecker (Universität Bremen)	Physik multimedial — Lehr- und Lernmo- delle für das Studium der Physik
06.05.04	Prof. Dr. HJ. Freund (Fritz-Haber-Institut Berlin)	Nanoteilchen als Modellsysteme in der Katalyse
13.05.04	Prof. Dr. G. Wunner (Universität Stuttgart)	Neue Entwicklung in der Kosmologie
03.06.04	S. Kümmel (Max-Planck-Institut komple- xer Systeme, Dresden)	Dichtefunktionaltheorie: Chance oder Sackgasse?
10.06.04	Prof. Dr. J. Peinke (Carl von Ossietzky Uni- versität Oldenburg)	Turbulenz und Turbulenzen am Finanz- markt
23.06.04	C. Deutsch (U Paris-Sud)	Interaction of Intense Relativistic Elec- tron Beams with Plasmas (Greifswald-Rostock-Seminar)
24.06.04	Prof. Dr. G. Gerber (Universität Würzburg)	Laser-optimierte Femtophysik/-chemie: Quantenkontrolle durch lernfähige Femtosekunden-Laser

01.07.04	Prof. Dr. Schwalm (Max-Planck-Institut für Kernphysik Heidelberg)	Kosmologie und Experimente der Teilchenphysik
08.07.04	Prof. Dr. C. Hagner (Institut für Experimentelle Physik Hamburg)	Neutrinos — Massen, Mischung und Os- zillationen
14.07.04	M. Roth (TU Darmstadt)	Intensive Laser- und Ionenstrahlen (Greifswald-Rostock-Seminar)
07.10.04	Dr. T. Tschentscher (DESY Hamburg)	Freie-Elektronen-Laser
08.10.04	Prof. Dr. Q. Rahman (Industrial Toxicology Re- search Center, Lucknow, India)	Problems Associated with Ultrafine Par- ticles
04.11.04	PD. Dr. M. Zacharias (Max-Planck-Institut für Mikrostrukturphysik, Halle)	Confinement Systeme und Nanostruk- turen — die neue Perspektive für Silizium
05.11.04	Dr. P. Cea (University of Zaragoza, Spanien)	The Langmuir-Blodgett Technique: A Multidisciplinary Research Field with Im- plications in Chemistry, Physics, Biology and Engineering
08.11.04	Prof. Dr. HO. Peitgen (Universität Bremen)	Ordnung im Chaos — Chaos in der Ord- nung
11.11.04	Prof. Dr. M. Arndt (Universität Wien)	Molekülinterferometrie und Nanophysik
12.11.04	PD Dr. F. Bufler (Institut für Integrierte Sys- teme, ETH Zürich)	Monte Carlo Simulation of Semiconductor Devices
25.11.04	Prof. Dr. U. Heinzmann (Universität Bielefeld)	Zeit- und phasenaufgelöste Photoelektro- nenspektroskopie — ein Beitrag zum Jubiläum: 100 Jahre Photoeffekt
02.12.04	Prof. Dr. Forchel (Universität Würzburg)	Quantenpunkte in Mikroresonatoren
09.12.04	Prof. Dr. R. Dörner (Universität Frankfurt)	Von tanzenden Elektronen und zitternden Kernen — Quantendynamik von Wenig- Teilchen-Systemen
10.12.04	Prof. Dr. W. Hoyer (TU Chemnitz)	Structure and Properties of Molten Metallic Alloys
14.12.04	Milutin Stepic (Universität Clausthal)	Unusual properties of optical solitons in photorefractive nonlinear waveguide ar- rays

16.12.04	Prof. Dr. Ebeling (Humboldt-Universität zu Berlin)	Schwärme von Insekten, Fischen und Vögeln — aus der Sicht des Physikers
07.01.05	Prof. Dr. B. Nestler (University of Applied Sci- ences, Karlsruhe)	Modelling and Simulation of Phase Trans- formations
11.01.05	Prof. Dr. H. Kantz (MPI PKS Dresden)	Extreme Ereignisse: Eine Heraus- forderung an das Verständnis komplexer Systeme
20.01.05	Prof. Dr. M. Fleischhauer (TU Kaiserslautern)	Quantenelektrodynamik in Medien mit negativem Brechungsindex
21.01.05	Prof. Dr. G. Heinrich (Leibniz-Institut für Polymer- forschung, TU Dresden)	Polymer Materials Research: from Basic to Industrial Applications
26.01.05	Prof. Dr. J. Harff und Prof. Dr. H. Burchard (Leibniz-Institut für Ostsee- forschung Warnemünde)	Tsunamis
14.04.05	Dr. O. Stachs (Augenklinik Rostock)	Konzepte zur Wiederherstellung der hu- manen Akkomodationsfähigkeit
12.05.05	Prof. Dr. D. Michel (Universität Leipzig)	NMR-Untersuchungen von Ordnungs- und Unordnungsphänomenen in Festkör- pern mit strukturellen Phasenübergängen
19.05.05	Prof. Dr. W. Rozmus (Alberta, USA)	Theory of Thomson Scattering
02.06.05	Prof. Dr. G. Rempe (MPI für Quantenoptik, Garching)	Wo Einstein irrte und doch Recht hatte: Vom Photoeffekt zur Photonenpistole
16.06.05	Prof. Dr. W. Lauterborn (Universität Göttingen)	Blasen aus Schall und Licht
19.06.05	Prof. Dr. D. MacFarlane (San Diego, USA)	Matter-antimatter asymmetries in B decays
23.06.05	Prof. Dr. S. Solanki (Direktor des MPI für Sonnensystemforschung in Katlenburg-Lindau)	Was hat das Magnetfeld der Sonne mit Einstein und unserem Klima zu tun?
07.07.05	Prof. Dr. L. Kipp (Universität Kiel)	Von Einsteins Photoeffekt zur Forschung mit dem Freie-Elektronen-Laser
18.10.05	Dr. V. Gryaznov (Institute of Problems of Chemical Physics, Chernogolovka, Rußland)	Equation of state of solar plasma with SAHA-S model

10.11.05	PD Dr. Steinmeyer (Max-Born-Institut, Berlin)	Ultrakurze Lichtpulse
22.11.05	Prof. Dr. Z. Hradil (Universität Olomouc, Tschechien)	Quantum measurement and estimation
24.11.05	Dr. M. Betz (TU München)	Ultraschnelle Ladungsträgerdynamik in Halbleiter-Nanostrukturen
08.12.05	Prof. Dr. G. Meijer (Direktor am Fritz-Haber- Institut der MPG)	Deceleration and trapping of neutral po- lar molecules
15.12.05	Prof. Dr. W. Däppen (University of Southern Cali- fornia Los Angeles, USA)	Helioseismologie — Physik der Sonne
12.01.06	Prof. Dr. L. Wöste (Freie Universität Berlin)	Künstliche Lichtblitze in der Atmosphäre
26.01.06	Prof. Dr. W. Heil (Universität Mainz)	Polarisiertes <sup>3</sup> He in physikalischer Grund- lagenforschung und medizinischer Anwen- dung
14.02.06	Prof. Dr. T. Brabec (Universität Ottawa, Kanada)	Extreme Nonlinear Optics: Atto meets Nano
06.04.05	Prof. Dr. E. Suraud (Universität Toulouse, Frankreich)	Dynamics of embedded and deposited clusters
04.05.06	Prof. Dr. Dirk Timmermann (Institut für Angewandte Mikroelektronik, Universität Rostock)	Herausforderungen für CMOS-Schal- tungen im Nanobereich
18.05.06	V. Bitukov und I. Luba- shevsky (Moskau)	Research and Teaching at Radio- Engineering Faculty at MIREA/Moscow
22.06.06	Dr. S. Glenzer (Lawrence Livermore Natio- nal Lab)	Erste Experimente zur Laser-getriebenen Kernfusion
29.06.06	Prof. Dr. DG. Welsch (Friedrich-Schiller-Universität Jena)	Quantenelektrodynamik in passiven Medien
06.07.06	Prof. Dr. T. Lohse (Humboldt-Universität Berlin)	Explodierende Sterne und Schwarze Löcher: Gammastrahlungsastronomie mit dem H.E.S.STeleskop
13.07.06	Prof. Dr. M. Koch (TU Braunschweig)	Terahertz-Wellen und ihre Anwendungen

19.10.06	Prof. Dr. P. Wölfle (Universität Karlsruhe)	Der Kondoeffekt: Von magnetischen Legierungen zur Nanoelektronik
04.11.06	Prof. Dr. H. Burchard (Institut für Ostseeforschung Warnemünde)	Wie viele Brücken und Windparks verträgt die westliche Ostsee?
07.11.06	Dr. P. Hilse (EMAU Greifswald)	Beschreibung der Wechselwirkung intensiver Laserstrahlung
15.11.06	Prof. Dr. M. Kira (Universität Marburg)	Quantum Degenerate Exciton States
16.11.06	Prof. Dr. V. Stepanyuk (Max-Planck-Institut für Mikrostrukturphysik Halle)	Mirages, Interactions and Spin Polariza- tion in Quantum Resonators
21.11.06	Dr. W. Hoyer (Universität Marburg)	Characterisation of Disorder in Semicon- ductors via Single-Photon Interferometry
30.11.06	Prof. Dr. R. Collins (University of Alaska, Fair- banks)	LIDAR-Messungen in polaren Breiten
07.12.06	Prof. Dr. E. Polzik (Niels-Bohr-Institut Kopen- hagen)	Quantum teleportation from light to mat- ter
12.12.06	Prof. Dr. M. Tolan (Universität Dortmund)	Weihnachtskolloquium: "Geschüttelt, nicht gerührt! James Bond im Visier der Physik"

## 1.5 Scientific Meetings organized by the Institute

The titles, periods of time and organizers were:

## 2004

"2nd Workshop on Semiconductor	14.04	Prof. Dr. Stolz
Quantum Optics",	17.04.2004	
Sellin, Rügen / Germany		
"Laehnwitzseminar on	07.06	Prof. Dr. Schick
Calorimetrie", Rostock / Germany	10.06.2004	
DFG-Kolloquium "Cluster in Kon-	17.06	Prof. Dr. Meiwes-Broer
takt mit Oberflächen",	19.06.2004	
Bad Honnef / Germany		
"Alpha Condensation",	10.08	Prof. Dr. Röpke
Rostock / Germany	12.08.2004	
DAAD-Sommerschule	05.09	PD Dr. Mahnke
"Modelling of Strongly Correlated	19.09.2004	
Many-Particle Systems",		
Ekaterinburg / Russia		
WE-Heraeus-Ferienkurs	04.10	Prof. Dr. Redmer,
"Korrelierte Materie im Strahlungs-	15.10.2004	Prof. Dr. Meiwes-Broer,
feld: Von der Femtosekunden-		Prof. Dr. Stolz
spektroskopie zum Freie-Elektronen-		
Laser", Rostock / Germany		

## 2005

"Lasertag",	26.01.2005	Prof. Dr. Mitschke
Rostock / Germany		
DFG-Kolloquium "Cluster in Kon-	24.02	Prof. Dr. Meiwes-Broer
takt mit Oberflächen",	25.02.2005	
Bad Honnef / Germany		
Material Days 2005,	23.05	Prof. Dr. Burkel
"Interfacial Effects in Functional	24.05.2005	
Materials",		
Technologiezentrum		
Rostock-Warnemünde / Germany		
"International Linear Collider:	01.06.2005	Prof. Dr. Schröder
ILC physics and detector meeting",		
Rostock / Germany		
"Alpha Condensation",	18.08	Prof. Dr. Röpke
Rostock / Germany	19.08.2005	
Workshop	30.09.2005	Prof. Dr. Edwards,
"Metal-insulator transitions in solids		Prof. Dr. Dr. Hensel,
liquids and plasmas",		Prof. Dr. Redmer
In honor of the 100 <sup>th</sup> birthday of Sir		
Nevill Francis Mott,		
Rostock / Germany		

Workshop I	18.11.2005	Prof. Dr. Burkel
"The Cell Material Dialogue",		
Hohe Düne, Rostock / Germany		
Workshop II	16.12.2005	Prof. Dr. Burkel
"The Cell Material Dialogue",		
Hohen Luckow near Rostock / Ger-		
many		

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Workshop	28.02	PD Dr. Tiggesbäumker,
"Coulombexplosion gespeicherter	01.03.2006	Prof. Dr. Schweikhard,
Cluster", Rostock / Germany		Prof. Dr. Meiwes-Broer
"School on Stochastic Dynamics:	16.03	PD Dr. Mahnke
From Wiener Process to Econo-	19.03.2006	
physics", Güstrow / Germany		
Material Days 2006	23.05	Prof. Dr. Burkel
"Functional Materials by	24.05.2005	
Nanostructuring",		
Technologiezentrum		
Rostock-Warnemünde / Germany		
International Conference	28.05	Prof. Dr. Meiwes-Broer
"Clusters and Surfaces",	02.06.2006	
Rostock-Warnemünde / Germany		
Kick-off Meeting des Landes-	03.06.2006	Prof. Dr. Gerber
schwerpunktes "Regeneration des		
Knochens", Rostock / Germany		
"Laehnwitzseminar on	07.06	Prof. Dr. Schick
Calorimetrie", Rostock / Germany	10.06.2006	
Mini-Workshop	15.06.2006	Prof. Dr. Redmer,
"Strongly Coupled Plasmas and In-		Prof. Dr. Meiwes-Broer
tense Radiation Fields",		
Rostock / Germany		
"Alpha Condensation"	15.08	Prof. Dr. Röpke
Rostock / Germany	16.08.2006	
"Third International Workshop on	05.10	Prof. Dr. Stolz
Quantum Optics in Semiconductor	07.10.2006	
Nanostructures",		
Würzburg / Germany		

## 2 Current Research

## 2.1 Optics and Laser Physics

### 2.1.1 Nonlinear Optics

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### General Outline of the Field of Research

We study nonlinear dynamical processes in the realm of optics. *Nonlinear* means that optical properties of a material are modified by the irradiated light so that light propagation is influenced. *Dynamical* refers to short time scales; we routinely deal with femtosecond processes. Lasers are a central concept here in a twofold way: They provide the light required to excite nonlinear processes, but inside they rely on nonlinear processes themselves.

Our focus during the report period has been on the nonlinear interactions which occur when a short pulse of light travels down an optical fiber (the group head has published a textbook on fiber optics [1]). Given the right conditions, very special pulses called solitons can arise. A quarter century after their first experimental demonstration, solitons have now found their way into commercial applications in optical telecommunication. One aspect of our work deals with the fundamental limitations of the data-carrying capacity of fibers, and with ways to extend that limit using soliton concepts.

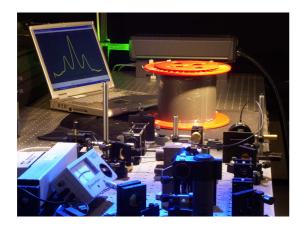
In the broader picture, we envision that optical technologies will advance our society's communication and data handling needs and abilities, and that in the near future 'photonics' will become similarly important to our lives as electronics already is.

#### Laser Instabilities

A longstanding question in laser physics was why lasers with homogenous gain line so stubbornly avoid to operate in a single mode. Conventional wisdom said they should, but experiments prove otherwise. Through a series of systematic experiments in conjunction with theoretical modeling by colleagues in Spain and Italy we could provide an explanation in terms of the so-called Risken-Nummedal-Graham-Haken instability [2, 3].

Soliton Molecules Optical communication is all about robust pulse structures: Signal pulse shapes must be stable over long distances so that the message arrives intact. This makes solitons so valuable because they have the property of 'self-healing' after perturbation. We have studied a type of fiber now favored by telecom providers called dispersion-managed fibers [4]. These fibers have several technical advantages: There are certain signal disturbances which are subtle for the individual data stream but become a concern when many data streams are transmitted simultaneously, as is done in today's high performance systems. It has been known for a few years that the soliton concept remains useful in these fibers. With the ever increasing data rates used today, however, a fundamental limit is soon reached that cannot be exceeded as long as data are encoded in a binary format, i.e. as 'on' and 'off'. We discovered that there exists a stable solution which is a compound state of several solitons. It was

then a major breakthrough that we accomplished an experimental demonstration [5]. This compound, called the soliton molecule, may provide a viable means to extend the range of symbols, thus avoid the limitation.



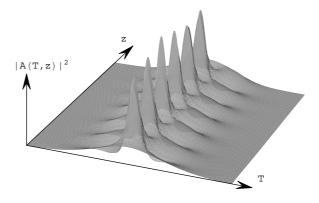
Partial view of the setup to generate and investigate soliton molecules in a fiber (on red spool).

This result was surprising and immediately prompted researchers elsewhere to pursue this concept further. In an extension of the concept we could also show that dark solitons in dispersion managed fibers can have bound states, too [6]. In 2006 the group head has written a review article on this field [7].

#### Soliton Analysis

One of the fundamental aspects of soliton physics is that almost always some linear radiation is generated along with the soliton. To tell linear and solitonic contribution apart is usually done with a complex mathematical technique known as Inverse Scattering Transform (IST). IST is, however, only applicable in the absence of loss – sometimes a viable, but often an impossible approximation.

We found a more intuitive method to tell solitons and radiation apart which is called soliton radiation beat analysis. We start by interpreting the oscillations of the pulse shape when a solitons and linear waves propagate together as a beat between both, and evaluate this beat signal to draw conclusions about the quantitative properties of both. This method makes no a priori assumptions about presence or absence of loss, constancy of parameters, etc., and is therefore much more universally applicable. This has been demonstrated in situations where IST cannot provide an answer: We could readily identify a higher-order soliton in a dispersion-managed fiber (it was unclear before whether this even exists) [8], and we could show how a soliton emerges from a pulse with an arbitrary shape [9].



Oscillating pulse shape when solitons and linear waves propagate together. The temporal power profile  $|A(T)|^2$  varies with propagation distance z.

#### 2.1.2 Theoretical Quantum Optics

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#### Nonclassicality

The characterization and application of nonclassical effects was studied. Based on the full information on a given quantum state, we have derived nonclassicality conditions. These conditions have been related to observable quantities.

We have further developed our approach to formulate nonclassicality criteria by using observable characteristic functions [10, 11], on whose basis we could completely characterize nonclassical Glauber-Sudarshan P-functions. It has been shown that the phase-dependence of the nonclassical characteristic functions can be important even for the characterization of phase-independent quantum states [12].

Alternatively the nonclassicality conditions have also been formulated in terms of moments, which also yields a complete characterization of nonclassical effects. This approach has first been developed for moments of Hermitian quadrature operators [13]. Later it was shown that the moments of non-Hermitian annihilation and creation operators are very useful for the formulation of nonclassicality conditions [14]. This has been demonstrated for a higher-order generalization of the well-known squeezing effect [15].

#### **Characterization of Entanglement**

In particular we were interested in conditions for entanglement. Entanglement is a special but important nonclassical feature. It is considered to be the key resource for quantum information processing and quantum computation.

For the characterization of entanglement, the Peres-Horodecki (partial transposition) criterion is an important approach. This criterion could be completely reformulated in terms of observable moments [16]. This allows one to completely characterize an important class of entangled quantum states in terms of a continuous-variable description of systems in infinite dimensional Hilbert spaces. Later on, we have also generalized this method to describe properties of the more complex multipartite entanglement [17].

#### Quantum theory of optical measurements

Based on our previously developed methods of homodyne measurement and quantumstate reconstruction we have further studied efficient measurement principles. In particular, the advantages of correlation techniques have been analyzed, with emphasis on the detection of general correlation properties of light and matter. These methods are of great interest in the context of the characterization of nonclassical and entangled quantum states.

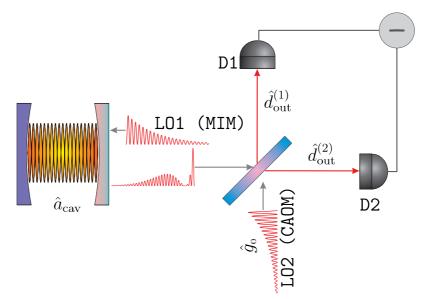
Early proposals to observe anomalous correlation properties of light by homodyne correlation measurements have been further developed to detect different kinds of moments of radiation fields [16]. A balanced homodyne correlation technique has been proposed that renders it possible to observe arbitrary correlation functions of radiation

up to high orders in the field strength [18]. This method unifies the advantages of balanced homodyne detection with those of correlation measurements.

#### Cavity QED

We have studied the description of realistic cavities by taking into account the unwanted scattering and absorption losses. The strong atom-field coupling under such conditions is of particular interest.

The description of imperfect cavities has been developed both from the viewpoint of quantum field theory [19, 20, 21] and by methods of quantum-noise theory [22]. In this context we have analyzed in detail the development of the quantum state, including its mode structure, during the outcoupling process from the cavity [19, 20]. Measurement techniques for characterizing such quantum states have been developed [22]. A cascaded homodyne technique, as shown in Fig. 1, turned out to be very useful for such applications.



Cascaded homodyne detection scheme for measuring the quantum state of a cavity field (after [22]).

#### **Trapped Ions**

Nonlinear effects in the atom-light interaction of trapped ions, caused by the quantized center-of-mass motion, are one of our main research fields for more than ten years. In the period under consideration we have studied the preparation of stable trapping states in the quantized motion, which result from the corresponding nonlinearities in the atom-radiation interaction [23]. Moreover, we have studied the motion-induced nonlinear effects in a system of three ions [24]. In such a case we could identify two different situations in which the dynamics of the system can be solved exactly.

#### Molecular Dynamics and Trapped Bosonic Gases

One of the former members of the Quantum Optics group, Dr. Sascha Wallentowitz, was supported by the DFG by the Emmy-Noether grant, a program for outstanding young scientists. The Emmy-Noether grant also included the financial support of two PhD students. The group was studying the laser manipulation of the rotational dynamics of molecules [25, 26, 27, 28]. Moreover, the cooling of trapped bosonic gases has been investigated [29, 30, 31, 32], as well as some aspects of quantum information processing [33].

#### 2.1.3 Semiconductor Optics

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The main topics of our research are the study of fundamental quantum processes in semiconductors and their interaction with light on ultrashort time scales down to some femtoseconds  $(10^{-15}s)$ , especially with respect to future applications in computer and communication technology and the investigations of the optical properties of semiconductors with reduced dimensionality by light scattering methods. During the report period, the main focus of our research has been the study of quantum optical properties of the light emission from these structures, finacially supported by the Deutsche Forschungsgemeinschaft in the research group "Quantum optics of low dimensional semiconductors". Since 2005, we also participate in the collobarative research activity SFB 652 of the Deutsche Forschungsgemeinschaft "Strong correlations and collective effects in radiation fields: Coulomb systems, clusters and particles" with three projects on dense exciton systems.

#### Quantum Optics of low dimensional Semiconductors

This research project aims to explore the quantum properties of the light emitted from semiconductors under resonant excitation. This reradiation is commonly referred to as resonance fluorescence (RF). In semiconductor systems, quasiparticle excitations, like excitons, are fermions at the composite level. Since Coulombic many-body effects are usually strong in semiconductors, one may expect significant fermion contributions also in excitonic RF [36]. As a first step, we have inverstigated the RF from disorder localized excitons in high quality quantum wells and have been able to observe single excitonic RF for the first time (see Fig. 1). This opens up to study the dependence of the spectrum of RF on the intensity of excitation, where we expect to see strong changes due to the coupling to the light which will be significantly different whether excitons behave like bosons or more like fermions. The quantum statistical properties of this RF is expected to show sub-Poissonian statistics and the possibility of squeezing below the quantum noise level. For quantum wells we have also measured the optical first order correlation function of light emitted into left and right side, where we found interesting interferenc effects that can be interpreted in analogy to the well known which-way-experiments in quantum mechanics [37] and indicate an entanglement between emitted photon and the entire many-body system.

#### Dense Exciton Systems

In semiconductors a new state of matter could be generated by exciting electron-hole pairs with intensive laser pulses. This state is similar to that of common matter due to many aspects: Bound states, very similar to the hydrogen atom, can build up which are called excitons. These could further form molecules (biexcitons) or even larger aggregates under adequate circumstances. Due to their tiny mass - the exciton mass is more than three orders of magnitude smaller than that of the hydrogen atom - excitons show up pronounced quantum properties already at temperatures of a few

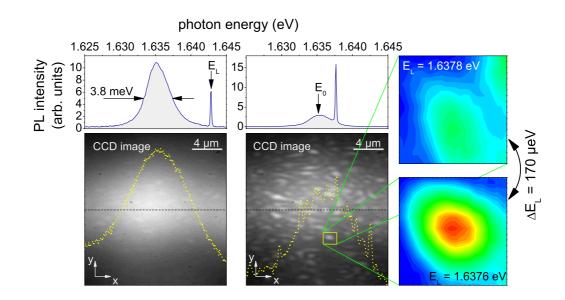


Fig. 1: Spatially resolved resonance fluorescence of excitons in single quantum well excited by a single frequency laser. The left part shows the photoluminensce under non-resonant, the middle under resonant excitation. The left side shows an enlarged image of the RF under resonant and off-resonant excitation. The breakup of the luminescence into differtn spots due to single excitons is clearly visible. The size of the spots is determined by the optical resolution of the microscope (< 1µm), the actual exciton sizes beeing still one order of magnitude smaller. From [48].

Kelvin which is quite different to common matter where temperatures of a few micro Kelvin are necessary. In the focus of this project are the thermodynamical properties of dense exciton systems. Especially, the existence of a theoretically proposed Bose-Einstein condensate and its interaction with the light field is of particular interest. Here we expext advances in the near future, when a new magnetokryostat system will be available, which allows to reach temperatures below 100 mK and magnetic fields up to 7 T. In the course of this project we are investigating two different types of systems:

a) High quality cuprous oxide samples [53] which shall be excited resonantly in magnetic fields at temperatures of some ten milli Kelvin. Due to the long exciton lifetime in this system, the dense exciton matter shall build up in the intense laser focus. These excitons will be further confined into shallow strain-induced traps to allow for quasi-thermal equilibrium.

b) Strong inhomogeneous electric fields shall be applied to high quality semiconductor quantum well samples which generate a parabolic-like potential in the quantum well plane such that the exciton motion becomes directed onto the potential minimum where the dense exciton matter shall arise. Furthermore, the excitons become aligned along the growth direction in the potential center due to band shifts along the electric field. Therefore, the wave function overlap between electron and hole will be reduced, so that the radiative decay of the excitons will be suppressed. This leads to a longer

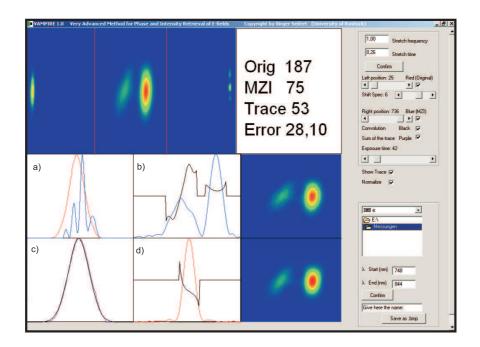


Fig. 2: Screenshot of the VAMPIRE measurement and analysis software to determine the amplitude and phase of ultrashort laser pulses. Shown is clockwise from the above left corner clockwise: CMOS camera picture, retrieval quality parameters, measured VAMPIRE trace and reconstructed trace, a) spectra of the input pulse and filtered pulse, b) field and phase derivative of the filtered pulse, c) comparison of the frequency marginal of the VAMPIRE trace and convolution of input and filtered spectrum, d) final retrieval result: amplitude and phase derivative of the input field. On the right hand side, several parameters for the reconstruction process can be adjusted.

life time in which quantum correlations can build up. The excitons in these systems can be analyzed with the method of phase-sensitive reflection spectroscopy which we have developed for states in zero electric field [41, 44, 47].

#### Amplitude and Phase Characterisation of Ultrafast Laser Pulses

One of the main problems in ultrafast laser physics is the reliable determination of the complex electric field amplitude and phase of the laser pulse. A direct observation like in a conventional oscilloscope is not possible up to now due to the time resolution of femtoseconds necessary. Therefore indirect schemes that are based on a nonlinear interaction of the laser pulse either with itself or with a known reference pulse have to be applied. These schemes in general require the reconstruction of the field by a inversion procedure (retrieval), which per se is numerically highly unstable and in most cases not unique. We have been able to develop a new measurement scheme called Very Advanced Method of Phase and Intensity Retrieval of Electric fields [57] that allows to overcome this uniqueness problem (see Fig. 2). It is based on the conditions under which the uniqueness of the retrieval can be shown mathematically [35]. With this method, almost arbitrary complicated ultrashort laser pulses can be characterized completely.

#### 2.1.4 Theoretical Solid-State Optics

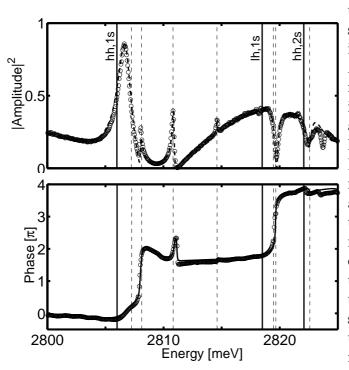
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#### Phase behaviour of the reflected light at semiconductor layers

The optical properties of semiconductors are strongly influenced by carriers, which have been injected by a pump pulse. We have investigated this effect by studying the amplitude and phase of the light field reflected from ZnSe layer in cooperation with the experimental group of Prof. Stolz (University Rostock). While we found [58, 59] only weak changes in the amplitude with increasing excitation, the phase changed drastically. In case of the non-excited sample the phase exhibits a global change at the heavy-hole exciton resonance by  $2\pi$  towards the band edge. A detailed analysis shows, that it can be decomposed into an abrupt, nearly step-like jump by  $\pi$  and a smooth increase to higher energies up to  $2\pi$ . This behaviour can be described by interfering polariton waves including their spatial dispersion. Increasing the intensity of the pump, the step-like jump changes its direction to  $-\pi$ , whereby the global jump by  $2\pi$  vanishes. We have explained this behavior within a quantum-kinetic manybody theory by a subtle increase of the excitonic linewidth, which results from (i) a counterbalance of diagonal and off-diagonal dephasing and (ii) memory effects in the scattering between excited carriers and the laser-induced polarization.

Further investigations [60, 61, 62] were performed with heterostructures, where the



active ZnSe layer was cladded by two ZnSSe layers. These samples show very small exciton resonances in comparison to those used above. As a result we found a whole series of polariton interferences being reflected in strong changes of amplitude and phase of reflected light. This is demonstrated in the Figure, where vertical solid lines mark the single exciton resonances and the vertical dashed lines mark the position of the single polariton modes. Experimental results (circles) are in good agreement with those of the theoretical investigations (thick dashed lines). The measurement of both phase and amplitude enables a very accurate determination of

the dielectric parameters of the sample. The study of the influence of excited carriers is subject of further investigations, which will give more inside into the microscopic processes in an excited semiconductor.

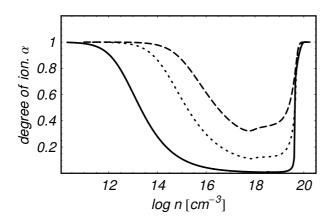
#### Ionization equilibrium and Mott effect in electron-hole plasmas

The carriers in a highly excited semiconductor – electrons (e, occupied conduction band states) and holes (h, empty valence band states) together with their bound states (excitons, X) can be regarded as a partially ionized two-component plasma. Such a system may be described either in a physical picture (only electrons and holes as basic constituents which occur in bound or scattering states) or in a chemical picture where the bound states are introduced as a new basic particle species. The latter picture requires to consider the chemical equilibrium  $e + h \rightleftharpoons X$ , the condition of which leads to a mass action law and, in the nondegenerate case, to the Saha equation. Furthermore, the degree of ionization can be defined by  $\alpha = n_e^*/n_e$ , where  $n_e^*(n_e)$  is the free (total) electron density.

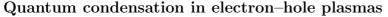
On the other hand, in the physical picture the total density follows from  $n(\mu, T) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{d\omega}{2\pi} a(\mathbf{p}, \omega) f(\omega)$ . Applying for the spectral function *a* the extended quasiparticle approximation, the density can be split into free quasiparticle, scattering, and bound state contributions.

Since the excitons as composite particles consisting of two fermions should exhibit a Bose-like behavior, one can expect the occurrence of Bose–Einstein condensation (BEC). The investigation of the ionization equilibrium in the e-h plasma is, therefore, of particular interest in order to determine the domain of existence of excitons (small  $\alpha$ ) as a precondition for the observation of BEC.

We have analyzed the degree of ionization in the density-temperature plane. The ex-



istence region of excitons turns out to be not only restricted to higher temperatures (thermal ionization) but also to higher densities due to an abrupt breakup of the bound states caused by the Mott effect. We observe a sudden transition (Mott transition) from an exciton gas ( $\alpha \approx 0$ ) to a fully ionized plasma ( $\alpha \approx 1$ ) (solid line: T = $0.1R_X$ , dotted line:  $0.15R_X$ , dashed line:  $0.2R_X$ ).

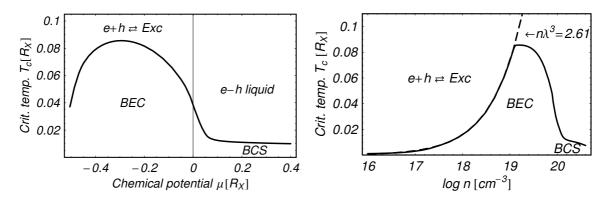


Since the e - h plasma consists of Fermi particles which form Bose-like bound states, one can expect the occurrence of Bose–Einstein condensation of the excitons as well as the formation of a BCS condensate of Cooper-like pairs of unbound electrons and holes. A unified description of both types of quantum condensation can be given in the framework of real-time Green's functions [63]. Starting point is the two-time two-particle Keldysh Green's function which, if quantum condensation occurs, exhibits an additional contribution surviving for  $t - t' \rightarrow \pm \infty$  (time long range order, LRO). The LRO concept allows to derive Kadanoff–Baym equations with an additional (LRO) self-energy contribution and generalized Gorkov equations, respectively. The key quantity is the gap function  $\Delta$  determining the BCS energy gap and being closely connected to the BEC macro wave function. For  $\Delta$ , a nonlinear integral equation has been derived which, for vanishing gap, determines the critical temperature of quantum condensation, too.

In the left hand figure below, the critical temperature  $T_{crit}$ , i.e., the phase boundary of

quantum condensation, is shown vs. the chemical potential. Obviously, at  $2\mu = E_b = -1$  (in excitonic units; equal masses) the Bose–Einstein condensation of excitons sets in. After reaching a maximum,  $T_{crit}$  drops again but remains finite for  $\mu > 0$ . In that region, a BCS state of e - h pairs exists. Thus, both BEC and BCS condensate are described by a single phase boundary with a smooth crossover between the two states.

Further investigations have been done to analyze the phase boundary in dependence on the particle density, i.e., eliminating the chemical potential. Starting from the spectral function in extended quasiparticle approximation, we have derived an expression for  $n(\mu, T)$ . The result for  $T_{crit}(n)$  is shown below in the right hand figure.



Generalizing the radiation laws of Kirchhoff and Planck to nonequilibrium: Exact relation between absorption and emission for steadily excited media Emission and absorption of excited media are considered by describing light and matter quantum-mechanically as an interacting many-body system in nonequilibrium. Applying Poynting's theorem to slab geometry yields at given frequency  $\omega$  and inplane wave vector  $\mathbf{q}_{\perp} = (q_y, q_z)$  for a classical absorption experiment the relation

$$1 - |r|^2 - |t|^2 = a$$

between the incident (~ 1) and re-emitted intensities (reflected ~  $|r|^2$ , transmitted ~  $|t|^2$ ) on the one hand and the absorption within the slab a on the other hand. Emission as a pure quantum effect is given by

$$e = (b - n)a,$$

where n and b are globally defined nonequilibrium distributions of field and matter, respectively. This relation balances spontaneous emission  $e_{sp} = ba$  [which results already from vacuum fluctuations if no radiation (n = 0) is present] and stimulated absorption (a > 0) or gain  $(a < 0) e_{stim} = -na$ . Assuming e = 0, i.e., vanishing energy flow between medium and its surrounding yields b = n, which generalizes Kirchhoff's law to nonequilibrium. Then, for thermodynamic equilibrium b develops to a Bose distribution and Planck's radiation law is rediscovered.

Quite generally spoken, the distribution  $b(\omega, \mathbf{q}_{\perp})$  generalizes Planck's radiation law to nonequilibrium. It can be investigated experimentally by measuring simultaneously spontaneous emission and classical absorption. Theoretically, it is given by the recombination rate of the medium.

#### 2.1.5 Optics of Clusters and Nanostructures

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Finite size, large surface fraction, limited capacity for heat and charge, and discrete electron states: these are characteristics of metal clusters and nanoparticles, addressed in the field of cluster physics. Our research is aimed at the remarkable consequences many of which are accessible by spectroscopic means. Free clusters in a beam allow for the investigation of the pure cluster properties where the coupling to the environment may be neglected. When deposited on a surface the cluster-substrate interaction becomes crucial and is a topic of intense research.

#### Spectroscopy of metal clusters embedded in helium droplets

Embedding clusters in helium droplets leads to extremely low system temperatures of 0.37 K. Under these conditions we investigated small neutral silver clusters. With the combination of resonant two-photon ionization and photoelectron spectroscopy, it could be demonstrated that after an electronic transition the systems undergo relaxations on the picosecond timescale. It is the first time photoelectron spectroscopy on dopants embedded in helium droplets has been performed and the first time photoelectron spectra for small neutral silver clusters could be measured. The low temperature of the matrix enables the preparation of metastable states. In the case of Ag<sub>2</sub>, we measured the absorption for excitations originating from the lowest triplet state. This allowed the identification of three excited triplet states unaccessible by prior gas phase spectroscopy. Recent measurements on helium droplets doped with Mg atoms indicate that more exotic metastable states can be prepared. The atoms do not form a compact cluster but are isolated from each other by a thin layer of helium. A new type of condensate is created which opens a new field of manyparticle physics.

#### Interaction of strong laser light fields with clusters

A strongly nonlinear situation is probed in clusters when exposing free particles to intense laser pulses of up to  $10^{16}$  W/cm<sup>2</sup>. Partly, the studies were performed on clusters isolated in helium nanodroplets. The violent interaction leads to the emission of energetic photons and particles. The dynamics is probed by feeding in dual pulses leading to extreme charging of the clusters. This can be controlled by a suitable choice of the laser intensity and the optical delay between the pulses. In the final state of the Coulomb explosion, highly charged (up to Z=28) atomic ions with huge recoil energies of several hundreds of keV leave the interaction region. In addition, electrons are emitted with up to 400 eV, which is orders of magnitude higher compared to the corresponding ponderomotive or thermal energy. Analyzing the photoemission in more detail, the angular intensity distribution shows a pronounced peaking in the direction of the laser polarization axis. In order to clarify the physical processes contributing in the absorption dynamics, Vlasov simulations were performed and a novel plasmon-assisted acceleration mechanism in clusters (SPARC) was identified, see Fig. 1. Moreover, the calculations proved the generation of short attosecond electron bursts.

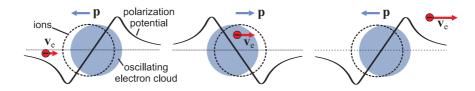


Fig. 1: Cascade-like acceleration of electrons through surface-plasmon assisted rescattering in clusters (SPARC): continuous acceleration for three laser half-cycles can be achieved when electrons recollide in phase with the cluster polarization potential. A prerequisite for high energy gain are large amplitude collective oscillations of bound electrons.

#### Core-level photoelectron spectroscopy on mass-selected metal clusters at the free-electron laser FLASH

Despite enormous progress of analytical tools in cluster science, detailed knowledge of geometrical and electronic structures and dynamics is still scarce. Whereas a wealth of information could be obtained from valence band photoelectron spectroscopy in the past, core-level spectroscopy on mass-selected clusters became only now possible with the advent of the VUV free-electron laser FLASH at DESY in Hamburg. Within a collaboration of seven groups from German universities headed by the Rostock group, a dedicated experiment has been set up. First experiments at FLASH in 2005 and 2006 using 38 eV (32 nm) photons revealed a size-dependent lead 5d core-level shift. This shift is in accordance with both, a classical metal sphere model and LDA calculations for larger clusters. However, the strong deviation from that behavior at a cluster size of N = 19 and below may be interpreted as a metal-to-nonmetal transition, which has not been conclusively observed in valence band spectroscopy before, but is in agreement with earlier theoretical work. The interplay of electronic structure and geometry appears as a covalent to metallic transition which comes along with a structural reorientation from a more layered to a compact, fcc-like atomic arrangement.

#### Magnetism of clusters and nanostructures

A different question concerns the magnetic properties of supported clusters. Our homebuilt arc cluster ion source (ACIS) has been used for studies on magnetic nanoparticles being deposited in situ onto single crystalline substrates. X-ray absorption experiments carried out at BESSY (Berlin) have revealed enhanced magnetic orbital moments in e.g. pure iron and cobalt particles. Furthermore a significant influence of the substrate on the magnetic moments has been found and is potentially important when attempting to tune the properties of magnetic nanostructures for future technical applications. More recently these experiments could be extended toward studies on individual nanoparticles by means of photoelectron emission microscopy (PEEM) at the Swiss Light Source. Significant variations in the shape of x-ray absorption spectra of individual cobalt particles have been detected as seen in Figure Fig. 2 (right). In the future, such experiments will enable detailed studies on the magnetic coupling of individual clusters and their interaction with magnetic and non-magnetic substrates.

#### Tunneling transport through deposited clusters and metal islands

The charge transport through deposited metal clusters is highly determined by the combined electronic structure of the cluster/surface system, including interface effects. Low-temperature scanning tunneling microscopy (STM) offers a tool for imaging the shape and the local density of states of single clusters in real space. Currently we focus on the investigation of metal particles on semiconducting surfaces, particularly Ag and Co on Germanium and Silicon surfaces, see Figure 2 (left). The observation of regularly shaped facets at the top of single clusters - as shown for the case of Co clusters on Ge(100) - is an important prerequisite for developing geometric models. Spectroscopic STM data reveal a continuous lateral transition between semiconducting and metallic regions on single clusters, thus defining the clusters' electronic area of influence. Such effects are expected to play a crucial role for potential electronic devices based on nanoscopic metal-semiconductor interfaces.

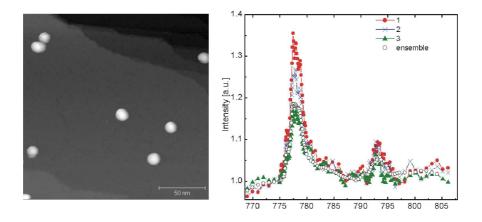


Fig. 2: Experiments with clusters at surfaces: cobalt particles are generated in a plasma source, size selected and deposited onto ultraclean surfaces. Left: STM image with resolved Si(111) surface steps. Randomly distributed clusters create nano-sized Schottky contacts. Right: Magnetic properties of single particles studied by photoemission electron microscopy (PEEM) at the Swiss Light Source. X-ray absorption spectra at the Co  $L_{2,3}$  edges are shown as a function of the incident x-ray energy for three different single particles.

The work is supported by the Deutsche Forschungsgemeinschaft (DFG) (within the Sonderforschungsbereich 652: "Starke Korrelationen und kollektive Phänomene im Strahlungsfeld: Coulombsysteme, Cluster und Partikel", the Graduiertenkolleg 567 "Stark korrelierte Vielteilchensysteme", the Sonderforschungsbereich 198 "Kinetik partiell ionisierter Plasmen", the Priority Program SPP 1153, and basic funding projects), the Growth Programme of the European Union, several projects of the Bundesministerium für Bildung und Forschung (BMBF), and the State of Mecklenburg-Vorpommern.

### 2.2 Physics of Nanomaterials

#### 2.2.1 Physics of New Materials

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The main scientific activities of our group focus on the development of novel functional materials. Nano-, micro- and macrostructures with special physical properties are prepared using various techniques. A large spectrum of analysis methods, mainly based on synchrotron radiation scattering, allow us to analyse the formation and phase stability of nanostructured materials and explore the magnetic, electronic or dynamic properties of advanced functional materials with focus on the following areas:

- I. Nanocrystallization dynamics and atomic structure formation at grain-boundaries in nanocrystalline VITROPERM alloys
- II. New nanocrystalline Co-rich magnetic alloys
- III. Spark plasma sintering of nanomaterials
- IV. Biocompatible titanium alloys with surface porosity and antibacterial functionality
- V. Magnetic Layer

Scientific Results

#### I. Nanocrystallization dynamics and atomic structure formation at grainboundaries in VITROPERM alloys

This research focused on the use of in-situ synchrotron radiation methods to investigate structural changes of the grain boundary (GB) regions in nanocrystalline alloys. A well-known soft-magnetic alloy (Vitroperm, Vakuumschmelze AG) was chosen as model system for these investigations. The as-cast VITROPERM specimens are melt-spun ribbons consisting of amorphous  $Fe_{73}Si_{16}B_7Nb_3Cu_1$ , i.e., an Fe-Si-B based metallic glass with Nb and Cu additions. Upon annealing at 550°C,  $\alpha$ -Fe<sub>3</sub>Si crystallites form (D03 structure, mean crystallite size 10 to 20 nm, volume fraction between 75 to 80 %). The grain boundaries are typically 1-2 nm wide and mainly consist of an amorphous  $Fe_{55}Nb_{14}B_{31}$  phase.

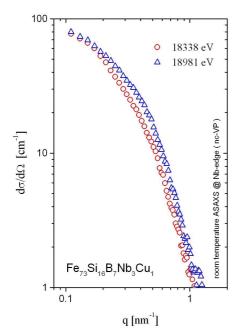


Fig. 1: Room temperature ASAXS curves at two energies near the Nb-edge (nanocrystalline ribbon).

Time-resolved high-temperature X-ray diffraction experiments were performed at the DESY/HASYLAB (Hamburg) synchrotron radiation facilities. The samples were additionally characterized by thermal analysis (Univ. Rostock) and high-resolution electron microscopy (Max Planck Institut, Stuttgart). The most recent experiments were concerned with the time- and temperature-resolved observation of structure formation in nanocrystalline Vitroperm (Fig.1) by in-situ anomalous smallangle X-ray scattering (ASAXS). ASAXS experiments were rarely performed in-situ to analyse nanocrystallization processes at high temperatures. The main advantage is the monitoring of time-/temperature-dependent diffusion processes leading to nanocrystallization, with chemical selectivity, i.e. the participation of a certain constituent element to precipitation, cluster formation or crystallization events can be accurately resolved.

#### II. New nanocrystalline Co-rich magnetic alloys

The work on cobalt-rich nanocrystalline magnetic alloys took place in the framework of the European Marie Curie Development Host Project Synthesis of Nanostructured Materials under Extreme Conditions (HPMD-CT-2001-00089) in Rostock. Structural stability is a critical aspect for the technological application of bulk amorphous and nanocrystalline alloys. It is therefore of great importance to know how structural stability is influenced by thermo-mechanical treatments. The phase transformations under various pressure-temperature conditions were followed by in-situ synchrotron radiation experiments and differential scanning calorimetry. The structure of samples was determined by electron microscopy and X-ray diffraction. Ribbon and powder materials were consolidated at elevated temperatures, yielding bulk specimens which will later be used as targets for thin-film deposition by magnetron sputtering. Magnetic measurements performed by vibrating sample magnetometer (VSM) were used to explore the process of mechanically-induced crystallization / amorphisation in Cobased materials. The main alloy systems investigated were CoFeZrB, CoFeSiB and CoFeTaB. Amorphous  $Co_{56}Fe_{16}Zr_8B_{20}$  and  $Co_{70.3}Fe_{4.7}Si_{10}B_{15}$  alloys in the form of thin ribbons were prepared by melt spinning. These ribbons were cut into small pieces (10x5 mm2) and ball-milled using planetary ball mill RETSCH PM400. CoFe and CoFeTaB alloys were prepared by wet milling.

The alloy structures were determined using high-energy transmission XRD. Phase transitions in the above-mentioned ball-milled powders were investigated by in-situ X-ray diffraction also under different pressure conditions. Complementary experiments, such as differential scanning calorimetry and vibrating sample magnetometery were also performed.

**Co-Fe-Zr-B alloys:** in-situ XRD experiments at constant heating rate (ambient pressure) were performed up to 800°C at the B2/HASYLAB station (Fig.2). The crystallization onset of as-quenched alloy is observed at 590°C: at this temperature the amorphous matrix crystallizes into a mixture of bcc Co(Fe) and hexagonal  $ZrCo_3B_2$  phases.

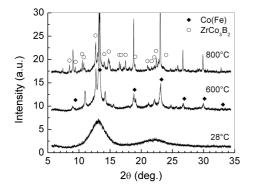


Fig. 2: Crystallization of as-quenched Co-Fe-Zr-B alloy into Co(Fe) and ZrCo3B2 phases upon heating.

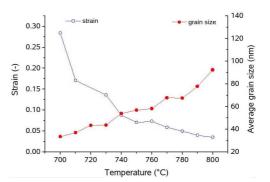


Fig. 3: Temperature evolution of strain and mean grain size for ball-milled Co-Fe-Zr-B alloy.

To follow the grain size growth of  $\alpha$ -Fe(Co) phase during *in-situ* XRD experiments, the profiles of (110) and (220) lines were fitted using Voigt functions. Applying the 'double Voigt' method to fitted profiles, the corresponding grain size distributions were obtained. From Fig.3 it is clearly visible that the level of strain decreases with increasing temperature whereas the average grain size shows an opposite behaviour From a series of EDX patterns it could be further derived that the crystallization of amorphous Co-Fe-Zr-B ribbons under <u>applied pressure</u> of 0.6 GPa occurs at 675±5°C and that the crystallization temperature  $T_x$  is influenced by the applied pressure p. An initial increase of pressure causes the  $T_x$  to increase and  $T_x$  reaches its maximum at pressure of 1.27 GPa. Further increase of external pressure tends to lower  $T_x$  at a slower rate.

**Co-Fe-Ta-B alloys:** based on the experience achieved during the project we have decided to proceed with the development of a new alloy derived from Co-Fe-Ta-B master alloy system. The target properties are here the superplastic behaviour coupled with improved magnetic properties, to allow for ex. the synthesis of complex shaped nanostructured bulk magnets. Mechanical alloying resulted in formation of partially amorphous alloys containing fractions of nanocrystalline  $Co_{0.7}Fe_{0.3}$  and  $Co_{20.82}Ta_{2.18}B_6$  phases. Typical XRD patterns are shown in Fig.4.

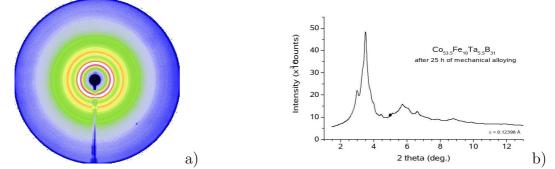


Fig. 4: XRD patterns of Co<sub>53.5</sub>Fe<sub>10</sub>Ta<sub>5.5</sub>B<sub>31</sub> alloy a) as recorded using a 2D detector (mar345) in symmetric mode and b) after integration to 2-theta space using Fit2D software package.

### III. Spark plasma sintering of nanostructured materials

For the synthesis of bulk nanostructured materials, new sintering procedures must be developed to overcome the difficulties in achieving densities in excess of 95% for materials with ultrafine grain sizes below 100 nm. Most promising approaches are spark plasma sintering and microwave sintering techniques. The potential of these technologies was comparatively tested in several series of experiments performed at the group's partner institutes or companies located in Europe and in the United States.

The powder materials investigated included nanocrystalline magnetic alloys (HIT-PERM, NANOPERM, Co-rich alloys), lightweight alloys (TiAlV, AlCuFe), hydrogen storage materials, Ti-based implant alloys (see also §IV), as well as special ceramics for applications like high-temperature coatings, photocatalysis (metal-doped titania, titanates), or metal-ceramic nanocomposites.

# IV. Biocompatible titanium alloys with surface porosity and antibacterial functionality

The potential of advanced nanomaterials synthesis (mechanochemistry, sol-gel techniques) and sintering procedures (SPS, microwave sintering) was used to design new alloys and composite nanomaterials for biomedical applications. We have recently tested the SPS technology in achieving bulk Ti-alloy parts with variable surface porosity and chemical composition. This interdisciplinary research aims to optimize the surface chemistry and topography of the implants so as to support cell adhesion, proliferation and bone regeneration, while maintaining the necessary isoelastic mechanical properties of the implant. Bulk titanium alloy parts were prepared by powder metallurgy routes (ball milling followed by SPS) and further tested for biocompatibility using osteoblast cell assays.

#### V. Tuning the remanent spin structure of exchange coupled magnetic films

The information density of magnetic storage devices is not only limited by the spatial extension of the magnetic memory cells, but also by the number of distinguishable magnetic states that can be realized in each cell. Conventional magnetic storage devices rely on the realization of two magnetic states for encoding information. One could expect a significant increase of the storage density for digital data, if multiple states per memory cell could be generated. A potential route towards this goal is the controlled adjustment of different coupling angles between two exchange coupled magnetic films.

A generic phenomenon that is observed if two layers of different magnetic materials are coupled to each other is the exchange-bias effect with features like a shifted hysteresis loop or an enhanced coercive field of the involved ferromagnetic material. These phenomena are not restricted to coupled ferromagnetic/antiferromagnetic layers but can also be observed for exchange-coupled magnetic layers with different magnitudes of their coercive fields, e.g. as in the case of soft magnetic and hard magnetic materials. Such layer systems are often referred to as exchange-spring magnets where the minor loops (i.e. the hysteresis loops where the field is cycled within limits below the switching field of the hard magnetic layer) exhibit the exchange-bias phenomenology. We identified the relevant parameters of exchange coupled hard/soft magnetic layer that allow for an exact adjustment of the coupling properties and showed that the remanent magnetization direction of the soft magnetic layer can be controlled by temporally applied external magnetic fields due to the competition between the exchange bias field and the soft layer coercive field.

The sample used was a polycrystalline trilayer consisting of Fe(10 nm)/Cu(0.6...6.4 nm)/FePt (30 nm), deposited by rf-magnetron sputtering on a superpolished Si substrate with an amorphous Ta seed layer (10 nm) and capped by 3 nm of Ta<sub>2</sub>O<sub>5</sub>. For a continuous variation of the coupling across the samples, the Cu spacer layer was wedge shaped. The surface quality of the layers was controlled via x-ray reflection in grazing incidence geometry. The FePt layer was transformed into the magnetically hard  $L_{10}$ -phase by high vacuum annealing. The polycrystalline character of the FePt layer was confirmed via atomic force microscopy and x-ray diffraction.

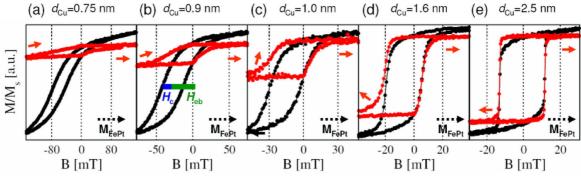


Fig. 5: Minor hysteresis loops (black curves) of the Fe/Cu/FePt trilayer, recorded via MOKE, for various values of the Cu interlayer thickness.

The magnetic properties of the layer systems were studied by longitudinal magnetooptical Kerr-effect (MOKE) measurements at room temperature. Figure 5 shows selected minor magnetic hysteresis loops of the layer system for different interlayer thicknesses  $d_{Cu}$ . While the black curves are conventional loops, the red curves are remanent loops where the field was only temporarily applied (for t = 1 s) and then the MOKE signal afterwards measured in zero field. From the conventional loops (black curves) we have determined the exchange bias field and the coercive field as a function of interlayer thickness, as displayed in figure 6. The bias field decreases exponentially with increasing interlayer thickness. Such behaviour points to a mainly magnetostatic interaction between both films.

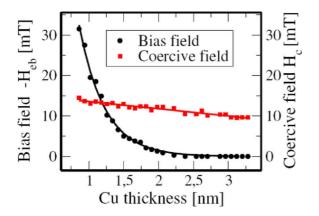


Fig. 6: Exchange bias field Heb and coercive field Hc of the minor loops versus the Cu interlayer thickness, indicating an exponential respectively a linear decrease with increasing interlayer thickness. The solid line for Heb is a fit.

Hereby, the ratio Heb/Hc determines the maximum range of coupling angles that can be remanently adjusted via an external field. Therefore, for the ratio Heb/Hc = -1the coupling angle assumes all values between 0 and 90 degrees while proceeding from

positive to negative fields along the remanent loop. This immediately prompts potential applications in magnetic data storage technology, because in this way multiple states per memory cell could be realized as schematically shown in figure 7(a). In such devices, the information is then written via the magnitude of temporarily applied external fields and is stored as in the coupling angle between the magnetization vectors of the films.

In future applications, conventional techniques like MOKE or magneto-resistance effects (e.g. GMR or TMR) could be used to read out the stored information encoded inside the coupling angle.

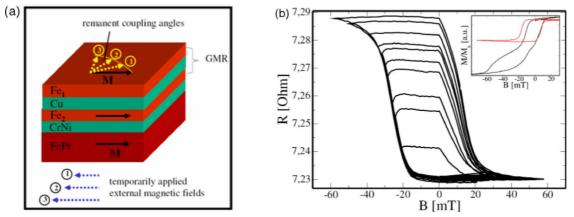


Fig. 7: (a) Sketched minor loops, measured in the conventional way (black curve) and using the etched layer system and working principle of a novel storage device application based on interlayer coupled magnetic films with a GMR(Fe1/Cu/Fe2) element for information reading. (b) Experimental proof of this principle, where 10 different levels could be induced, illustrated by the GMR remanent mode minor loops. The inset displays the corresponding MOKE remanent mode technique (red curve).

Therefore, the sample system was modified by implementing a supplemental GMR layer system  $Fe_1(7 \text{ nm})/Cu(2.5 \text{ nm})/Fe_2(7 \text{ nm})$ , on top of a hardmagnetic FePt (30 nm/NiCr (0.5 nm) bilayer like schematically sketched in figure 7(a). For an increasing GMR signal, 0.5 nm Co are deposited at both Cu/Fe interfaces. In the layer system, the Fe<sub>2</sub> layer is stronger coupled than Fe<sub>1</sub> layer and the inducible coupling effects are only between the magnetizations of Fe<sub>1</sub> and Fe<sub>2</sub>. The inset of figure 7(b) is shown the MOKE minor loops, measured in the conventional (black curve) and in the remanent mode (red curve). Here, the ratio Heb/Hc admit only for the Fe1 layer inducible coupling angles as one can see in the remanent minor loop. To clarify the potential for future applications, we measured GMR (current in-plane geometry)minor loops also in the remanent mode, as described above. Different GMR minor loops where only the maximum of the applied field is varied are displayed in figure 7(b). As illustrated, 10 different levels - and hereby 10 different information - can be remanently stored for externally applied fields within a range of about 40mT. Due to improved GMR or TMR layer systems as functionalized reading elements, one can image a very low signal-to-noise ratio which allows applications for multilevel and/or analogue recording.

This approach allows one to read out these magnetic states via magneto-optical techniques or magneto-resistance effects, thus providing the potential for miniaturization far below the length scales of conventional analogue magnetic recording technology.

# 2.2.2 Polymer Physics

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# Major Research Topics (grants)

Melting and crystallization of polymers (EU and DFG) Glass transition in confining geometries (DFG) Polymer / inorganic nanocomposites (DAAD) Heat capacity spectroscopy at the glass transition (DFG) Fast scanning calorimetry and calorimetry of thin films (DFG, Sonion AS, DK) Improvement of differential scanning calorimetry (PerkinElmer Instruments, USA) New micro calorimeter for high throughput characterization of polymers (AIF)

The major research topic is on the structure properties relationships of polymers and low molecular weight organic compounds. Morphology changes in semi crystalline compounds and chemical modifications are possible strategies for the variation of the structure for new materials with new properties. They can be studied by different spectroscopic techniques like dielectric, dynamic mechanical and modern calorimetric methods. Our main focus is on new calorimetric setups as chip calorimetry for fast and sensitive measurements developed in our group.

# Ultra fast scanning chip calorimetry (1.000.000 K/s)

Investigations of melting/crystallization and reorganization phenomena needs methods to be able to follow this sometimes fast processes. As another point the processing conditions relevant in industry are also faster than usual calorimeter devices. So we focused on the development of ultrafast calorimetry. Recently commercially available chips especially designed for fast scanning calorimetry allow heating and cooling rates up to 1.000.000K/s. Combining different devices about 10 orders of magnitude in scanning rate is covered. The reorganization and crystallization behavior was studied during scanning and isothermal experiments. During melting the rate dependent superheating of the polymer crystals is observed which shows a saturation for high heating rates (see figure 1B) for some polymers.

# Nano sized AC chip calorimetry

With a differential AC-calorimeter based on a commercially available chip sensor from Xensor Integrations, which is also used fast scanning calorimetry we achieve a sensitivity in the pico Joule per Kelvin range allowing to measure samples below one nanogram. Consequently the limit for film thickness is in the range of one nanometer. Because of the small total heat capacity (addenda + sample) not only a high sensitivity is achieved but AC measurements at relative high frequencies are possible too. The calorimeter allows heat capacity measurements in the frequency range 1 Hz to 1 kHz also below 10 nm film thickness. Main fields of investigation are the thickness

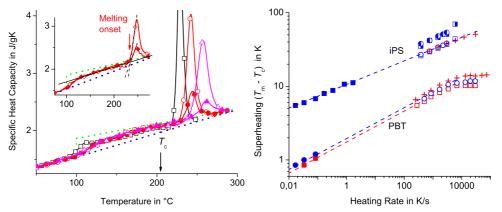


Figure 1: (A) Temperature dependence  $c_p(T)$  of iPS in the melting region measured at 1.7 K/s (DSC),  $4 \cdot 10^2$  K/s, and  $3 \cdot 10^3$  K/s after melt crystallization at 205°C for 16 h (open symbols) and 1 h (filled symbols). Dotted lines correspond to completely amorphous and crystalline material. Detection of the melting onset at  $8 \cdot 10^2$  K/s is shown in the insert. (B) Rate dependence of superheating  $\Delta T = (T_m - T_c)$  from DSC (filled symbols) and fast-scanning calorimeter (open symbols) for iPS crystallized at 205°C for 16 h (squares), 1 h (circles and crosses) and PBT crystallized for 15 min at 200°C (circles), and 180°C (squares and crosses), respectively. Dashed lines correspond to the power law  $\Delta T(R) = A \cdot R^{\beta}$  (iPS:  $\beta = 0.16$ , A = 10.6 K; PBT:  $\beta = 0.21$ , A = 1.95 K and 1.75 K at  $T_c = 200$ °C and 180°C, respectively). The shift of the melting peak  $\Delta T_{max} = (T_{max} - T_c)$  for iPS is shown by semifiled symbols.

dependence of glass transition and the identification of glass transitions in comparison with dielectric spectroscopy. In figure 2 the thickness dependence of glass transition in nanometer thin polystyrene films are shown.

#### Nanocomposites

Nanocomposites offer a unique opportunity for new materials with enhanced properties. Beside technological interests they are also interesting for basic research. Their similarities with semi crystalline polymers offer an opportunity to study the devitrification of the immobilized fraction (RAF) without interference of melting of crystals. The immobilized fraction in nanocomposites can be determined from heat capacity as it is common for the rigid amorphous fraction in semi crystalline polymers (see figure 3).

It was found that the interaction between the  $SiO_2$  nanoparticles and the PMMA is so strong that no devitrification occurs before degradation of the polymer even by lowering the glass transition of MAF by plasticization. The results obtained for the polymer nanocomposites support the view that the reason for the restricted mobility must disappear before the RAF can devitrify. For semi crystalline polymers this means that rigid crystals must melt before the RAF can relax. Only for semi crystalline polymers with significant chain mobility inside the crystals RAF may devitrify before melting.

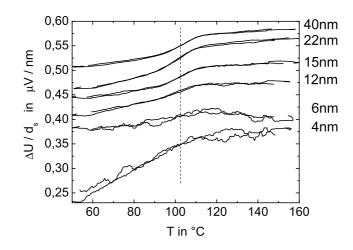


Figure 2: Normalized AC-calorimetric response  $\Delta U/d_s$  as function of temperature for six different film thicknesses  $d_s$ . The scanning rate for all measurements was 2 K/min and the frequency 40 Hz. The heating and cooling curves for the second heating cooling cycle 50°C - 150°C - 50°C are shown. The dashed line indicates the glass transition temperature.

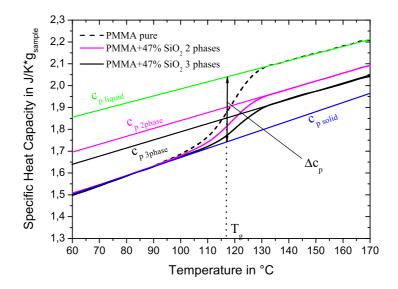


Figure 3: Specific heat capacity of PMMA with 47 wt%  $SiO_2$  nanocomposite; straight lines are for solid and liquid states for the pure polymer (green) and polymer nanocomposite according to two (magenta) and three phase (black) model

## 2.2.3 Physics of Glasses

Head: Prof. Dr. Rainer Kranold

Staff: Dr. Uwe Hoppe Dr. Günter Walter Ursula Heyer

#### Main research area

The work concentrates on investigations of non-crystalline and partially crystalline materials. In this field, special interest has been directed to processes of the formation of crystalline and amorphous nanoscaled phases in glasses and alloys as well as the short- and intermediate-range order in single-phase oxide glasses.

#### Methods

Besides X-ray diffraction experiments (SAXS, WAXS, XRD) performed in the laboratory, synchrotrons (HASYLAB, Hamburg; BESSY, Berlin) and neutron scattering facilities (RAL, Chilton; HMI, Berlin) are utilized. The latter experiments are aimed at extending the measuring range to extremely large magnitudes of the scattering vector as well as applying contrast variation techniques (ASAXS, SANSPOL, WAXS/WANS). In situ SAXS experiments at temperatures up to 1000°C are carried out as well. Computer methods for evaluating and simulating the scattering data have been continuously developed.

# Concentration fluctuations in mixed metaphosphate glasses

Frozen-in fluctuations in concentration and/or topological density are inherent in any glass and determine the zero-scattering vector limit, S(0), of the structure factor. Among the phosphate glasses, most interest has been directed to those with metaphosphate composition,  $Me(PO_3)_n$  where n is the valency of the metal ion Me. The structure of metaphosphate glasses can be described in terms of anionic phosphate chains and/or rings possessing no cross-links; charge compensation requires a well-balanced distribution of the Me cations around the anionic chains. Thus, for most of the binary metaphosphate glasses, concentration fluctuations can be neglected in comparison with the fluctuations in density, i.e. these glasses can be interpreted as pseudo one-component systems. Here, we extend this approach to ternary metaphosphate glasses which, consequently, are treated as pseudo two-component systems. Effects of substitution of BaO for SrO and BaO for Na<sub>2</sub>O in mixed metaphosphate glasses have been studied. Using the Bhatia-Thornton formalism, the quantity  $S_{cc}(0)$ was evaluated from the S(0) values obtained by X-ray diffraction. The compositional dependence of  $S_{cc}(0)$ , which represents the mean square fluctuations in concentration, is discussed in terms of ideal and regular mixture models. Fig. 1 indicates a preferred neighbourhood of dissimilar metaphosphate groups for the Ba-Sr system:  $S_{\rm cc}(0) < S_{\rm cc}(0)^{\rm im}$ . By contrast, in Fig. 2 the tendency toward segregation of NaPO<sub>3</sub> and Ba(PO<sub>3</sub>)<sub>2</sub> units is indicated:  $S_{\rm cc}(0) > S_{\rm cc}(0)^{\rm im}$ . The dashed line, calculated for a regular mixture of the components, corresponds to a critical temperature of about 340K which is much lower than the glass transition temperature. We suggest that the observed deviations from an ideal mixture behaviour of the components are determined by the different types of intermediate-range order existing in alkali and alkaline earth metaphosphate glasses.

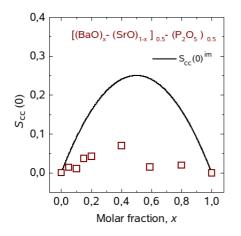


Fig. 1: Compositional dependence of the  $S_{\rm cc}(0)$  values ( $\square$ ). The solid line represents  $S_{\rm cc}(0)$  for an ideal mixture of  $\rm Sr(PO_3)_2$  and  $\rm Ba(PO_3)_2$  units.

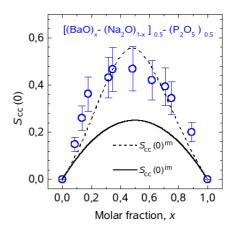
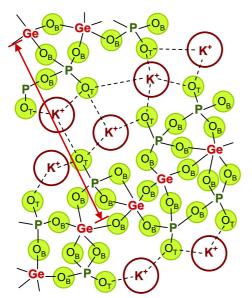


Fig. 2: Compositional dependence of the  $S_{\rm cc}(0)$  values (O). The solid line represents  $S_{\rm cc}(0)$  for an ideal mixture of NaPO<sub>3</sub> and Ba(PO<sub>3</sub>)<sub>2</sub> units. The dashed line indicates  $S_{\rm cc}(0)$  for the model of a regular mixture.

# The atomic structure of potassium germanophosphate glasses

It has been shown by X-ray and neutron diffraction experiments of high resolving power that the short-range structure of potassium germanophosphate (KGP) glasses of compositions close to that of the KGeOPO<sub>4</sub> crystal differs from that of its ordered counterpart. For example, the mean number of oxygen neighbors of the Ge atoms is



 $O_B$  and  $O_T$  indicate O atoms in bridging and terminal (non-bridging) sites.

Fig. 3: Scheme of the atomic structure of KGP glasses with compositions close to that of the KGeOPO<sub>4</sub> crystal.

five in the glass instead of six as found for the crystal structure. This difference needs to assume fractions of non-bridging oxygen atoms for the glass. Such O sites do not exist in the crystal structure. Since only a single length of P–O bonds is detected for the  $PO_4$  tetrahedra in the glass the existence of P-O-P bridges can be excluded and P-O(-Ge) or P–O( $\cdot \cdot \cdot K$ ) bonds dominate. Moreover, pairs of K atoms (or Ge atoms) must share oxygen neighbors and, consequently, Kand Ge-rich substructures are formed as outlined in Fig. 3. The distance of repetition of like regions amounts to  $\sim 1$  nm and is indicated by a long arrow. This length is related with the first peak in the scattering intensities found at a magnitude of scattering vector 7nm<sup>-1</sup>. This value is the smallest which of has ever been reported for a first sharp scattering peak of an oxide glass. (For comparison: The first Bragg reflections belonging to the related KGeOPO<sub>4</sub> crystal appear only at values  $>10 nm^{-1}$ .)

# 2.2.4 Electron Scattering – Insulator Physics

Head: Prof. Dr. Hans-Joachim Fitting

Staff: Dr. Andreas von Czarnowski Dipl.-Phys. Roushdey Salh Elke Prandke

The research group is dealing with electron scattering, mainly in wide-gap dielectrics and insulators; here the electron energy range covers meV up to keV. Consequently, eleastic and ineleastic interactions of electrons with atoms, core and valence band electrons as well as the collective interactions with plasmons and phonons have to be taken into account.

All these scattering mechanisms have been transformed into Monte-Carlo (MC) simulations accompanying our experiments of electron emission, spectroscopy, and microscopy in thin layers and structured solids as well as the hot and ballistic electron transport in semiconductors and dielectric layers. Here basic materials of micro- and optoelectronics are under investigation: e.g. compound semiconductors like BN, AlN, GaN or ZnS and high attention is also payed to the conventional SiO<sub>2</sub>-Si system modified by special ion implantations.

Already in 1980 we have started to calculate the energy balance of hot electrons in  $SiO_2$  by means of respective Monte Carlo simulations and 1990 we first have investigated the vacuum emission (VE) and spectroscopy of ballistic electrons emitted from planar ZnS structures. Especially for dielectric materials like SiO<sub>2</sub>, ZnS, GaAs and applied electric fields a special MC version is developed based on the electron scattering with optical and acoustic phonons, intra- and intervalley scattering and impact valence band ionization, see Fig.1.

The experimental work is performed mainly in a digital scanning electron microscope (SEM) equipped with energy-dispersive X-ray analysis (EDX), cathodoluminescence (CL), electron beam induced conductivity (EBIC) and field-controlled vacuum emission (VE) of hot and ballistic electrons. Furthermore we use Fourier transform 20 infrared spectroscopy (FTIR) for investigation of local defects in amorphous networks of dielectrics. During the last years, in cooperation with French groups in Lyon and St. Etienne, special attention was payed to electron beam charge injection into high-insulating ceramics and the respective selfconsistent charge transport and charging processes in these materials.

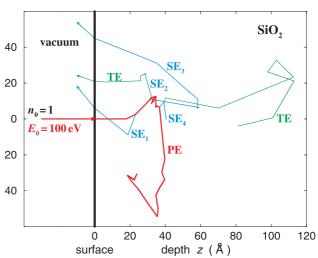


Fig. 1: Monte Carlo simulation of an incident primary electron (PE) scattering and trajectories in SiO<sub>2</sub> with excitation of secondary electrons (SE) also cascading often to tertiary electrons (TE).

Ionizing radiation in dielectric and optically transparent materials produces defect luminescence and modifies the electronic and optical properties of these materials, e.g. of  $SiO_2$ . In this context cathodolumi–

nescence (CL) spectroscopy in a scanning electron microscope (SEM) is a powerful technique enabling high sensitivity and high spatial resolution detection of defect centers in dielectric and insulating materials, especially in small volumes and thin layers. The main luminescent centers in  $SiO_2$  are the red (R) luminescence (650 nm, 1.9 eV) of the non-bridging oxygen hole center (NBOHC), the blue (B) band (460 nm, 2.7 eV) and the ultraviolet (UV) luminescence (290 nm, 4.3 eV) both related commonly to oxygen-deficient centers (ODC). In  $SiO_2$  we have either enhanced or replaced the second constituent oxygen isoelectronically by additional oxygen or sulfur implantation. In Fig. 2 (top) we see the typical CL spectra of pure  $SiO_2$  as explained above. Surpricingly, in additional oxygen and sulfur implanted samples identical multimodal spectra appear as shown in Fig. 2 (middle and bottom).

There are strong reasons to favour the interstitial oxygen molecule  $O_2^-$  and its electronic-vibronic optical transitions for the multimodal CL structure. In case of sulfur implantation, the oxygen is likely released from the SiO<sub>2</sub> network, and probably, substituted by sulfur atoms, leading to free oxygen and finally to molecules on interstitial sites.

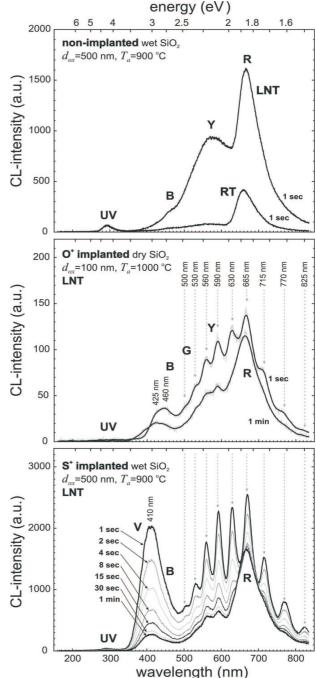


Fig. 2: Cathodoluminescence spectra of a pure  $SiO_2$  layer in comparison to oxygen  $O^+$  and sulfur  $S^+$  ion implanted  $SiO_2$  layers appearing with a sharp multiplet structure.

## **International Cooperation:**

Université de Nantes, Ecole Centrale de Lyon, Ecole Nationale de Mines de St.Etienne (France); University of Latvia in Riga (Latvia); Ioffé Physico-Technical Institute St. Petersburg, and Ural State Technical University (USTU) in Ekaterinburg (Russia); as well as the Institute of Ion Beam Physics / Research Center Rossendorf - Dresden in Germany.

# 2.2.5 Physics of Nanomaterials

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## Nanostructure Processing of Advanced Biomaterials

The main topic of our research is the structure analysis and development of nanoscaled materials. The investigations are performed using X-ray tomography, X-ray diffraction (SAXS and WAXS), scanning and transmission electron microscopy including spectroscopy (EDX and EELS) and electron diffraction.

The sol-gel-process is our the key technique for manufacturing nanostructured material.

The improvement of the acceptance of a synthetic material in living tissue is of great importance. Therefore we developed a synthetic nanostructured biomaterial with spe-

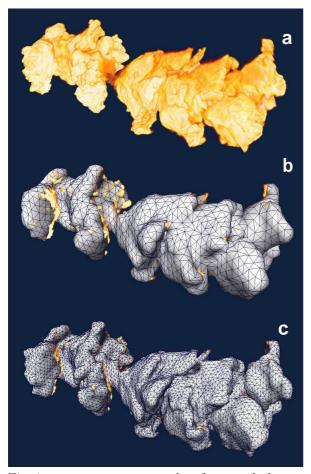


Fig. 1:  $\mu$ -computer tomography of a granule from a bone grafting material (a). Covering of the surface area with triangles of different size (b and c).

cial properties. The interaction between the synthetic material and autological proteins is achieved by using a synthetic matrix of defined porosity. The special properties of the matrix are the reason for a high bioactivity. This activity stimulates the differentiation of adult stem cells and the formation of various tissues.

The interdisciplinary research projects are cross-disciplinary efforts that draw together working groups of our faculty and the faculty of medicine, including physicists, chemists, biologists and physicians.

Two examples are given to demonstrate the fields of our interest.

# Surface design of a synthetic bone grafting material

A simple example shows how a special surface structure can influence the properties of biomaterials. Figure 1a gives the granule of a bone grafting material. The surface was designed for an optimal tissue contact. This goal was achieved creating a fractal surface. The surface of the granule can be covered by triangles with different areas, given in Fig.

1b and 1c. Figure 2 shows the plot logarithm from number of triangle versus log-

arithm from size of triangles. The resulting linear dependence indicates a fractal surface, in this case with Dimension  $D_f=2.2$  (Hausdorff Dimension). Animal experiments documented the potency of the designed surface. Figure 2b shows a micrograph of a demineralised histological section from a sample 6 weeks after implantation. The granule located upper right is surrounded by newly formed bone tissue.

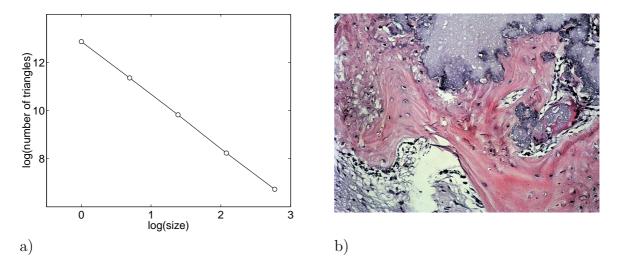


Fig. 2: a) Plot of the logarithm from number of triangle versus logarithm from size of triangles. The value of the slope is the fractale dimension with  $D_f = 2.2$ . b) Micrograph of a demineralised histological section from a sample 6 weeks after implantation (Hematoxylin-eosin, 25x).

#### Interaction of proteins with a synthetic biomaterial

NanoBone<sup>®</sup> is characterized by nanocrystalline hydroxiapatite (HA) that is embedded in a highly porous matrix of silica gel. As has been detected by means of scanning electron microscopy and EDX (figure 3 a and b), this silica gel matrix is degraded in vivo within a short time period without the granule losing its outer shape. This rapid degradation process is unusual because the solubility of SiO<sub>2</sub> in H<sub>2</sub>O is very low at a pH of 7, so that this degradation cannot be a mere solubility process. Using demineralised histological sections, it was demonstrated that HA is tied in the granule by an organic matrix which has formed in vivo in parallel with SiO<sub>2</sub> degradation. The transmission electron micrograph shows that the organic matrix is unstructured and that there are only a few isolated collagen fibrillae (figure 3 d).

Specific immunohistochemical examinations showed an immunoreactivity for osteopontin, osteocalcin (shown in figure 3 d as an example), BMP2 and other proteins which are involved in the osteogenesis.

Within 5 weeks, the completely synthetic inorganic biomaterial changed into a material which is similar to the extracellular bone matrix. Contrary to bone, however, the organic matrix of  $NanoBone^{(R)}$  granules contains almost no collagen fibrillae. For that reason, this material cannot have the same tensile strength as natural bone. In its mechanical properties, it is not comparable with natural bone. This example show, that the nanostructuring of synthetic biomaterial can control the physiological reaction of the tissue.

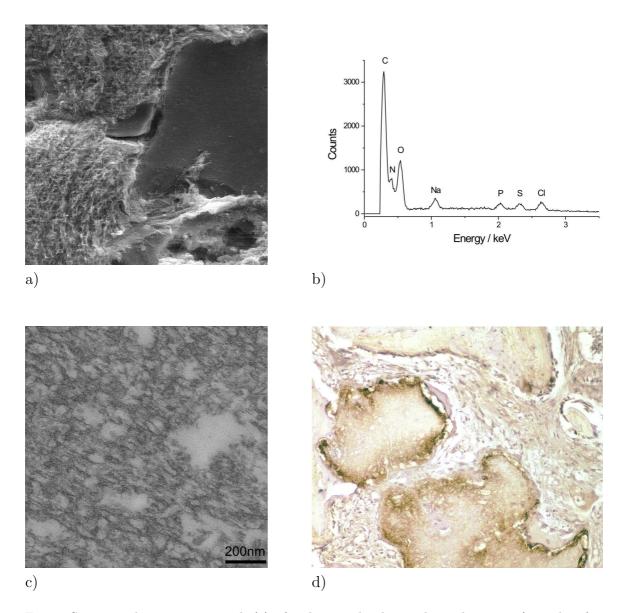


Fig. 3: Scanning electron micrograph (a) of a demineralized granule in the tissue (5 weeks after implantation) and EDX spectrum (b) of the granule. Owing to the demineralization process, calcium phosphate cannot be detected any longer. Neither is it possible to detect silicon from the matrix of the silica gel, although the demineralization process does not attack SiO<sub>2</sub>. The granule contains nothing but organic constituents. Transmission electron micrograph (c) of the granule 5 weeks after implantation and after demineralization. The samples have been contrasted (osmic acid and uranyl acetate) and embedded in epoxy resin. There is the typical newly formed amorphous organic matrix, which contains holes representing the sites where HA crystallites have been dissolved out. Immunoreactivity towards osteocalcin in the demineralized section (5 weeks after implantation). The brown coloration indicates osteocalcin which can be detected in high concentration at the surface of the granule (d).

# 2.3 Physics of Particles and Fields

# 2.3.1 Quantum Theory of Many-Particle Systems

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#### **Optical and Transport Properties in Dense Plasmas**

Within a many-particle linear response theory, the dielectric function is related to a dynamical collision frequency which is expressed in terms of force-force correlation functions. We use quantum statistical methods to evaluate the equilibrium correlation functions and compare with MD simulations. In particular, we find that perturbation theory can be applied to nonideal plasmas with coupling strength smaller than 2. MD simulations are based on a classical approach incorporating quantum effects via a pseudopotential, but work at any coupling strength.

Our approach allows for calculations of quantities related to radiation - matter interaction of dense plasmas. Investigations are performend for Thomson scattering, which is used as a diagnostic tool for warm dense matter, reflectivity in shock compressed plasmas, electrical conductivity and Hall factor, see Fig. 1. In particular, experimental results for inert gases are now well described. Also, of particular interest is the transition from bulk properties to finite cluster properties.

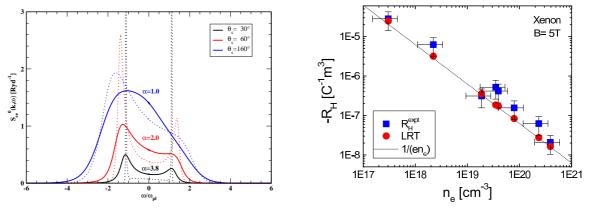


Fig 1: Left: Structure factor of free electrons in dependence of frequency, normalized with plasma frequency  $\omega_{\rm pl}$  at free electron density  $10^{21}$  cm<sup>-3</sup>, temperature 2 eV and incoming radiation with wavelength of 4.13 nm, dotted line - collisionless plasma (RPA), full line - inclusion of collisions (figure by R. Thiele). Right: Hall coefficient in dependence of the electron density for xenon. -Experimental results by Shilkin. -Results of linear response theory (LRT) calculated in a five moment approximation for partially ionized plasmas in a magnetic field of 5 Tesla (figure by J. Adams).

The influence of particle correlations on the bremsstrahlung spectrum in non-ideal plasmas is investigated. Single-particle correlations are accounted for using the concept of the single-particle spectral function determined in self-consistent (GW) approximation, see Fig. 2. Self-energy and vertex corrections for the free-free absorption coefficient are evaluated.

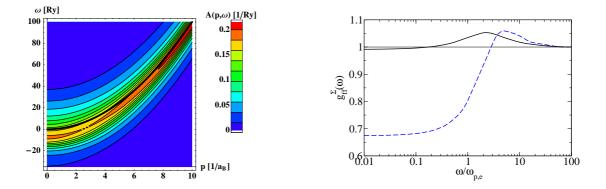


Fig. 2: Left: Contour plot of the self-consistent electron spectral function in GW approximation for the self-energy at solar core conditions as a function of the frequency  $\omega$  and the wave vector p. For small wave vectors, considerable broadening is observed. *Right:* Self-energy and vertex corrections to the free-free absorption coefficient as a function of the frequency  $\omega$  (figures by C. Fortmann).

#### Spectral Line Profiles in Dense Plasmas

Due to the interaction with surrounding particles, spectral lines in dense plasmas are strongly modified compared to their isolated, atomic counterparts. The spectral line shape for neutral helium and He-like ions is investigated using a quantum-statistical many-particle approach. Shift and broadening of several lines are obtained for various density and temperature conditions, see Fig. 3. Using the same methods, the spectra of He- $\alpha$  and He- $\beta$  in dense and hot, laser-induced carbon plasmas are used for diagnostic purposes.

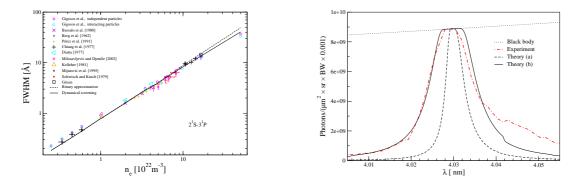


Fig. 3: Left: Stark FWHM for the He I 5016 Å line as a function of the electron density. Our approach is termed 'dynamical screening'. Measured data and other theoretical approaches are included. Right: Comparison of the measured He- $\alpha$  profile of laser-heated carbon. A synthetic spectra with density  $n_e = 4.5 \times 10^{26} \,\mathrm{m}^{-3}$ , temperature  $T = 3.3 \times 10^6 \,\mathrm{K}$ , and thickness  $d = 400 \,\mu\mathrm{m}$  reproduces the measured profile (figures by B. Omar).

The features of chlorine K-lines (see Fig. 4) have been investigated to develop X-ray probes for Compton scattering on warm dense plasmas. The shapes of these spectral lines have been studied at different laser energies by irradiation of thin saran foils by an intense ultra-short-pulse laser beam. The observed positions of  $K_{\alpha}$  and  $K_{\beta}$ lines undergo a red shift due to a laser induced plasma environment. With increasing intensities the shift changes direction and turns into a blue shift caused by a higher contribution of K-transitions occuring in highly excited or ionized atoms. A theoretical approach on the level of a static plasma potential is outlined to describe this inversion. Plasma polarization effects are taken into account as well as different ionization stages of the X-ray emitter within a warm dense plasma.

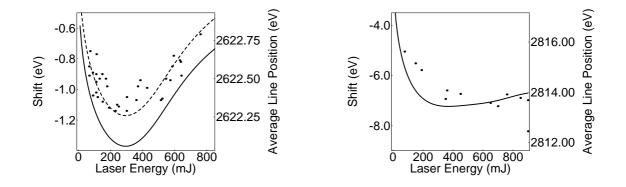


Fig. 4: Shift of average line positions of Cl  $K_{\alpha}$  (left) and  $K_{\beta}$  (right) at different laser energies. Dots: experimental data. Lines: calculated results. Dashed line: results for  $K_{\alpha}$  shifted by 0.2 eV (figures by A. Sengebusch).

#### Clusters and Quantum Condensates in Nuclear Matter

The equation of state (EoS) of nuclear matter at finite temperature and density with various proton fractions is considered, in particular the region of medium excitation energy given by the temperature range  $T \leq 30$  MeV and the baryon density range  $\rho_B \leq 10^{14.2}$  g/cm<sup>3</sup>. Standard approaches such as Dirac Brueckner Hartree Fock (DBHF) or Relativistic Mean Field (RMF) are not applicable in that region. In addition to the mean-field effects, the formation of few-body correlations, in particular light bound clusters up to the  $\alpha$ -particle ( $1 \leq A \leq 4$ ) have to be taken into account. The calculation is based on a many-particle approach, the medium modification of the light clusters is described by self-energy and Pauli blocking effects. Comparison is made with different theoretical approaches as well as with recent experimental analysis of moderate-temperature nuclear gases produced in violent heavy-ion collisions.

#### Kinetic Theory and Decoherence in Quantum Systems

Kinetic equations and linear response approach are extended to relativistic systems. The elaboration of the quantum field theory for nonequilibrium systems is one of the challanging problems in future research. Generalized quantum master equations have been derived for open systems, in particular for Rydberg atoms in a plasma. Decoherence in the time evolution of the open quantum system leads to localisation and the transition from quantum to classical behaviour. Quasiclassical approaches give an adequate description of transition rates for highly excited atoms coupled to a radiation field and interacting with a plasma.

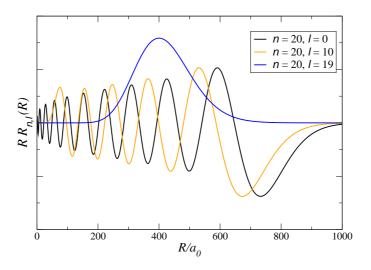


Fig. 5: Radial part of hydrogen's wave function for fixed main quantum number n and different secondary quantum numbers l (figure taken from dissertation thesis by Ch. Gocke).

## Traffic Flow Theory

Microscopic traffic models based on follow-the-leader behaviour are strongly asymmetrically interacting many-particle systems. We investigate the flux of mechanical energy to evaluate the energy balance out of the given nonlinear dynamical system of vehicular particles. In order to understand the traffic breakdown as transition from free flow to congested traffic we estimate the total energy per car at low and high densities and observe the energy of jam formation, see Fig. 6.

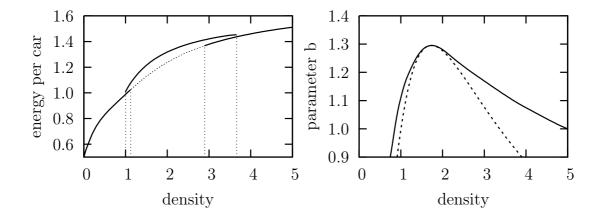


Fig. 6: Left: Total energy per car as sum of kinetic and potential energies over vehicular density  $\tilde{c}$  and fixed control parameter b = 1.1. Dotted lines mark the region of unstable free flow  $1.00 < \tilde{c} < 3.66$ . Right: Region of congested traffic below the critical point ( $\tilde{c}_{cr} \simeq 1.714, b_{cr} \simeq 1.295$ ) bounded by lines of traffic breakdown from heterogeneous flow (solid curve) or homogeneous flow (dashed curve). Numerical calculations and graphics done by Ch. Liebe.

# 2.3.2 Statistical Physics

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#### Equation of state (EOS) of warm dense matter

The properties of hydrogen (or deuterium), helium and their mixtures at high pressure are of great interest for models of the interiors of stars and giant planets as well as for inertial confinement fusion experiments. A precise knowledge of the EOS of hydrogen and helium is, therefore, needed for a large domain of densities and temperatures, especially for high densities as typical for condensed matter and for temperatures of several eV, i.e. for *warm dense matter*.

The EOS of hydrogen and helium is obtained within a chemical model which treats the elementary charged particles (electrons, ions) and neutral bound states (atoms, molecules) on an equal footing. The chemical equilibrium for dissociation and ionization processes is solved accounting for nonideality corrections via laws of mass action. In this way, EOS data and Hugoniot curves but also transport coefficients and the reflectivity are calculated for a wide range of relevant parameters.

Furthermore, a transition from nonmetallic to metallic behaviour is derived from the strong increase of the electrical conductivity and reflectivity above 40 GPa in hydrogen. Some theoretical models predict that this electronic transition is accompanied by a thermodynamic phase instability, the plasma phase transition (PPT), which would affect models of planetary interiors and the evolution of giant planets strongly.

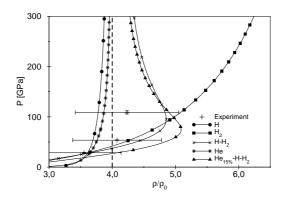


Fig. 1: Hugoniot curves as function of the compression ratio for hydrogen (atomic, molecular,  $\text{H-H}_2$  mixture with dissociation), atomic helium and a hydrogen-helium mixture (15% He mass fraction) within a chemical model (Redmer et al. 2006). We compare with experimental data for deuterium.

#### Ab initio molecular dynamics simulations

The physical properties of fluid alkali metals are of great interest as prototypical simple metals. The most interesting feature in fluid metals compared with Lennard-Jones systems is the density dependence of the interaction potential between the charged particles. This leads to a strong state dependence of the thermodynamic properties and to a metal-to-nonmetal transition along the thermal expansion. This electronic transition is a result of a relocalization of free conduction electrons at nuclei with decreasing density. Although this qualitative explanation is simple it nevertheless requires the treatment of fundamental problems of many-particle physics such as disorder and correlations for a more detailed description. Furthermore, the dense vapor is not monoatomic as in noble gases but consists also of dimers and further neutral and charged clusters.

We have performed finite-temperature density functional calculations for expanded fluid Rb and Cs to clarify the origin of this continuous transition from metal to nonmetal along the expansion. We compare the calculated pair correlation functions with results derived from neutron and X-ray scattering experiments. The experimentally observed structural changes with the density and temperature are well reproduced.

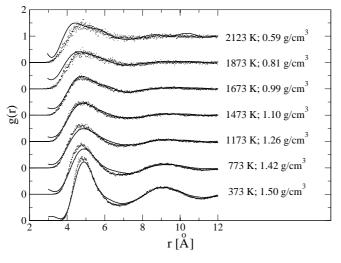


Fig. 2: Pair correlation function for expanded fluid Rb: Ab initio molecular dynamics simulations (data points) are compared with x-ray diffraction experiments (solid lines). The first and second peak are weakened along the expansion of the liquid towards the vapor. The slight structures in these peaks below 1 g/cm<sup>3</sup> are due to the onset of dimerization (Kietzmann et al. 2006).

#### Interaction of plasmas with electromagnetic fields

The growing interest in understanding the properties of matter under extreme conditions requires the development of new experimental techniques for the measurement of temperatures, densities, and charge states. During the recent years, X-ray Thomson scattering has become such a powerful experimental method demanding, however, substantial theoretical input for a proper interpretation of the measured spectra. The scattering of intense X-ray radiation with the electrons is essentially determined by the response function which was calculated in a joint effort at the U Rostock together with partners at the FSU Jena and DESY Hamburg within the so-called Born-Mermin approximation (Redmer et al. 2005). This approach goes beyond the usual Random Phase Approximation (RPA) for the dielectric function and accounts for collisions. The new theoretical results have allowed to derive plasma parameters from novel experiments on warm dense matter for the first time (Gregori et al. 2006).

A further topic was the quantum kinetic description of collisional absorption in dense plasmas. A general expression for the electron-ion collision frequency valid for arbitrary field strengths has been derived and discussed both in the weak-field (linear response) and high-field regime. Molecular dynamics simulation were performed which confirm qualitatively the analytical results for two-temperature plasmas.

Numerical results for collisional absorption of laser energy in aluminum have been calculated covering a broad temperature range, especially the region of intermediate temperatures which cannot be described by the high- and low-temperature asymptotes. Ionic correlations affect the electron-ion collision frequency quantitatively at not too high temperatures and small laser frequencies (corresponding to long wavelengths). For short-wavelength lasers such as the free electron laser at DESY Hamburg (FLASH), the linear response theory works up to rather high intensities. Our approach to collisional absorption in laser fields provides an efficient tool for studies

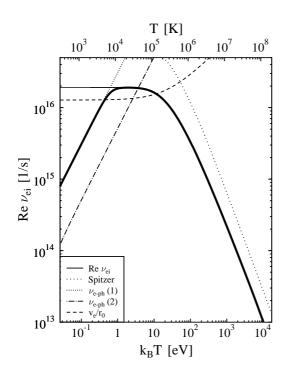


Fig. 3: Dynamic collision frequency vs. electron temperature with  $T_i = T_e$  for aluminum and a laser wavelength of  $\lambda =$ 800 nm in the weak field case (Semkat et al. 2006). The analytical theory is compared with limiting results for the electron-phonon interaction in the lowtemperature range and the Spitzer result for the high-temperature plasma case. The dashed line gives an estimate where the mean free path is equal to the mean interionic distance.

of warm dense matter. It can also be used as input in hydrodynamic simulations of solid-density matter at arbitrary temperatures.

## High-field electron transport in semiconductors

We have performed extensive ab initio band structure calculations for semiconductors such as Si, GaAs, GaN, and ZnS within density functional theory using an exact exchange formalism with a local density approximation for correlations (EXX-LDA). These results were processed in full-band ensemble Monte Carlo simulations of highfield electron transport in these materials, considering all relevant scattering processes including impact ionization. Especially, the wave-vector dependent impact ionization rate was calculated, and a strong asymmetry of this microscopic scattering rate as well as a pronounced influence of the band structure was found. Results were obtained for the drift velocity, the mean kinetic energy, the valley populations, and the ionization coefficient dependent on the applied electrical field.

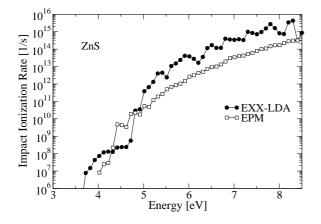


Fig. 4: Impact ionization rate for ZnS using EXX-LDA and the empirical pseudopotential method (EPM) (Kuligk et al. 2005).

## 2.3.3 Physics of Elementary Particles

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## Experiment BABAR

Since summer 2000 the group is participating in the BABAR-experiment at the Stanford Linear Accelerator Center (SLAC) in Stanford, USA. This experiment studies multi-particle final states produced in the electron-positron-annihilation at a center of mass energy of 10.580GeV. At this energy, the  $\Upsilon(4S)$ -resonance is produced, which decays exclusively into a pair of heavy *B*-mesons. The principal aim of the experiment is the investigation of a time dependent CP asymmetry (particle-anti-particle asymmetry) in the decay of neutral *B*-mesons. The main achievement of BABAR was the first observation of this CP asymmetry in 2001. In the three years covered by this report, subsequent studies have revealed more details and improved the precision of the parameters of the Cabibbo-Kobayashi-Maskawa matrix which are responsible for this effect.

Also direct CP violation (an asymmetry in time-integrated decay rates) was observed in 2004 as an asymmetry in the decay probability for  $B^0 \to K^+\pi^-$  compared with the anti-particle decay  $\overline{B}^0 \to K^-\pi^+$  (see Fig. 1).

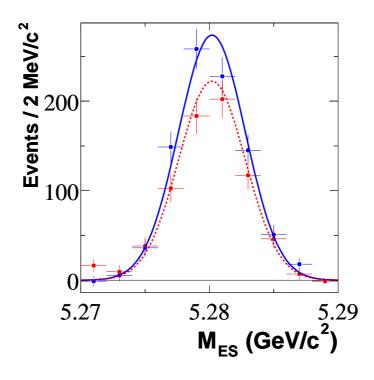


Fig. 1: Direct CP violation is observed as an asymmetry between the decay rate  $B^0 \to K^+\pi^-$  (blue solid line, blue data points) and  $\overline{B}{}^0 \to K^-\pi^+$  (red dashed line, red data points). The peaks centre at the *B* meson mass of 5.28GeV/ $c^2$ , the widths are given by the mass resolution of the analysis method.

In addition to these key questions, the BABAR experiment offers an almost unlimited potential for the study of charmed mesons, charmed baryons, tau leptons, exclusive final states from radiative  $e^+e^-$  annihilation, and the 500 million  $B\overline{B}$  pairs collected so far are used to analyze the details in decays of this heavy particle. The recent focus of our group's investigations is the production of baryons in *B*-meson decays, which is unique to very few heavy mesons like the  $B^+$  and  $B^0$ .

## **Experiment OPERA**



Fig. 2: The OPERA spectrometer. The aluminum pipes providing tracking information of charged particles are 8 meters long. The black part consists of thousands of emulsion bricks.

The OPERA neutrino detector at the underground Gran Sasso Laboratory (LNGS) was designed to perform the first detection of neutrino oscillations in appearance mode, through the study of  $\nu_{\mu}$  to  $\nu_{\tau}$  oscillations. The apparatus consists of a leadand emulsion-film sandwich target complemented by electronic detectors. It is placed in the high-energy, long-baseline CERN to LNGS beam (CNGS) 730 km away from the neutrino source. In August 2006 a first run with CNGS neutrinos was successfully conducted. A first sample of neutrino events was collected, statistically consistent with the integrated beam intensity.

The German groups in the OPERA-experiment (University of Hamburg, University of Münster, University of Rostock) were constructing the muon spectrometer of the OPERA detector. The Rostock group developed, produced and commissioned the TDC-read-out electronics of the muon spectrometer (see Figure 2).

# The International Linear Collider (ILC) Project

The next generation of particle accelerators will operate at 1000 GeV centre-of-mass energy and above (Terascale). The most urgent questions of interest are: i) What is the origin of masses of the elementary particles? More precisely, what is the nature of the electroweak symmetry breaking? Is the Higgs mechanism the correct description? ii) What is the structure of space at small scales? Are there hidden dimensions? iii) What is the nature of dark matter and dark energy?

Our group participates in the detector development and the physics program of the ILC which is under exploratory studies and complementary to the Large Hadron Collider (LHC) that starts operation in 2008.

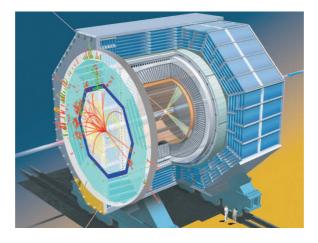


Fig. 3: Large detector concept of the ILC. Central part of the detector shows the Time Projection Chamber (TPC). Front end shows an event expected for the Standard Model Higgs.

# Monte Carlo Studies for ILC

High precision analysis of physics questions such as the electroweak symmetry breaking requires a close collaboration of experimentalists and theorists. This is realized by simulating the complex experimental set-up in depth, starting from an effective Lagrangian quantum field theory that provides the ideas via event generation, hadronisation, detector simulation and finally reconstruction of signal events embedded in a realistic Standard Model background. This study shows sensitivity to new physics encoded in the effective Lagrangian.

# **Detector Research and Development**

The main tracking detector of the Large Detector Concept is a large Time Projection Chamber (TPC, Figure 3), which should allow us to measure with high precision charged tracks originating in the  $e^+e^-$  interaction. Our group studies a novel type of read-out electronics which is based on Time-to-Digital-Converters (TDC) and should meet the stringent requirements of the proposed TPC with more than one million read-out channels. The study is embedded in the European network EUDET.

# Matter under extreme conditions

During the evolution of the early universe or in the interior of compact stellar objects such as neutron stars temperatures of more than  $10^{12}$  K and matter densities of  $10^{15}$ g/cm<sup>3</sup> can be reached. Considerable difficulties of lattice calculations of Quantum Chromodynamics (Lattice QCD) at finite densities (viz. chemical potentials) lead us to develop a novel relativistic statistical description based on light front quantization of QCD. The framework has been proven to work for a simple Nambu Jona-Lasinio model. It is presently applied to QED and QCD with the objective to explore the critical behavior of QCD at the confinement-deconfinement transition.

# 2.4 Physics of Atmosphere and Oceans

#### 2.4.1 Leibniz Institute of Atmospheric Physics, Kühlungsborn

Name of the facility:	Leibniz-Institut für Atmosphärenphysik e. V. (IAP)
	an der Universität Rostock
Address:	Schlossstr. 6, 18225 Ostseebad Kühlungsborn, Germany
Director:	Prof. Dr. Franz-Josef Lübken
Telephone:	-49-38293-68-0
Fax:	-49-38293-68-50
Web:	www.iap-kborn.de
Source for more information:	Institute report (updated every two years)
Other locations:	Außenstelle Juliusruh, Drewoldke 13
	18556 Juliusruh, Germany

## Main Areas of Research

The main task of the Institute of Atmospheric Physics (IAP) at the Rostock University is to conduct research in the field of atmospheric physics. The atmosphere is a multi-faceted and often quite variable medium of complex behaviour. Its great variety gives us the opportunity to seek "market niches" in international research activity where even comparatively small investments can yield distinctive and interesting contributions to a deeper understanding of the atmosphere. The IAP emphasizes research in the areas of (a) the mesosphere, in particular at Arctic latitudes, (b) the dynamical coupling between the troposphere, stratosphere, and mesosphere, and (c) long-term changes ("trends") of the thermal and dynamical structure in the upper atmosphere. In 1996 the institute moved into a new building at Kühlungsborn which provides modern offices and laboratories. Field measurements are performed primarily at the institute's site at Kühlungsborn, its field station at Juliusruh (at the island Rügen) and at the ALOMAR observatory in Northern Norway. ALOMAR is located at 69°17′N and 16°01′E, hence 2° poleward of the arctic circle. All instruments located at ALOMAR were built and are now operated in international cooperations, of which the IAP is a partner. The IAP also operates a mobile lidar (= light radar) in a container which was stationed in Teneriffe  $(28^{\circ}N)$  and in Spitsbergen  $(78^{\circ}N)$ . The instrumentation at IAP mainly consists of lidars at various frequencies from the infrared to the ultraviolet range of the electromagnetic spectrum and several radars with frequencies between 2 and 54 MHz. Furthermore, instruments are installed on sounding rockets to measure dust, and neutral and plasma number densities in the mesosphere and lower thermosphere. The experimental investigations are accompanied by model calculations and theoretical studies.

## Supplemental Information

By December 2006, 59 individuals were employed at the IAP, amongst them 19 scientists and 19 students. In the period 2004-2006 six staff members of the IAP, namely Prof. Dr. F.-J. Lübken, Prof. Dr. G. Schmitz, Prof. Dr. E. Becker, Dr. habil. U. Achatz, Dr. habil. D. Peters, and Dr. habil. M. Rapp gave courses and seminars at the Rostock University in the field of physics of the atmosphere. They also provided opportunities for students to work at the IAP for their bachelor, master, diploma or ph. d. thesis.

In the following we provide some details from typical research projects in the three departments of the IAP. A list of papers published by IAP scientists during the years 2004-2006 can be found in the appendix of this report.

#### Section "Optical and Rocket Borne Soundings of the Atmosphere"

Head: Prof. Dr. Franz-Josef Lübken
Scientists: Dr. Gerd Baumgarten, Dr. Uwe Berger, Prof. Dr. Götz von Cossart, Dr. Jens Fiedler, Dr. Michael Gerding, Dr. Josef Höffner, PD Dr. Markus Rapp, Dr. Armin Schöch, Dr. Gerd Sonnemann, Dr. Boris Strelnikov, Dr. Cord Fricke-Begemann, 8 PhD students, 5 master thesis students

Main areas of research are the exploration of (a) the arctic middle atmosphere (approximately 10 to 100 km altitude), (b) the thermal structure of the mesopause region at various latitudes (mesopause = pronounced temperature minimum near 90-100 km altitude), (c) aerosol layers in the mesopause region known as "noctilucent clouds", and (d) turbulence and dust in the mesophere. Field measurements are performed by a number of lidars and by instruments mounted on sounding rockets.

In the following, we present some results from Spitsbergen performed with the SOUSY VHF radar and with our mobile potassium lidar. This lidar measures temperatures in the 90-110 km region, as well as 'noctilucent clouds' (NLC) and potassium densities. NLC were first observed at mid latitudes by naked eye in the summer season more than 100 years ago. Today we know that NLC consist of water ice particles which can only exist in the very cold summer mesopause region at mid and high latitudes where temperatures can drop below  $-140^{\circ}$ C. Since several years NLC are detectable by lidars even within the polar circle, i. e. during full daylight. Only the 'large' part of the ice population with radii larger than  $\sim 20$  nm leads to sufficient light scattering. Strong radar signals known as 'polar mesosphere summer echoes' (PMSE) are also related to (charged) ice particles but are less sensitive to particle size. In Figure 1 we show the occurrence rates of NLC at Spitsbergen and demonstrate that 'large' ice particles (NLC and PMSE) basically remove all potassium atoms from the vapor phase, whereas small particles (PMSE only) still reduce K densities significantly.

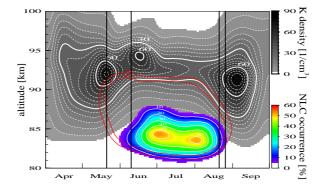


Fig. 1: Seasonal and height variation of potassium densities (grey contours), compared with the occurrence rate of NLC (color contours) and PMSE (red isolines). Potassium disappears in the presence of large ice particles (NLC and PMSE) and gets significantly reduced by small particles (PMSE only) (from Lübken and Höffner, Geophys. Res. Lett., 31, 2004.)

This demonstrates that ice particles in the upper atmosphere can significantly alter the abundance of trace constituents thereby influencing the photochemistry in this region. This result was highlighted on the cover page of *Geophysical Research Letters*, volume 31, 2004. It is important to understand the physical processes leading to NLC since they are very sensitive to background temperatures and may indicate long term anthropogenic changes in the upper atmosphere.

Except from observations by lidar we also study the creation of particles and their morphology by models dealing with microphysical processes and with the spatial and temporal variability of the atmosphere. Furthermore, we have for the first time measured dust particles in the mesosphere by rocket borne instruments and by new radar applications.

## Section "Radar Soundings of the Atmosphere"

Head: Dr. Jürgen Bremer

Scientists: Dr. Norbert Engler, Dr. Peter Hoffmann, Dieter Keuer, Dr. Ralph Latteck, Dr. Werner Singer, Dr. Marius Zecha, Dr. Andrej Serafimovich, 2 PhD students, 3 master thesis students

The main target is the investigation of the structure and dynamics of the mesosphere and lower thermosphere (60-100 km altitude) by means of radar systems at different frequencies in the MF-, HF-, and VHF-ranges. But also at lower heights radar observations are carried out (in the troposphere and lower stratosphere, 2-18 km altitude). The radar measurements are made not only at mid-latitudes (Kühlungsborn and Juliusruh) but also at polar latitudes in northern Norway. Therefore, atmospheric information in dependence on latitude can be derived. The phenomenon of strong radar echoes in the VHF-range during summer months at polar latitudes (PMSE: polar mesosphere summer echoes) and their corresponding echoes in mid-latitudes (MSE: mesosphere summer echoes) are closely connected with the existence of ice particles in the mesopause region (80-90 km). Therefore, these radar echoes contain essential information about the background atmosphere of this height region, mainly about its temperature and water vapour content. Since such information is very important in a global scale the results of radar observations at different places in the world are compared. Therefore, it is necessary to remove those parts of the detected radar echoes which depend on individual technical radar details and derive e. g. radar volume reflectivities of the (P)MSE since such values depend only on atmospheric conditions. The method to calibrate different radars has successfully been developed during the last years. In Figure 2 the results of two absolutely calibrated VHF radars at 69° latitude in the southern (Davis) and northern hemisphere (Andenes) are shown. The normalized height distribution of both observations and the seasonal variation of both data series are presented. The PMSE heights are approximately 1 km higher in the southern hemisphere and the PMSE occurrence rate is markedly smaller than in the northern hemisphere. This result is a strong indication that the temperature in the mesopause region in the southern hemisphere is slightly higher than at the same latitude in the northern hemisphere.

Furthermore, investigations of long-term variations of PMSE and MSE have been carried out. The occurrence rate as well as the seasonal duration increase, indicating a slight decrease of the temperature or an increasing water vapour content of the background atmosphere. Other topics were directed to investigations of mesospheric VHF radar echoes in winter which are more seldom than the corresponding summer echoes mentioned above, the influence of stratospheric warming effects on the mesosphere, the derivation of atmospheric gravity wave parameters during a sounding rocket campaign in northern Norway, the solar influence on the mesospheric wind field and trends

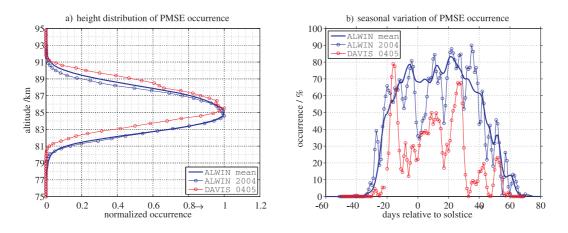


Fig. 2: a) Normalized height distribution of PMSE occurrence and b) seasonal variation of PMSE occurrence above Andenes (thin blue lines for the summer 2004, thick blue lines for mean summer derived from 7 years observations) and Davis (red lines for the summer 2004/2005)

in different atmospheric and ionospheric parameters.

## Section "Theory and Modeling"

Head: Prof. Dr. Erich Becker

Scientists: Dr. Ulrich Achatz, Dr. Axel Gabriel, Dr. Norbert Grieger, PD Dr. Dieter Peters,

Dr. Heiner Körnich, Dr. Christoph Zülicke, 2 PhD students, 1 master thesis student

The department's general field of research is the dynamical coupling of the troposphere, stratosphere, and mesosphere/lower thermosphere (MLT, altitude range from 50 to 120 km). This coupling is controlled by atmospheric waves found on vastly differing temporal and spatial scales. Generally, these waves originate in the troposphere, propagate upward, and dissipate at higher altitudes, giving rise to wave-mean flow interaction. By this mechanism, atmospheric waves drive a global circulation that induces substantial deviations from radiative equilibrium seen in the winter stratosphere and particulary in the summer MLT around 80-90 km.

In recent years, the department has investigated the excitation, propagation, and turbulent dissipation of gravity waves which dominate the wave-mean flow interaction in the MLT. Due to their comparatively small spatial and temporal scales, atmospheric gravity waves can hardly be resolved in conventional comprehensive climate models including the MLT. Instead, gravity waves are usually parameterized which invokes strong assumptions and even serious theoretical uncertainties. The department is therefore working on a better understanding and parameterization of gravity waves with regard to both their generation in the troposphere and the transition to turbulence in the MLT. In addition, a mechanistic global climate model has been developed that allows to explicitly simulate an important part of the gravity-wave spectrum. This has been achieved by using a sufficient spatial resolution and a new formulation of anisoptropic turbulent diffusion based on Smagorinsky's generalized mixing-length approach.

In the following we briefly discuss an example where this model concept is applied to explain unusual observations of the MLT obtained at the site of the ALOMAR observatory (69°N) in summer 2002. Figure 3 shows the model response for this unusual season relative to 'normal' summer seasons. The simulated changes in the polar summer MLT ultimately result from diabatic heating perturbations in the tropical and southern troposphere. These perturbations induce a global intensification of gravity-wave generation, which in turn leads to wave dissipation at lower altitudes in the summer MLT. This downshift can consistently explain all climatological changes observed in the northern summer MLT in 2002.

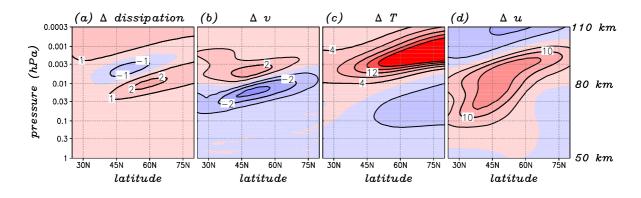


Fig. 3: Differences of (a) dissipation, (b) northward wind, (c) temperature, and (d) eastward wind in northern summer 2002 relative to a 'normal' summer season. Shown are climatological averages from a sensitivity experiment performed with a mechanistic climate model as described in the text. The contour intervals are (a)  $0.5 \text{ Kd}^{-1}$ , (b)  $1 \text{ ms}^{-1}$ , (c)  $5 \text{ ms}^{-1}$ , and (d) 4 K.

# 2.4.2 Baltic Sea Research Institute, Warnemünde

(Institut für Ostseeforschung Warnemünde (IOW) an der Universität Rostock) Director: Prof. Dr. Bodo v. Bodungen

# Department of Physical Oceanography and Instrumentation

Head: Prof. Dr. Wolfgang Fennel Deputy: Prof. Dr. Hans Burchard

#### Introductory remarks

The Baltic Sea Research Institute Warnemünde is a member of the Science Association Gottfried Wilhelm Leibniz. The Director is Prof. Bodo von Bodungen. It is jointly funded by the federal government and the state of Mecklenburg-Vorpommern and is associated with Rostock University where the IOW department heads contribute to the teaching of biology, chemistry and physics. The two professors in the department of marine geology teach at Greifswald University. The institute has an interdisciplinary profile comprising the four basic disciplines of marine sciences in the department of physical oceanography, marine chemistry, biological oceanography, and marine geology. The research is focused on marine systems in coastal and marginal seas using the Baltic Sea as an example. For more detailed information we refer to the annual reports of the IOW and invite the reader to visit our web site (www.iowarnemuende.de).

The department of physical oceanography is linked to the Institute of Physics of the faculty of mathematical and natural sciences of the University of Rostock. Six members of our department, Prof. Fennel, Prof. Burchard, Dr. habil Hagen, Dr. habil. Lass, Dr. Umlauf and Dr. Seifert are teaching in the university of Rostock.

The oceanographic research encompasses four elements: Observations with research vessels and moored instruments, theoretical studies and numerical modelling, satellite oceanography and work in the Baltic Monitoring Programme. Further activities outside the Baltic are mainly focussed on the Benguela Current System off Namibia, South Africa and Angola. The department is also strongly involved in multidisciplinary modelling of marine ecosystems.

This report focuses on research related to the water exchange between the Baltic Sea and the ocean on different time scales, turbulence modelling and theoretical developments with respect to modelling marine ecosystems. Moreover, the application of satellite remote sensing for different system (Baltic, Indonesia, South Africa and Namibia) is addressed and results of our oceanographic research on the coastal oceans off Namibia are briefly outlined.

#### Longterm observations in the central Baltic Sea

# E.Hagen and R.Feistel

The Baltic Sea is relatively young and its environment has always been subject to changes on different spatio-temporal scales. It is located in the humid climate belt of the mid-latitudes. On the climate scale, two types of the general weather situation may be distinguished. The continental type advects dry air masses from Eurasia towards the Baltic Sea, while the maritime type conveys humid air masses in the belt of westerlies from the North Atlantic towards West Europe. Associated variability in the Baltic Sea climate peaks during the winter season due to intensified westerlies. Thus, there exists an exceptional positive correlation between the well known North Atlantic Oscillation (NAO), which describes changes in intensity of the westerlies over the North Atlantic Ocean and West Europe, and the filling level of the Baltic Proper from January until March. However, the impact of the NAO on the Baltic Sea climate decreases with increasing eastern longitude. To address this issue, Hagen and Feistel (2005) proposed the 'Winter Baltic Climate Index (WIBIX)'. It is based on winter anomalies (January-March) of (i) differences in air pressure at sea level between Gibraltar and Reykjavik (NAO), (ii) filling level of the Baltic Proper (Landsort sea level), and (iii) maximum Baltic ice cover. Due to the global nature of changes in the Baltic Sea climate, the obtained index series also reflects long-term changes in land-surface air temperatures of the whole Northern Hemisphere.

On shorter time scales of several days and few weeks, drastic anomalies in sea level changes of the Baltic Proper well reflect in-outflow conditions via exceptional gradients between the south-western Baltic Sea and the Kattegatt. Triggered 'Major Baltic Inflows' affect the hydrographic state of intermediate and deep layers in the whole Baltic Sea and modify the embedded ecosystem on much longer time scales. Such scarce events are able to renew completely the water in deep basins of the Baltic Sea. However, their sequence is separated by stagnation periods lasting several years and the resulting overall residence time of Baltic deep water is about 20 years, but it exceeds 100 years in the absence of such effective deep water intrusions. This was established by numerical circulation models as well as from the analysis of long-term hydrographic trends observed by the Baltic Monitoring Programme at central stations in deep Baltic basins, Feistel et al. (2006).

Power spectra of long-term current records made 20 m above the sea bed of the northeastern topographic flank of the Eastern Gotland Basin (EGB) showed a significant energy gap at a period of about 18 days, Hagen and Feistel (2004). Two significant peaks dominate this period range. The first of them corresponds to the so-called synoptic cycle with periods between 3 and 5 days due to quasi-rhythmic changes in actual weather conditions. The second one exhibits accumulation of kinetic energy for a period of about 10 days and is probably caused by corresponding changes in the westerlies. Long-term current measurements in the deep EGB, which started in 1999 and are continued, suggest that the westerlies maintain a persistent cyclonic circulation with topographically steered deep rim currents. The core velocity is about 3cm/s but accelerates by a factor of about two or three during the winter season.

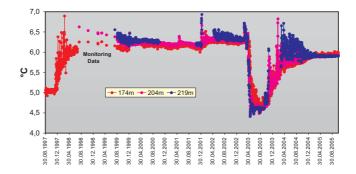


Fig. 1: Daily temperature series from the north-east position (NE) of the Eastern Gotland Basin [EGB - 224 m water depth; modified from Feistel et al. (2006)].

Most of the recording time was characterised by stagnant deep water conditions established by a strong warm water intrusion in the winter 1997-1998, Fig. 1. The deep water conditions were dramatically changed by the cold inflow event of the winter of 2002-2003, Feistel et al. (2006), and a series of subsequent warm water intrusions, Feistel et al. (2004). It could be shown that background changes in the strength of the cyclonic deep circulation react synchronously on changes in the filling level of the Baltic Proper, especially during stagnation periods, see Fig. 2. Typical changes of  $\pm 10 \, cm$  in the Landsort sea level release fluctuations in deep volume transports of about  $\pm 5 \, km \, day^{-1}$  due to a barotropic response of deep motions on suddenly changed winds. However, it also became evident that baroclinic dynamics enter the deep circulation during/after the inflow events.

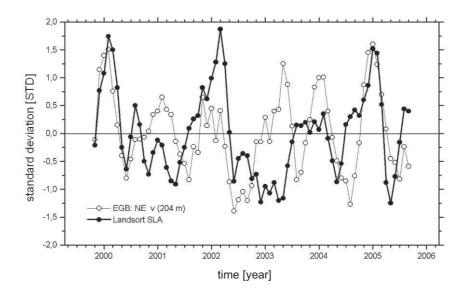


Fig. 2: Three monthly running averages of standardized series (mean=0, standard deviation STD=1) of the Landsort sea level anomaly (SLA) reflecting changes in the filling level of the Baltic Proper and the along-slope currents (v) recorded 20 m above the sea bed at the mooring site denoted NE in Fig. 1; note the general similarity of both curves during so-called stagnation conditions while great discrepancies point to other relevant dynamics during and after the strong inflow reported for the winter 2002-2003.

This point will be further analysed with the help of numerical circulation models and the deployed current meter arrays.

#### Water mass transformation through mixing in the Arkona Sea

L. Umlauf, H. Burchard, H.U. Lass and V. Mohrholz

Saline inflows originating in the North Sea are of essential importance for the ventilation of the deep basins of the Baltic Sea, and therefore their exploration forms one of the central research topics at IOW. Crucial for the pathway of these saline bottom currents, in particular with regard to their potential to reach the deepest and deoxygenated layers, is their dilution by entrainment of less saline, and therefore less dense, water masses. It is obvious that man-made construction elements like off-shore wind farms or bridge piles are additional mixing agents that may strongly enhance the natural entrainment. So far, however, it has not been possible to clearly quantify these additional mixing effects, and illustrate their basin-scale effect on the ecosystem.

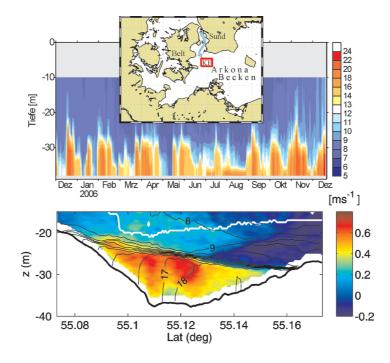


Fig. 3: Upper panel: Long-term measurements of salinity in the channel north of Kriegers Flak (marked by 'KF' in the inlay). Orange/red shading indicate near-bottom inflow events of saline waters. Lower panel: Down-channel currents speed across the channel (colors), and density anomaly in  $kg m^{-3}$  (black contour lines). The width of the channel is approximately 10 km.

The question about the natural and the antropogenically modified dynamics of saline inflows is currently being investigated at IOW in the framework of the two projects QuantAS-Nat and QuantAS-Off. Using advanced measuring techniques, these measurements are focused on the Belt Sea area and the Akona Basin (Fig. 3). Here, a small submarine channel north of a shallow region called Kriegers Flak (Fig. 3) plays a key role since the major part of saline water masses entering through the Sound have to pass it. Long-term measurements in this important constriction have been obtained recently by IOW researchers, and show, for the first time, a detailed illustration of the temporal distribution of occurrence, strength, and dynamics of saline gravity currents. One of the main results was that these inflow events occur much more frequently than previously thought (Fig. 3) Detailed current measurements across the channel have shown that these density driven bottom currents may reach quite high velocities (Fig. 3), and have therefore the potential to transport large amounts of salt into the Baltic Sea. The tilting and spreading of the interface are manifestations of the effects of Earth's rotation on the current field (Coriolis acceleration plays the major role here), and according investigations have been discussed in, e.g., Sellschopp et al., 2006). The observations could be well reproduced with numerical simulations of the Western Baltic Sea see Fig. 4.

First *in situ* investigations of the effects of man-made constructions on the vertical mixing in a stratified flow have been conducted in 2006 during two research cruises

near the Great Belt bridge. Using high-resolution (both in space and time) measuring systems IOW researchers could demonstrate a considerable impact of individual bridge piles on the mixing behind the bridge. Streets of turbulent eddies were shown to exists even at large distances downstream from the bridge. These results were consistent with the mixing rates estimated from direct turbulence measurements, also indicating strongly enhanced mixing behind the bridge. Strong mixing implies a weakening of the vertical temperature and salinity stratification downstream from the bridge, which is clearly illustrated by the data shown in Fig. 5. It could also be demonstrated that the bridge piles generate a field of so-called internal waves that may travel over long distances before they break and eventually cause energetic mixing.

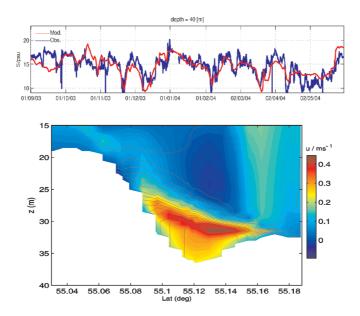


Fig. 4: Upper panel: Bottom salinity from the MARNET-Station in the central Arkona Basin (blue) and model data for the years 2003-2004. Lower panel: Cross-section across the channel north of Kriegers Flak. Shown are the modeled current speed (in color), and contours of constant salinity. Note the structural similarity with Fig. 3.

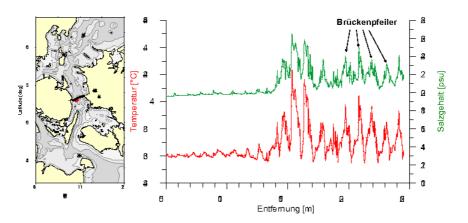


Fig. 5: Temperature and salinity at 5 m depth on a transect parallel to the Great Belt bridge. The peaks in the green and red curves mirror the effect of individual bridge piles.

## Modelling of Transport and Mixing in Coastal Seas

Hans Burchard and Lars Umlauf

Coastal seas which include shelf seas (such as the North Sea and the Baltic Sea), estuaries (river mouth areas) and small-scale coastal area such as the Wadden Sea are dynamically dominated by strong density gradients due to temperature and salinity differences interacting with currents due to wind, tides and density driven flows. For the quantification of transport and mixing processes in such coastal systems, realistic numerical models are needed which incorporate the major dynamic processes. For these purposes, numerical models are developed at IOW in close international cooperation. The General Ocean Turbulence Model (GOTM, see Umlauf et al., 2005, Umlauf and Burchard, 2005), is a one-dimensional Public Domain water column model, widely accepted as a community model for studying turbulent mixing in the ocean, for details see www.gotm.net. GOTM has also been used for studying advantages of adaptive vertical coordinates in ocean models, see Burchard and Beckers (2004).

In recent years, the water column model GOTM has been extended by a biogeochemical module, including several standard models of the NPZD type (Nutrient-Phytoplankto-Zooplankton-Detritus), see Burchard et al. (2006). Since some of the differential equations parameterising biogeochemical processes are stiff, i.e. they include a wide range of time scales, special numerical methods are needed in order to discretise the process terms. New stiff solvers have been developed by IOW, see Burchard et al. (2005).

The turbulence module of GOTM has been implemented into the three-dimensional General Estuarine Transport Model (GETM, see www.getm.eu). In GETM the coordinates can be constructed in a way that a number of near-bottom layers of horizontally homogeneous thickness allows for reproduction of plume dynamics without distortion by step-like bottom approximation or strongly varying layer thickness. High-order total variation diminishing (TVD) advection schemes for momentum and tracers allow for positive definite transport calculations with small numerical diffusion. Various three-dimensional simulations focussed on turbulent mixing have been documented in detail, see e.g. Burchard et al. (2004) for the tidal Elbe. Studies of the transport and mixing in the Western Baltic Sea showed that mixing is strongest in the sill areas (Drogden Sill between Copenhagen and Malmö, Darss Sill between Darss peninsula and island Falster, and Bornhom Channel between Sweden and Bornholm), Burchard et al. (2005), see Fig. 6. GETM has also been applied to mixing and transport in the Lake of Geneva, see Umlauf and Lemmin (2005), and in the framework of master theses at the University of Rostock for the Limfjord in Denmark Hofmeister (2006).

The combination of a water column turbulence model with a three-dimensional transport model with general vertical coordinates makes the system consisting of GOTM and GETM a unique Public Domain numerical tool for studying transport and mixing processes in coastal areas.

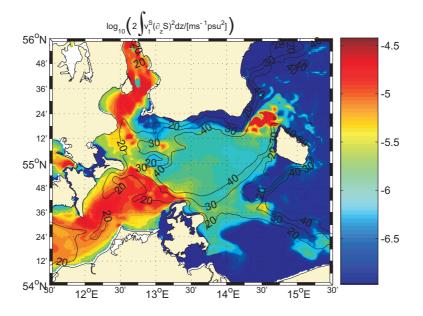


Fig. 6: Vertical mixing in the Western Baltic Sea quantified as the vertically integrated and time averaged decay of salinity variance.

# Ecosystem Model of the Baltic Sea

# Thomas Neumann and W.Fennel

In the last years the IOW ecosystem model has been developed further to facilitate a bridging of biogeochemical processes with the upper part of the marine food web. This has been done by implementing live cycles of copepods, the main secondary producers in the Baltic Sea, into the ecosystem model. The key for a successful simulation of copepods populations was the consideration of simple behaviour rules and specific life cycles. The behaviour rules control the vertical migration. An example of the downward migration of adult Pseudocalanus is shown in Fig. 7. The figure shows the abundance of adult Pseudocalanus at a meridional cross-section in the Baltic Sea. Pseudocalanus prefers higher salinities which it finds usually in the deeper water but have, at the same time, to prevent low oxygen which frequently also is a condition in deep waters, Neumann and Fennel (2006).

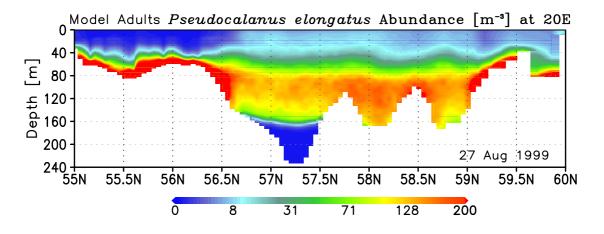


Fig. 7: Pseudocalanus abundance at a meridional cross-section in the central Baltic Sea.

A further field of action was the application of the ecosystem model to reconstruct the status of the Baltic Sea ecosystem for the period 1960-2000. Fig. 8 shows the time evolution of the reproductive volume for cod in the Bornholm Sea. The reproductive volume is a water volume characterized by a certain salinity range with an oxygen content not below 2 ml/l. This volume influences *inter alia* the recruitment of cod. The time evolution of the volume shows a strong inter-annual variability which is controlled mainly due to hydrographical conditions but also due to nutrient loads and primary production.

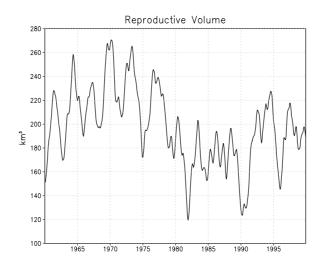


Fig. 8: Cod reproductive volume in the Bornholm Sea.

# Satellite Oceanography

#### H. Siegel

Remote sensing is the only method providing coherent pictures of oceanographic processes which leave signatures at the sea surface. Both the synoptic character and the high repeating rate allow the mapping of variable structures in space and time. The application of satellite data in the IOW was focussed on sea surface temperature (SST) development of the Baltic Sea, the development of phytoplankton blooms, dynamical processes, river discharge and monitoring. SST data derived from the Advanced Very High Resolution Radiometer (AVHRR) of the NOAA weather satellites are evaluated to investigate seasonal and inter-annual variations in the temperature development of the Baltic Sea. The seasonal development in each year is described in the yearly hydro-chemical assessments of the state of the Baltic Sea prepared by IOW (Nausch et al. 2004, 2005, 2006) and in the HELCOM fact sheets (Siegel and Gerth, 2004, 2005, 2006). The analysis of a 15 years SST time series was published by Siegel et al. 2006. The investigation period was characterised by a positive trend in the yearly mean SST with an increase of 0.8 K in 15 years. Summer and autumn dominate this positive trend. This trend continued due to the warm last years. Highest positive slope was found for July in the Northern Baltic Sea. Slight negative slopes were determined for March in the Baltic Proper. The temperature increase in the summer has the consequence of increasing cyanobacteria bloom. Seasonal variations in the satellite derived chlorophyll development are characterized by a spring bloom of diatoms and dinoflagellates and after a stagnation period in June by a summer bloom of cyanobacteria. The yearly course of the blooms is described in detail in the biological assessments of the state of the Baltic Sea since many years prepared by IOW (Wasmund et al. 2004, 2005, 2006). Intense cyanobacteria blooms correspond to warm years. Strong differences occur in the spatio-temporal development as observed in the summers 2005 and 2006. In summer 2005 the maximum intensity was reached on 13 July 2005 the warmest day of the year  $(23 - 25^{\circ}, C)$  in the central Baltic. In summer 2006 the bloom started also in early July in the central Baltic, but developed after mid July mainly in the southern and western parts and lasted until end of August. In the framework of the German-Indonesian Cooperation (SPICE) interdisciplinary pollution studies were performed in the Siak River, an important river in the Riau Province of East-Sumatra (Indonesia). Remote sensing investigations combined with ground-truth measurements in different seasons of the years 2004-2006 were focused on the identification of different sources of water masses in the tributaries and on the discharge into the estuary and Malacca Strait located between Malaysia and Sumatra. Sources of different water masses like humic substances dominated waters, erosion areas of high suspended matter concentration, and areas of limited bio-productivity in industrial regions were identified using satellite data and in situ measurements. High spatial resolution data provided insight into important sources of humic substances in the estuary. It was shown that the Siak River discharge patterns in the estuary are strongly related to tidal phases, the main transport is the outflow into the Malacca Strait and further in north-westerly direction.

In the coastal ocean off Namibia, the sporadic occurrence of milky turquoise was analysed on the basis of ocean colour satellite data. The features close to the coast are mainly due to the upwelling of hydrogen sulphide enriched waters oxidized to elemental sulphur, while offshore plumes outside the upwelling area are generated by phytoplankton of the group of coccolithophores, characterised by increasing the backscattering due to the calcite coccoliths. A bloom of the coccolithophore *Emiliania huxleyi* could be tracked by satellite data over 10 days (Siegel et al. 2005), see Fig. 9. A new multi-spectral classification algorithm for the evaluation of sulphur discolorations and the distinction from other existing features (Ohde et al. 2005). An analysis of sulphur outbreak events in 2004 and 2005 showed, for the first time, that the feature spread along the entire coast of Namibia between  $20^{O}S$  and  $26^{o}S$ , starting end of January and reaching their highest intensity in April. The life time of sulphide events ranges from one to six days.

# The Benguela Upwelling System

#### H.U.Lass and V.Mohrholz

The interaction of the subtropical gyre and the Subtropical Cell was studied with emphasis on the Benguela upwelling system by observations of sea surface height, surface wind vectors, and precipitation. Additionally, current profiles, drifter data, and hydrographic data were included in these studies. The subtropical gyre of the South Atlantic is governed by a Sverdrup balance between the curl of the wind stress and the planetary vorticity. The coastal and shelf edge upwelling of cold nutrient enriched

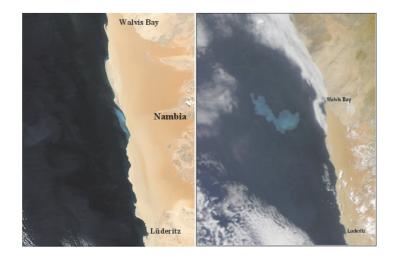


Fig. 9: MODIS quasi-true colour images demonstrate the occurrence of sulphur plumes on 20 March 2004 (left) and of a coccolithophore bloom on 31 March 2003 (right).

water in the Benguela are driven by the south-east trade winds and the negative curl of the wind stress concentrated at the shelf edge of the Benguela, respectively. The coastal upwelling is maintained by wind fluctuations in the coastal wave guide with time scales of less than 10 days since it is stopped and the associated jets are arrested by coastal Kelvin waves. The shelf edge upwelling is maintained by wind stress curl fluctuations with time scales less than a few months since it decays by radiation of long baroclinic Rossby waves into the open ocean. The compensation current of the Ekman offshore current ventilates the bottom water on the shelf of the Benguela more efficient in austral winter than in summer with well oxygenated Eastern South Atlantic Central Water which is advected equatorward by the Benguela current along the shelf edge from the southern tip of Africa, Fig. 10. The eastern part of the Angola Gyre, as part of the southern Subtropical Cell in the South Atlantic, is governed by a Sverdup balance between wind stress curl and planetary vorticity while its western part is modified by heat accumulated by upwelled water along its path from the shelf of Southwest Africa toward South America within the South Equatorial Current. The corresponding sea level elevation terminates the gyre at about  $20^{\circ}W$  and forms a ridge at whose southern edge the South Equatorial Counter Current develops. The upwelling in the Angola Gyre lifts its thermocline water into the euphotic zone causing high biologic productivity. The degradation of sinking plankton implies a suboxic thermocline water mass in the centre of the gyre with high nutrient concentration. The interaction between the subtropical gyre and the Subtropical Cell in the South Atlantic occurs on the West African shelf by poleward outbreaks of the Angola Current through the Angola-Benguela front carrying suboxic South Atlantic Central Water with high nutrient concentration into the northern Benguela. These outbreaks maintain the nutrient balance of the Benguela and are controlled by weak meridional wind stress in the Cape Frio cell and by elevated coastal sea level north of the Angola-Benguela front. Coastal sea level is elevated in September to November by the arrival of an equatorial downwelling Kelvin wave which is triggered by relaxation of zonal wind stress in the equatorial wave belt off Brazil and in February to April it is elevated by freshwater surplus due to precipitation in the eastern tropical Atlantic and river discharge at the African coast. The coincidence of outbreaks of the Angola current onto the shelf of the northern Benguela with weakened ventilation of the bottom water in austral summer supports the formation of oxygen depleted bottom water due to diffusion of hydrogen sulphide from the mud belt into the water column during austral summer.

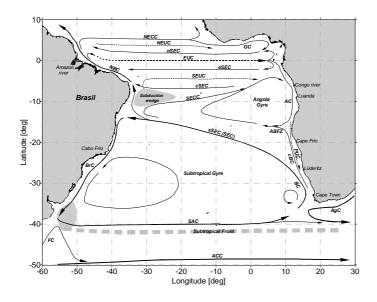


Fig. 10: Schematic map of the horizontal distribution of the near-surface circulation (full line) and the circulation in the thermocline (dashed line) in the equatorial and subtropical South Atlantic. Shown are the North Equatorial Counter Current (NECC), the North Equatorial Undercurrent (NEUC), the Guinea Current (GC), the northern (nSEC), equatorial (eSEC), central (cSEC), southern South Equatorial Current(sSEC), the Equatorial Undercurrent(EUC), South Equatorial Undercurrent(SEUC), the North Brazil Current (NBC), the South Equatorial Contercurrent (SECC), the Angola Current (AC), the Angola. Benguela Frontal Zone (ABFZ), the coastal (cBC) and the Benguela Current (BC), the Polar Undercurrent (PUC), the Brazil Current (BrC), the Falkland Current (FC), the South Atlantic Current (SAC) and the Agulhas Current (AgC).

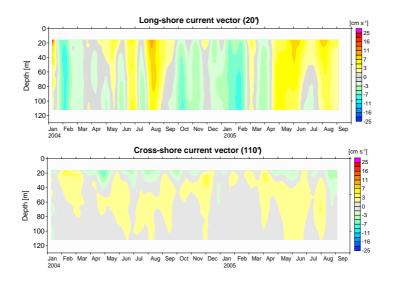


Fig. 11: Lowpass filtered time series of long shore component toward  $20^{O}$  true (upper panel) and cross shore component toward  $110^{o}$  true (lower panel) of current measured on the shelf off Walvis Bay. The cut off period is 30 days.

The seasonal variations in the advection and mixing of water masses in the northern Benguela were studied in relation to the oxygen minimum zone over the Namibian shelf. During intensive field campaigns hydrographic and current meter data were gathered with an oceanographic mooring 20 nautical miles off Walvis Bay, monthly CTD transects at the Namibian  $23^{\circ}S$  monitoring line and large scale hydrographic surveys. The current time series (Fig. 11) showed an intermittent southward continuation of the Angola current through the Angola-Benguela Frontal Zone (ABFZ) into the northern Benguela, commonly known as poleward undercurrent. In austral summer hypoxic, nutrient rich South Atlantic Central Water (SACW) from the Angola Gyre is transported into the northern Benguela, whereas during the winter season the oxygen rich Eastern South Atlantic Central Water (ESACW) spreads northward. The water mass analysis reveals a mixing between both water masses in the northern Benguela between the ABFZ and the Lüderitz upwelling cell  $(27^{\circ}S)$ . The oxygen balance over the Namibian shelf depends to a high extent on the water mass composition of the upper central water layer, controlled by the large scale and local circulation. The deviation of the measured oxygen concentration from its mixing concentration. calculated with the source water mass properties, was used to quantify the oxygen consumption. A new local definition of SACW was derived to exclude biochemical processes, taking place in the Angola Gyre. The oxygen deficit in the northern Benguela central water amounted to about 60 to 80  $\mu$  mol  $l^{-1}$  at the shelf edge and increased up to 150  $\mu$  mol  $l^{-1}$  on the shelf, due to local oxygen consumption. In the austral summer anoxic bottom waters are observed at the central Namibian shelf, which correlate to a SACW fraction of more than 55%. Periods with high SACW fraction in the water mass composition (Fig. 12) were congruent with hydrogen sulphide events detected by remote sensing.

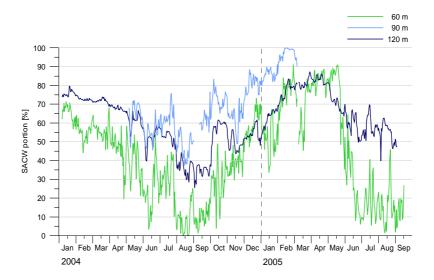


Fig. 12: Fraction of South Atlantic Central Water (SACW) on the watermass composition at the central Namibian shelf  $(23^{0}S, \text{ off Walvis Bay})$ . The high SACW content during austral summer (Dec-Apr) correlates with the season of hydrogen sulfide outbreaks.

# 2.5 Didactics of Physics

Head: Prof. Dr. Hans Erich Riedel

Staff: Dr. Heike Marchand PD Dr. Heidi Reinholz

### Multi-media teaching and training modules

Multi-media modules on topics of quantum physics were developed in cooperation with Cuban partners. The teaching and training software for the education of students in Havana and Rostock has been investigated with respect to education aspects.

Cuban partners:

Prof. Dr. Lazaro Pinol, Instituto Superior de Ciencias y Technologia Nucleares, La Habana, Cuba

Prof. Dr. Rene Hernandez Herrera, Prof. Dra. Victoria Arencibia Sosa, Direccion de Ciencia y Technica MINED, La Habana, Cuba

Prof. Dr. Alfredo Alvarez Dias, Instituto Pedagogico Latinoamericano y Caribenio, Playa, La Habana, Cuba

## School projects

In cooperation with schools and pre-school institutions, smaller projects on topics relevant for the considered age group and the curriculum have been developed and performed with student groups. Examples are *Thunder and Lightning* for pre-school, *What do you know about water?* for primary school children and *The latitude determined with a Foucault pendulum* for secondary school students.

### Textbooks for schools

The group is involved in rewriting textbooks according to changes in the school curriculum of Mecklenburg-Vorpommern and other federal states, e.g.

- H. E. Riedel, H. Marchand, *Mechanik* in Kuhn. Lehrbuch für Physik, Jahrgang 9/10 für Mecklenburg-Vorpommern, Niedersachsen und Rheinland/ Pfalz (Westermann)
- H. E. Riedel, H. Marchand, Nachschlagewerk *TÜF Tabellen*, *Übersichten*, *Formeln* für alle Bundesländer, für Sek I und Sek II sowie Studierende der Technik und Naturwissenschaften (Schroedel-Verlag)

## **Particle Concepts**

A focus of research is the introduction of particle concepts within the science subjects, in particular in physics and chemistry. Different models are used to describe different concepts, e.g. properties of states of matter, electricity or atomic physics. It would be desirable to teach using consistently developed and extended models throughout the science area.

# 3 Special Research Programs

# 3.1 Research Training Group 567: Strongly Correlated Many–Particle Systems

Head: Prof. Dr. Gerd Röpke

Graduiertenkolleg 567: "Stark korrelierte Vielteilchensysteme" Sprecher: Professor Dr. Gerd Röpke

## **Research** Topics

The research training group established on 1st October, 1999 ended after seven successful years in September, 2006.

The research of strongly correlated many-particle systems – in contrast to idealized simple models – shows the complexity of nature and enhances the cooperation between theory and experiment as well as simulation techniques. The topic of the area of research is broad enough to integrate recent and future disciplines of theoretical, experimental and applied physics. The aim of the research program is based on the further development of new methods in Statistical Physics of strongly correlated systems and its application to equilibrium and non-equilibrium quantum systems, dense plasmas, semiconductors, finite systems (clusters), nuclear and subnuclear matter at finite temperatures. Furthermore, the interaction between light and matter as well as the states of light fields are of interest.

The research program of the Training Group (Graduiertenkolleg) was essentially characterized by the represented PhD-topics. Theses topics are partly laid out spanned to intensify the cooperation between the research groups of the Institute of Physics as well as the Associated Institutes ("An-Institute") of the University of Rostock. In the framework of the 2nd and 3rd period of promotion of the Graduiertenkolleg, the following six basic chapters are of particular importance:

- 1. Quantum statistics of strongly correlated many-particle systems
- 2. Optical properties and transport processes in stimulated semiconductors
- 3. Elementary processes on smallest scales in finite systems
- 4. Particle- and Astrophysics
- 5. Nano-structured materials and dynamical structure factor
- 6. Nonlinear dynamical systems

## Seminars and Lectures

The educational activities of the Training Group were concentrated on seminars, lectures and workshops. We also performed interdisciplinary exchange. We organized weekly seminars in which scholarship holders and colleagues present their current work. Furthermore, workshops as well as presentations and lectures of guests were taking place. At the present time we are building up our post–graduate studies.

The research training group achieved the following results:

Several dissertations have already been defended. The research training group was also a further basis of the PHD–Program (graduating from universities in Germany, International Postgraduate Programs: IPP PHD-Program *Physics, Chemistry and Technology of New Materials*). The research training group provided a very good basis for the Collaborative Research Center (Sonderforschungsbereich) *Kinetics of partially ionized plasmas*.

The Research Training Group had different members, one is the group of staff as leaders of different projects:

Teachers:	Prof. Dr. Henneberger	Prof. Dr. Burkel
	Prof. Dr. Redmer	Prof. Dr. Fitting
	Prof. Dr. Röpke	Prof. Dr. Meiwes-Broer
	Prof. Dr. Vogel	Prof. Dr. Mitschke
	PD Dr. Mahnke	Prof. Dr. Schröder
		Prof. Dr. Stolz
		PD Dr. Beyer
		PD Dr. Waldi

together with associated colleagues from related institutions:

Teachers:	Prof. Dr. Blaschke	University of Bielefeld
	Prof. Dr. Dabrowski	University of Szczecin
	Prof. Dr. Burchard	An–Institut für Ostseeforschung
	Prof. Dr. Lübken	An–Institut für Atmosphärenphysik

The other participants are PhD–students with scholarship (scholarship holders; Stipendiaten) of German Research Foundation (DFG) from 2004 to 2006:

Students:	Frithjof Meinke	Andreas Przystawik
	Evgeny Shchukin	Roushdey Salh
	Nadine Nettelmann	Patrick Ludwig
	Jens Berdermann	Thomas Kampf
	Tomazs Denkiewicz	Julia Hinkel
	Banaz Omar	John Adams
	Stefan Strauss	

and more than 15 colleagues (Kollegiaten, PhD students without scholarship of DFG).

Each year these PhD students, Stipendiaten as well as Kollegiaten, carried out one *Graduiertenkolleg Summer Workshop*. In these workshops the participants and one invited speaker gave the presentations. The workshop was especially devoted to the research areas of the Stipendiaten. The talks have been of more general nature, in order to introduce the basic ideas and methods of the specific research area. The variety of the topics from philosophical up to theoretical and experimental descriptions

has been assured by the program. Furthermore, the workshop made a contribution to intensify the collaboration among the PhD students of our department.

Finally the research profile will be described by one particulare example of a manyparticle system with correlations from the working groups of PD Dr. Mahnke.

# One Example of Current Research of PhD–Students

## Julia Hinkel: Applications of Physics of Stochastic Processes to Vehicular Traffic Problems

## Supervisor: PD Dr. Mahnke

A many-particle system imitating the motion of the vehicular ensemble on a one lane road without crossroads is under study. Taking into account the properties of real traffic, both deterministic and stochastic approaches are applied in order to describe the system dynamics. Despite of the car interaction being local in nature, it gives rise to cooperative phenomena that manifests the formation, dissolution and joining of large car clusters. Such processes correspond to the different states of traffic flow which can be treated in terms of phase transitions.

In this connection, the theory of the three traffic states proposed by Kerner is taken as a hypothesis for present investigations. Starting from the microscopic level based on the optimal velocity ansatz, the detailed analysis of the possible traffic states is developed. In view of the fact that such an approach can describe either free flow or congestions, the problem of understanding and description of the intermediate states has been addressed within the framework of this thesis. The new approach is based on study of dynamical states controlled by kinetic coefficients taking into account their anomalous properties and their dependence on position in phase space. The interaction between the noise and the dynamical trap can cause certain anomalies in the system dynamics.

One of the main manifestations of the traffic congestion is the traffic breakdown phenomenon regarded as a random process developing via the cluster formation mechanism. In this manner, the probabilistic description based on the concept of first passage time is developed and the breakdown probability is calculated in terms of the solution of the corresponding Fokker–Planck equation given as a initial–boundary– value–problem. In order to interpret the obtained analytical result, its comparison with the empirical data is performed.

# 3.2 Collaborative Research Center (SFB 652) "Strong Correlations and Collective Effects in Radiation Fields: Coulomb Systems, Clusters and Particles"

Executive Board:	Prof. Dr. Karl-Heinz Meiwes-Broer	
	Prof. Dr. Ronald Redmer	• • • • • • • • • • • • • • • • • • • •
	Prof. Dr. Heinrich Stolz	
	Prof. Dr. Gerd Röpke	
Homepage:	http://www.physik.uni-rostock.de/sfb	SFB 652

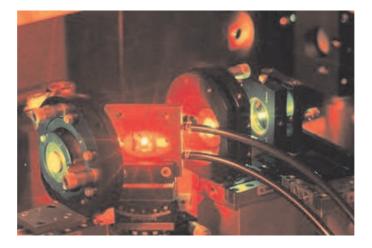
**Projects:** 

A1	Metal clusters in the light of the VUV- and X-FEL
	Prof. Dr. Ronald Redmer, Prof. Dr. Karl-Heinz Meiwes-Broer, PD. Dr. Josef Tiggesbäumker
A2	Thomson-scattering and correlation in warm dense matter
	Prof. Dr. Ronald Redmer
A3	Correlated processes upon photo excitation of trapped clusters and particles
	Dr. Gerrit Marx, Prof. Dr. Karl-Heinz Meiwes-Broer
A4	Many body quantum electrodynamics and dielectric response
	Prof. Dr. Gerd Röpke, PD Dr. Heidi Reinholz
A5	Controlled coupling of intense laser pulses to clusters and particles
	PD. Dr. Josef Tiggesbäumker, Prof. Dr. Karl-Heinz Meiwes-Broer
A6	Quantum kinetics of dense Coulomb systems in laser fields
	Prof. Dr. Manfred Schlanges, PD Dr. Thomas Bornath
A7	The phase of the light in optically excited semiconductor structures
	Dr. Günter Manzke, Prof. Dr. Heinrich Stolz
B1	Exciton matter in mesoscopic potentials
	Prof. Dr. Heinrich Stolz
B2	Microscopic description of quantum optics of many body systems
	Prof. Dr. Werner Vogel, Prof. Dr. Klaus Henneberger
B3	Excitonic clusters with strong coupling to light fields
	Prof. Dr. Holger Fehske, Prof. Dr. Heinrich Stolz
B4	Possibilities and signatures of BEC in structured electron hole systems
	Prof. Dr. Klaus Henneberger
B5	Collective excitonic phases in highly correlated electron hole systems
	Prof. Dr. Holger Fehske, Prof. Dr. Gerd Röpke
B6	Light field induced correlations in condensates of metal atoms
	Prof. Dr. Karl-Heinz Meiwes-Broer

"Collaborative Research Centres (Sonderforschungsbereiche) are long-term university research centres in which scientists and researchers work together within a crossdisciplinary research programme." (Deutsche Forschungsgemeinschaft)

**Overview:** In its first period (2005-2009) the SFB 652 comprises 13 research projects. The common goal of the research activities is to contribute to a deeper fundamental understanding of the role of strong correlations and collective phenomena for the interaction of radiation fields with material. By the joint experimental and theoretical investigation of corresponding signatures in a broad spectrum of systems including ultracold quantum condensates, exciton clusters in semiconductor quantum films, atomic clusters and nanoparticles, as well as warm dense matter, new frontiers in light-matter research are being explored. Along this line the center connects topical issues from various subjects, including physics of correlated Coulomb systems, semiconductor physics, quantum optics, and cluster physics in an interdisciplinary manner. State-of-the art light sources, such as stabilized optical cw-laser, ultraintense femtosecond lasers, as well as the DESY VUV free-electron laser (FLASH) are employed for the experimental investigations. In perspective, to attack new regimes regarding to the parameters of the radiation field, also the DESY X-ray free-electron

laser (X-FEL) as well as the BESSY free-electron laser will be used for the experimental investigations.



**Structure:** Thematically the projects are classified in two research complexes. Project complex A is devoted to the investigation of optical excitations of existent strongly correlated Coulomb systems while complex B addresses the generation of correlations by the radiation field itself. About 50 scientists collaborate on the above outlined topics, including several colleages from the University of Greifswald.

In the foreground of project complex A are the excitation and the analysis of dense Coulomb systems. Among those are cluster and particles, warm dense matter, dense electron-ion systems, and particle-hole systems in semiconductors. The theoretical investigations in projects A1, A2, A4, and A6 are grouped around three experimental topics. Those are: (i) the excitations of clusters and particles by radiation from freeelectron lasers (A1, A3), (ii) the controlled coupling of intense optical laser pulses to clusters and particles (A3, A5), and the phase of the light in optically excited semiconductor structures (A7). For the analysis of the systems as well as the exploration of new routes for future application of light-matter correlations cutting-edge control techniques, such as pulse optimization through genetic algorithms and pump-probe control schemes with phase-stabilized pulses are utilized. For the theoretical description modern approaches like quantum particle-in-cell methods (A1), quantum kinetic transport models (A6, A7), quantum molecular dynamics simulations (A2) as well as density-functional theory (A1) are applied.

Project complex B concentrates on the buildup of correlations in semiconductors, atom condensates, clusters, and nanoparticles. Semiconductors represent ideal targets for the study of many-particle effects in a wide density range because of the well-controlled elementary excitation of the excitons. A limiting factor is the finite lifetime of the excitons which, however, can be tuned over a wide range by the choice of the material or tuning an external confinement potential. Corresponding studies are a major issue within the projects B1-B4. Excitons in mesoscopic potential wells are investigates in project B1, being very promising candidates in this context. Essential for the realization and the control of the light-induced correlations is the development of theoretical concepts that provide a consistent connection of quantum optics with many-particle theory. This is subject of the projects B2 and B4. In project

B5 the formation of exciton-polariton quasiparticles through cooperative effects and the buildup of correlations at high pressures are investigated. Within project B6 the light-field induced formation of novel metal atom condensates in exotic and ultracold environments, such suprafluid helium droplets, is studied.

**Examples of research results:** Two published results from the current SFB period are given below. The first example illustrates the enhanced and correlated ion and electron emission through collective response effects in laser excited clusters as specimens for dense Coulomb systems, see Fig. 1. The second example on semiconductor systems shows the fingerprint of polariton modes in ZeSe - ZnS<sub>x</sub>Se<sub>1-x</sub> heterostructures which result in pronounced peaks in the intensity and the phase spectrum of the reflected light, see Fig. 2.

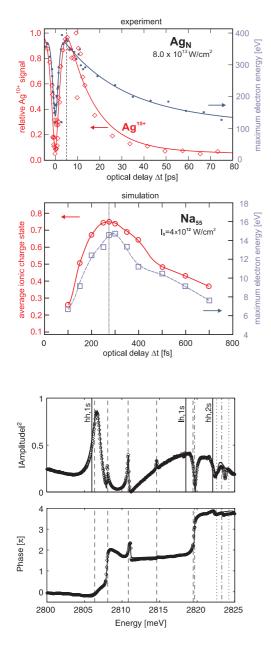


Fig. 1: Correlated emission of highly charged ions and energetic electrons from metallic clusters subject to intense dual femtosecond laser pulses. The optimal pulse delay reflects strongly enhanced laser-cluster coupling through resonant plasmon excitations. Experiment on silver clusters (upper panel); semiclassical Vlasov simulations on small sodium clusters as simplified model systems (lower panel); adopted from Döppner, Fennel, Radcliffe, Tiggesbäumker, and Meiwes-Broer, Phys. Rev. A **73**:031202R, 2006

Fig 2: Polariton interferences in the light reflected from  $ZeSe - ZnS_xSe_{1-x}$  heterostructures: square of the amplitude (upper part) and phase (lower part) of the reflection coefficient (experiment: circles, theory: solid line); adopted from Seemann, Kieseling, Stolz, Manzke, Henneberger, Hommel, Sol. State. Comm. **138**:457, 2006

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