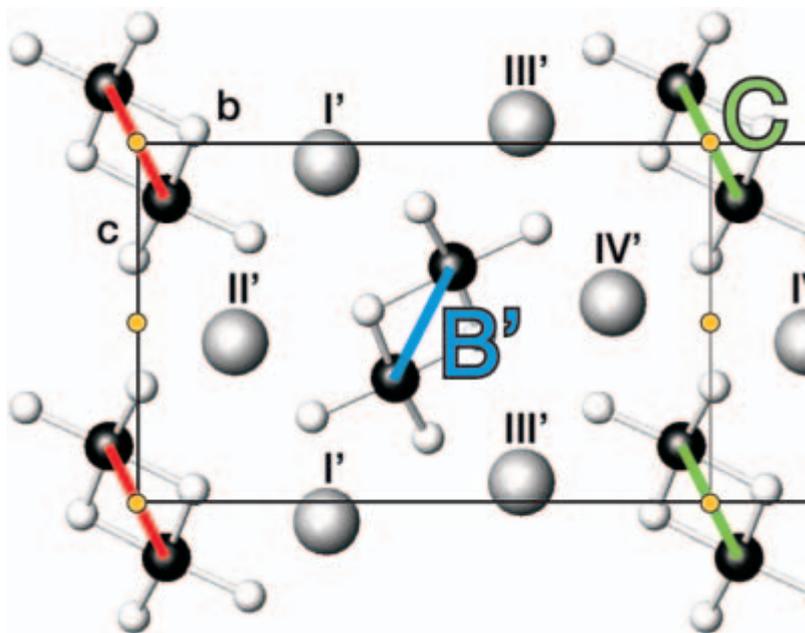
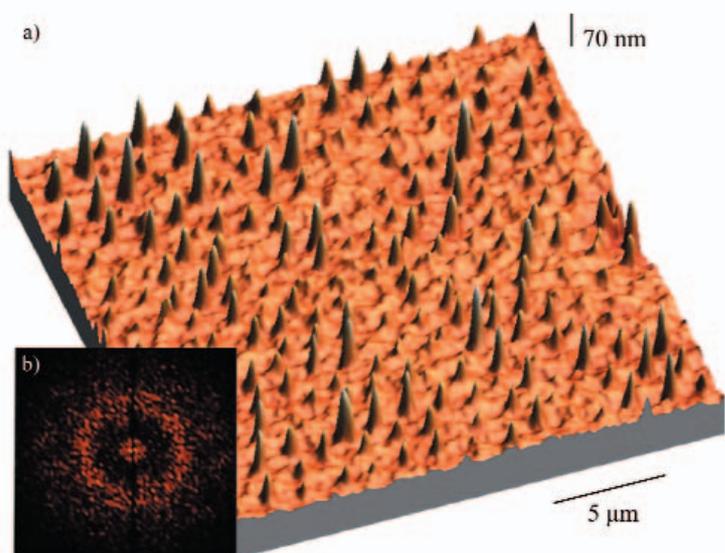
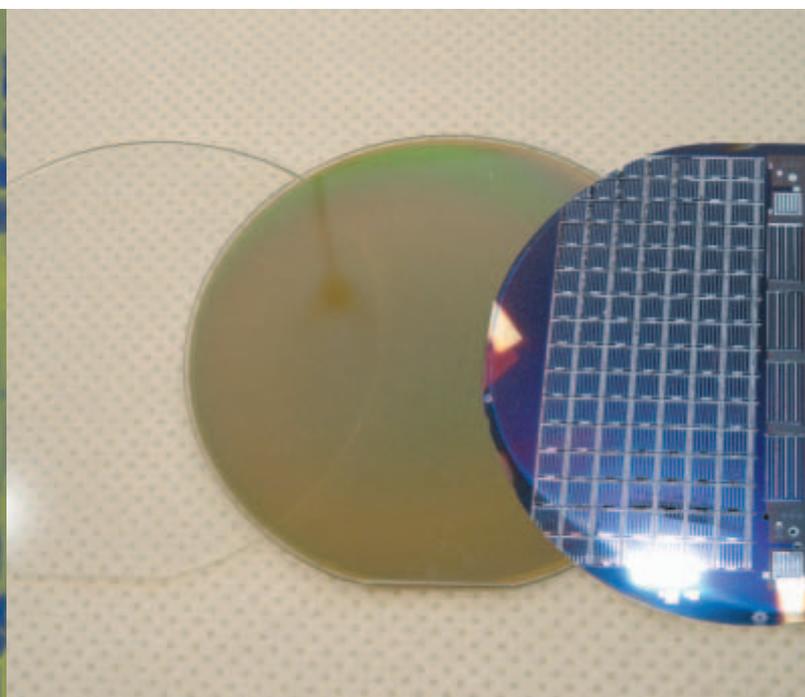
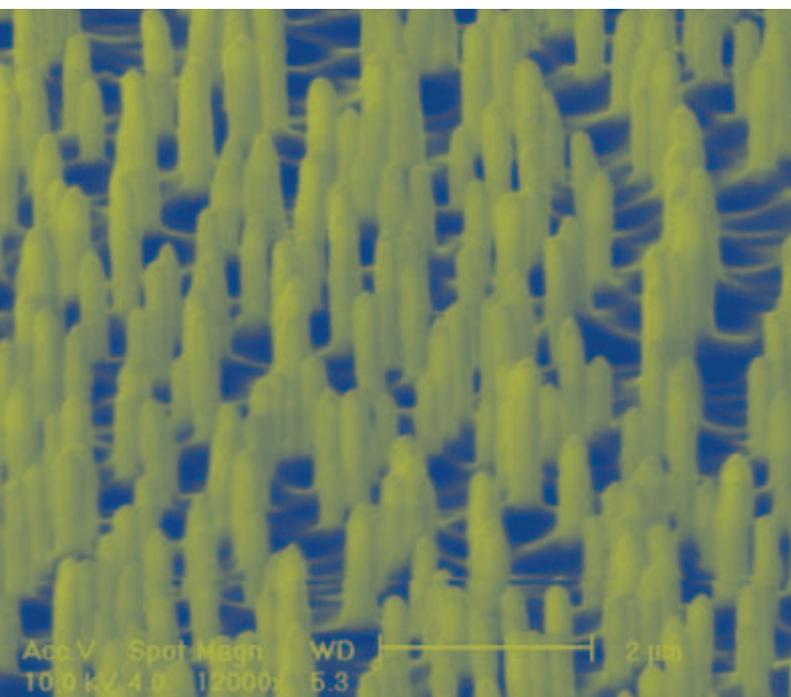


# Annual Report 2004 Selected Results



**Legend to Cover Figures:**

- top left:** *Nano-towers* produced by fast-ion irradiation in a thin NiO-layer deposited on a SiO<sub>2</sub> substrate. The *towers* have diameters of approx. 200 nm and heights of 1 μm. For details see p. 43.
- top right:** The three major steps to a poly-Si thin-film solar cell on glass (substrate – seed layer – epitaxy and cell processing)
- bottom left:** Surface morphology of laser crystallized poly-SiGe
- bottom right:** Low-temperature structure of NH<sub>4</sub>CuCl<sub>3</sub>.  
The interesting magnetic properties of this compound were investigated at HMI in 2004.

# Annual Report 2004

## Selected Results

Hahn-Meitner-Institut  
Berlin, 2005

# Table of contents

4	<b>Foreword</b>
6	<b>HMI in brief</b>
8	<b>News and Events 2004</b>
10	<b>People</b>
10	Two theorists leave HMI to take over professorships outside Berlin
10	Solar cells pioneer at SE3
11	New head of Department Magnetism
12	<b>New Neutron Guide Hall</b>
14	<b>Meetings and Workshops</b>
19	<b>Technology Transfer</b>
19	New application centre for industrial cooperation
20	Hahn-Meitner-Institut operates neutron scattering instrument in Munich
20	Contributing to the progress in proton therapy
21	Technology transfer prize goes to solar cell researchers
22	<b>Public Relations</b>
22	HMI's school lab inaugurated
23	HMI opens its doors to the public
24	Girls' Day 2004
24	Christoph Böhme receives Hahn-Meitner-Institut's Communicator Prize
25	<b>Instrumentation News</b>
25	First experiments at the 7 Tesla Wiggler beamlines
26	<b>User Service</b>
28	BENSC Operation
31	NAA Laboratory and Irradiation Service at BER II
32	ISL Operations and Developments
34	<b>Scientific highlights Structural Research 2004</b>
36	<b>BENSC User Service</b>
36	Magnetisation plateaus in the quantum magnet $\text{NH}_4\text{CuCl}_3$
38	Does antiferromagnetism survive in the superconducting phase of $\text{CeCu}_2\text{Si}_2$ ?
40	Tailoring surface coatings for protein immobilization
42	Structural explanation of the magnetoelectric phase transitions in $\text{HoMnO}_3$
44	<b>ISL User Service</b>
44	Nanoscale self-assembly of thin oxide films under swift heavy ion bombardment
46	10 years of materials analysis with heavy ions at ISL
48	<b>NAA User Service</b>
48	Investigation of heavy metal release during thermal waste treatment on a forward-acting grate using radiotracers irradiated at BER II
50	<b>SF1, Methods and Instruments</b>
50	Ordering upon melting dynamically enhanced
52	Search for scission neutrons using angular correlation method

54	■ SF2, Magnetism
54	■ Superconductivity? Just add water!
56	■ Competition of two AF structures in UNiAl single crystal
58	■ SF3, Materials
58	■ Metal foams
60	■ SF4, Structure and Dynamics
60	■ Magnetic anisotropy of Ni changed by extreme lattice expansion
62	■ Texture modification in nanocrystalline materials using swift heavy ions
64	■ Electronic energy-density effects in Auger angular distributions
66	■ SF5, Theoretical Physics
66	■ Melting of orientational order of colloidal molecular crystals on a triangular lattice
68	■ Force transduction in stiff polymers
70	■ SF6, Molecular Trace Element Research in the Life Sciences
70	■ Synchrotron light helps to elucidate the role of metalloproteins in health and disease
72	■ SF7, Nuclear Measurements
72	■ 25 years of the magnetic spectrometer Q3D
74	■ Chain states in $^{13}\text{C}$ and $^{14}\text{C}$ , nuclear polymers
76	■ Scientific highlights Solar Energy Research 2004
78	■ SE1, Silicon Photovoltaics
78	■ Laser-induced self-organization in Si-Ge alloys
80	■ Numerical simulation of thin-film heterojunction solar cells: open-source program AFORS-HET, version 1.2
82	■ Low-temperature Si epitaxy on polycrystalline Si seed layers on glass for thin-film Si solar cells
84	■ SE2, Heterogeneous Material Systems
84	■ Compositional and electronic characterisation of Zn(O,OH) by PES for a better understanding of interfaces in chalcopyrite solar cells
86	■ Time dependent charge separation in a nanoporous TiO <sub>2</sub> model system studied by surface photovoltage
88	■ Electrical activity at grain boundaries of Cu(Ga, In)Se <sub>2</sub> thin films
90	■ SE3, Technology
90	■ Production of CuInS <sub>2</sub> baseline modules on 5×5 cm <sup>2</sup> substrates with high yield
92	■ Thin film photovoltaics: diagnostics and repair
94	■ Prototype development – flexible high efficiency Cu(In,Ga)Se <sub>2</sub> thin film solar cells for space applications
96	■ SE4, Dynamics of Interfacial Reactions
96	■ Hot electrons at the interface of p-InP
98	■ Ultrafast electron dynamics measured with femtosecond two-photon photoemission
100	■ Improved structure and performance of the InP/GaAsSb interface in a resonance tunneling diode
102	■ SE5, Solar Energetics
102	■ Reactive magnetron sputtering of CuInS <sub>2</sub> : a new prospective deposition method for thin film solar cells?
104	■ Surface passivation of MoS <sub>2</sub> or WSe <sub>2</sub> for optimised photoconversion efficiencies
106	■ Polymer electrolyte membrane (PEM) fuel cells: new catalysts and bionic aspects
108	■ SE6, Electronic Structure of Semiconductor Interfaces
108	■ Spectromicroscopy: investigating the ALILE process
110	■ Band structure and effective masses for CuInS <sub>2</sub>
112	■ Organizational Chart
113	■ Imprint

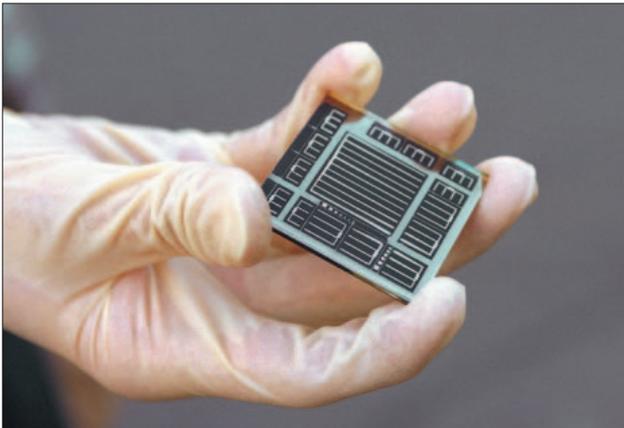
# Foreword

With the Annual Report 2004 of the Hahn-Meitner-Institut, we again can present only a selection of highlights out of a large number of results. Still, we hope to help the interested reader to get an idea of the breadth and high quality of the Institute's research. Intentionally, we present results achieved by both the scientists employed at the Hahn-Meitner-Institut and the users of our facilities. It is the intimate interplay of in-house and collaborative research, which is the backbone of the top-science produced in the Hahn-Meitner-Institut.



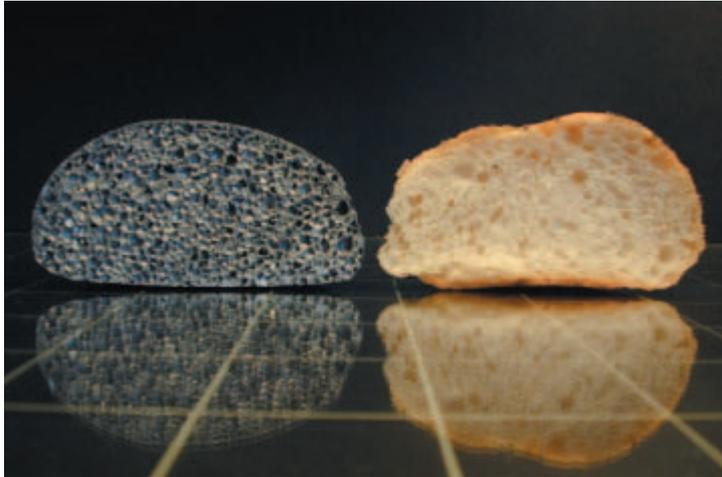
Photo: Sebastian Frenkel

For HMI and the entire Helmholtz Association, 2004 marked the completion of the new – *programme-oriented* – funding system. With *Structure of Matter* and *Key Technologies* the programmatic strategies of the remaining two out of six Helmholtz research fields were peer-reviewed. From 2005 on, the entire Helmholtz Association is funded according to the new scheme.



For Hahn-Meitner-Institut, the large-scale facilities and the major part of its division Structural Research were evaluated and the proposed programme for the period 2005–2009 got very good marks. This includes a strong support for our project N25T, to build a high- $T_c$ -superconductivity based magnet to provide a 25 Tesla sample environment for neutron scattering experiments.

Our delight was, however, seriously damped by the recommendation, due to lacking resources and despite its scientific success, to close the Ion Beam Laboratory ISL before 2008, and to concentrate the resources on the structural research with neutrons and synchrotron radiation. Meanwhile, the deciding bodies of Helmholtz and Hahn-Meitner-Institut confirmed the shut down of ISL by the end of 2006, and we started the difficult process to realize this decision for the benefit of the future potential of the institute.



We are happy that with Dr. Schock and Prof. Tennant we could welcome two new distinguished colleagues now heading the departments SE3 (*Technology*) and SF2 (*Magnetism*), respectively. The search for the new heads of departments SE1 and SF4 is well on the way.

On the other hand, we have to announce that Prof. Frey, head of the department SF5 (*Theoretical Physics*) left Hahn-Meitner-Institut to join the LMU Munich. We will do our best to assure a continuation of the activities he started at the Hahn-Meitner-Institut over the last years.

We hope that with this Annual Report 2004 we can communicate that thanks to the very high motivation of all the staff at Hahn-Meitner-Institut and the guests and collaborators from outside 2004 was a scientifically very successful year for HMI, too. This motivation is most gratefully appreciated.

Thanks go also to the funding authorities, the Federal Government, in particular the Federal Ministry of Education and Research (BMBF), the Senate of Berlin and all the third party funding agencies for their continuing support.

By no means diminishing the difficulties due to the shut down of ISL, we are confident that the scientific achievements together with our programmatic strategy and the competence of our staff are an excellent basis for the future of the Hahn-Meitner-Institut and its standing in the community.

Michael Steiner  
Scientific Director



## HMI in brief



The **Hahn-Meitner-Institut** (HMI) in Berlin is one of Germany's leading centres for research on solar energy conversion, condensed matter and materials science. It has approximately 800 employees, including almost 300 scientists – most of them physicists and chemists. Most of the institute's annual budget of roughly 70 Million € is provided by the German Federal Government and the City of Berlin in a ratio of 9 to 1.

The Hahn-Meitner-Institut is member of the **Helmholtz Association** of National Research Centres, an organisation representing fifteen of Germany's largest scientific institutions. The common mission of the Helmholtz centres is to develop, set-up and operate large-scale facilities, to solve complex – often multidisciplinary – scientific and technological problems in long-term proactive research programmes and to develop high technologies for the future. The Helmholtz Association concentrates its work in six research fields: *Energy, Earth and Environment, Health, Structure of Matter, Transport and Space* and *Key Technologies*. For each of these fields, scientists develop several research programmes for 5-year periods. These programmes are then evaluated by a group of international experts. This evaluation forms the basis for the programme-oriented funding, which distributes the financial resources to the scientific programmes of the Helmholtz research fields rather than to the institutes.



Scientific work at the Hahn-Meitner-Institut is organised in two divisions reflecting the two main fields of activity: Solar Energy Research and Structural Research. The Solar Energy Research is part of the programme *Renewable Energies* within the research field *Energy*. Most of the activities of the Structural Research Division are part of the programme *Large-Scale Facilities for Research with Photons, Neutrons and Ions* in the research field *Structure of Matter*. The eye tumour therapy and the research on trace elements are conducted in the Helmholtz programmes *Cancer* and *Environmental Health* within the research field *Health*.

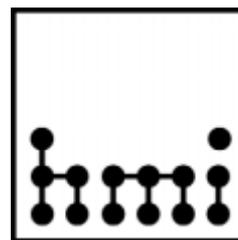
**Solar energy research** at the Hahn-Meitner-Institut is the largest effort in the field of sustainable energy within the Helmholtz Association and comprises approximately 25% of HMI's research and development efforts. As an interdisciplinary activity between solid state physics, material chemistry, optics and interfacial chemistry, it aims at creating scientific and technological preconditions for significantly increasing the contribution of sustainable energy to our energy supply over the next decades. This activity is taking advantage of an already well balanced research infrastructure and increasingly uses the unique measurement opportunities provided by the large scale facilities operated at the Hahn-Meitner-Institut.

At the centre of the solar energy research at HMI are materials and concepts for thin-film solar cells – activities covering the entire spectrum from basic research to the design of actual devices. The focus is on the currently most promising technologies, namely thin-film polycrystalline silicon and compound semiconductors of the I-III-VI<sub>2</sub> and III-V type. Research projects aim at the development of efficient photovoltaic solar cells which allow substantial reductions in the costs of solar power generation. The strategy is to develop existing thin-film technologies to a state of maturity and, in parallel, to explore new materials and concepts for solar cells of the future, e. g. nano-composite crystalline materials.



At the national level, the solar energy research programmes of the Hahn-Meitner-Institut, other Helmholtz centres, universities and other institutions are coordinated within the Solar Energy Research Association (ForschungsVerbund Sonnenenergie – FVS). In addition, the FVS represents the institutions jointly in the scientific, industrial and political communities and acts as a platform for numerous networking activities.

**Structural research** at the Hahn-Meitner-Institut is focused on experimental investigations of structures and materials using neutrons and fast ions as probes. These two probes are provided by two in-house large-scale facilities sited on the institute's grounds in Berlin-Wannsee: The 10MW research reactor BER II with the Berlin Neutron Scattering Center BENSC and the accelerator complex of the Ion Beam Laboratory ISL. In addition to that, the Hahn-Meitner-Institut makes use of a third complementary probe – synchrotron radiation – by operating instruments at the 3<sup>rd</sup> generation electron storage ring BESSY, an independent research institution in Berlin-Adlershof.



All facilities are primarily operated for a national and international user community. About 70 % of the beam time at the instruments is used by scientists from other research institutes, universities and industry from Germany and from abroad. It is HMI's policy to provide these users with full scale technical and scientific support, this way enabling them to make best possible use of the facilities. An outstanding highlight among the HMI activities are neutron scattering studies of samples in extreme sample environments such as very high magnetic fields and extremely low temperatures made possible by the institute's unique expertise on sample environment equipment.

At ISL, roughly a quarter of the beam time is used for the therapy of tumours in the human eye using 70MeV protons. The costs of the therapy are covered by the national health insurance companies.

Fields in the focus of in-house structural research are magnetic phenomena, properties and design of engineering components and materials, soft matter and biological systems as well as theoretical physics.



Photo: Sebastian Frenkel