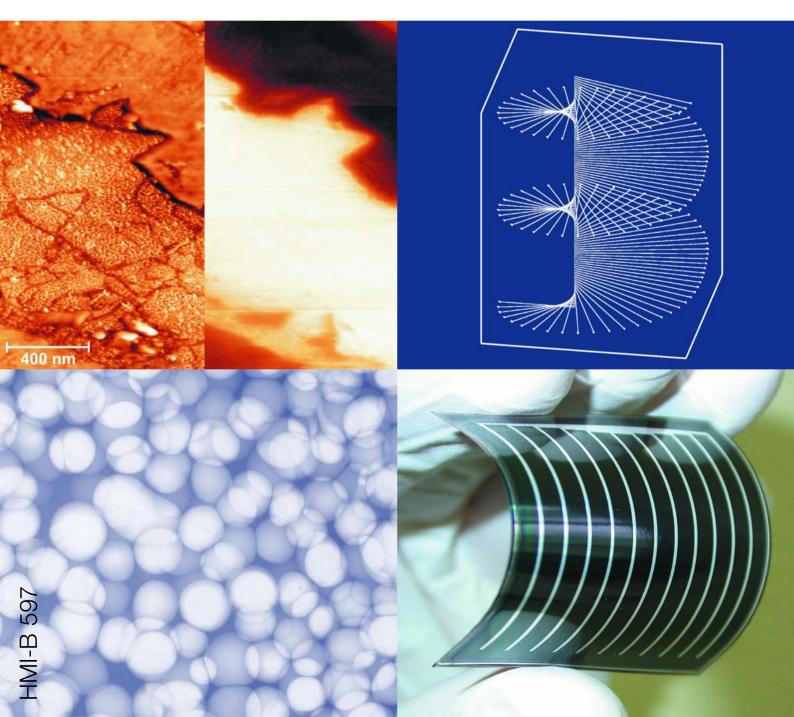
HIII

# Annual Report 2003 Selected Results



Legend to Cover Figures:

top left: Image of a CuGaSe<sub>2</sub> solar cell cross section (1000 x 2000 nm<sup>2</sup>): topography (left); workfunction (right). top right: Magnetic spiral in CsCuCl<sub>3</sub> at 7 T. bottom left: An x-ray radiograph of a 10 mm slice of aluminium foam. bottom right: Flexible solar cell based on Cu(In,Ga)Se<sub>2</sub> (area 16 cm<sup>2</sup>) on titanium foil.

# Annual Report 2003 Selected Results

Hahn-Meitner-Institut Berlin, 2004

## Table of contents

S. 4 HMI in brief S. 5 Foreword S. 6 News and Events 2003 HMI-theorist Martin Falcke receives the 2003 Erwin Schrödinger Prize S. 8 New Neutron-Guide Hall at HMI S. 9 HMI start-up: Sulfurcell wants to manufacture large area solar modules S. 10 ■ 5 Years of Experience in Proton Therapy for Ocular Tumours in Germany S. 11 Trace element research: Towards New Frontiers and Good-bye to an Old Campaigner S. 12 S. 14 Outstanding, rapidly done with open mind S. 14 First light from the 7-Tesla Wiggler S. 15 Materials department inaugurates new metal foam lab at TU-Berlin S. 16 HMI hosts Workshop on Orbital Physics and Novel Phenomena in Transition Metal Oxides S. 17 Development of a new Kelvin-Electronic for Omicron GmbH S. 17 Quantum Well structures measured by UHV-Kelvin Probe Force Microscopy in cooperation with KTH - Stockholm S. 18 User Service S. 20 BENSC Operation S. 23 NAA-Laboratory and Irradiation Service at BER II S. 24 ■ ISL Operations and Developments S. 26 Scientific highlights Structural Research 2003 S. 28 BENSC User Service S. 28 Antiferromagnetic order as a competing ground state for electron-doped high-transition temperature superconductors S. 31 Neutron diffraction and theoretical model studies of the field induced magnetic phases of the ErNi<sub>2</sub>B<sub>2</sub>C superconductor Boundary Lavers of Water at Polymer-Liquid Interfaces S. 34 S. 36 Neutron Autoradiography of the painting Armida abducts the sleeping Rinaldo (~1637) by Nicolas Poussin S. 38 ■ ISL User Service Plastic deformation of amorphous silicon under swift heavy ion irradiation S. 38 S. 40 Surface modification by irradiation with swift heavy ions S. 42 Tendaguru Sauropod Dinosaurs – Characterization of Diagenetic Alterations in Fossil Bone S. 44 NAA User Service S. 44 Fluid and particle retention in the hippos Kathi and Josef of the Berlin Zoo investigated by Neutron Activation Analysis S. 46 SF1, Methods and Instruments S. 46 EXED – an instrument in progress S. 48 Relaxation in a glassy magnet S. 50 Pre-equilibrium emission in 1.2 GeV proton-induced spallation reactions S. 52 SF2, Magnetism S. 52 Surface and interface magnetization of ultrathin films S. 54 Field distorted magnetic spirals: a neutron diffraction study of the magnetism in the frustrated quantum antiferromagnet CsCuCl<sub>3</sub>

S. 56 S. 56 S. 58 S. 60	<ul> <li>SF3, Materials</li> <li>Neutron tomography at HMI</li> <li>Characterisation of Precipitates in a Stainless Maraging Steel by Three-Dimensional Atom Probe and Transmission Electron Microscopy</li> <li>Pseudo-crystalline ordering of nanoparticles in ferrofluids induced by magnetic fields.</li> </ul>
S. 62 S. 62 S. 64 S. 66	<ul> <li>SF4, Structure and Dynamics</li> <li>Modification of the Ti Texture using swift heavy ions</li> <li>Nonthermal Melting of BeO Films Induced by Swift Heavy Ions</li> <li>TEMPOS – A universal ion track-based electronic building block</li> </ul>
S. 68 S. 68	<ul> <li>SF4, Cooparation SF3 and SF4</li> <li>Decomposition behaviour of as-received and oxidized TiH<sub>2</sub> powder</li> </ul>
S. 70 S. 70 S. 72	<ul> <li>SF5, Theoretical Physics</li> <li>Gelation in suspensions of "sticky" particles</li> <li>"W dip" in light-scattering of supercooled liquids experimentally confirmed</li> </ul>
S. 74 S. 74	<ul> <li>SF6, Molecular Trace Element Research in the Life Sciences</li> <li>Trace elements in the protection of the respiratory tract</li> </ul>
S. 76	Scientific highlights Solar Energy Research 2003
S. 78 S. 78 S. 80 S. 82 S. 84	<ul> <li>SE1, Silicon Photovoltaics</li> <li>Interface properties of a-Si:H/c-Si hetero-structures</li> <li>The nature of dangling bond recombination in silicon</li> <li>Hydrogen in ZnO</li> <li>Electronic functionalisation of Si surfaces by thin organic layers</li> </ul>
S. 86 S. 86 S. 88 S. 90 S. 92 S. 94 S. 96 S. 98 S. 99 S. 100 S. 102	<ul> <li>SE2, Heterogeneous Material Systems</li> <li>Do we really need another photoluminescence study on CuInSe<sub>2</sub>?</li> <li>A novel approach to chalcopyrite-based heterojunctions</li> <li>Novel approaches to the "lift-off" technology</li> <li>Understanding of the ILGAR-WEL/CIGSSe interface</li> <li>Over 11 % efficient ZnS/CIGSSe thin film solar cells without undoped ZnO</li> <li>Coherent manipulation of well-defined electron spins in solid state</li> <li>CuAIO<sub>2</sub> prepared from LiAIO<sub>2</sub> by ion exchange reaction</li> <li>Vertical nanowire field effect transistor in flexible template</li> <li>Synchrotron-based characterization of industrially relevant chalcopyrite solar device structures</li> <li>Solar cell cross section studied by Kelvin Probe Force Microscopy in ultrahigh vacuum</li> </ul>
S. 104 S. 104 S. 106 S. 108	<ul> <li>SE3, Technology</li> <li>Chalcopyrite solar cells on flexible substrates</li> <li>About the mechanism of CuInS<sub>2</sub> film formation</li> <li>Local diode parameters determined by infrared thermography</li> </ul>
S. 109 S. 109 S. 110 S. 112	<ul> <li>SE4, Dynamics of Interfacial Reactions</li> <li>Experimental proof for MOCVD-specific surface reconstruction of InP(100)</li> <li>Energy distribution of hot electrons in a semiconductor exposed to sunlight</li> <li>Solar cells with small band gaps built from III-V materials</li> </ul>
S. 114 S. 114	<ul> <li>SE5, Solar Energetics</li> <li>Chemical Surface Modification of Molybdenum, Tungsten-Dichalcogenides for Optimal</li> </ul>
S. 116 S. 118	<ul> <li>Photoeffects</li> <li>Noble metal free catalysts for the electroreduction of oxygen</li> <li>Characterization and improvement of semiconductors and semiconductor junctions for solar</li> </ul>
S. 119 S. 120	<ul> <li>energy conversion.</li> <li>On the Problem of (photo)-Degradation of Solid-State Nano-Composite Solar Cells</li> <li>Successful Electrochemical Removal of Cu-S phases from CuInS<sub>2</sub> (CIS) Films</li> </ul>
S. 122	Organisational chart
S. 123	Imprint

#### IHMI in brief

The Hahn-Meitner Institute (HMI) in Berlin is one of Germany's leading centres for research on solar-energy conversion, condensed matter and materials science. It has approximately 750 employees, including almost 400 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. HMI is member of the Helmholtz Association of National Research Centres, an organization comprising fifteen of Germany's largest scientific institutions.

Scientific work at HMI is organized in two divisions reflecting the two main fields of scientific activity: Solar-Energy Research and Structural Research.

Solar-energy research at the HMI 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, materials science, 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 the unique measurement opportunities provided by the large-scale facilities operated at HMI.

At the centre of the solar-energy research at HMI are materials and concepts for thin-film solar cells – activities covering the entire spec-



trum from basic research to the design of actual devices. The focus is on the currently most promising new 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 allowing for substantial cost reductions 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.

Structural Research at HMI groups around three large scale facilities providing three complementary probes to investigate structures and materials – neutrons, fast ions and synchrotron radiation. The three facilities are the 10 MW research reactor BER II with the Berlin Neutron Scattering Center BENSC, the accelerator complex of the Ion Beam Laboratory ISL and the 3rd generation electron synchrotron BESSY. BER II and ISL are run by HMI on the institute's grounds in Berlin Wannsee. At BESSY, an independent research institution in Berlin Adlershof, HMI operates several experimental stations designed for the particular requirements of structural research.

All facilities are in the first place operated for a national and international user community. About 70 % of the beam time at the instruments is provided to scientists from other research institutes, universities and industry from Germany and from abroad. It is the HMI policy to provide these users, if necessary, with full scale technical and scientific support, this way enabling them to make best possible use of the facilities.

Fields in the focus of Structural Research at HMI are magnetic phenomena, properties and design of engineering components and materials, soft matter and biological systems. Roughly a quarter of the beam time at ISL is used for the therapy of tumours in the eye using 70 MeV protons.

A particular highlight among the HMI activities are neutron scattering studies of samples in extremely high magnetic fields and/or very low temperatures made possible by the institute's unique expertise on sample environment equipment.

# Foreword

We are proud to present to you the Annual Report 2003 of the Hahn-Meitner Institute in its new format: we have selected highlights out of a large number of results in order to show the breadth and high quality of the Institute's research. This report presents results achieved by both the scientists employed at HMI and the users of our facilities. It is this combination of in-house and collaborative research, which is the backbone of the top-science produced in the Hahn-Meitner Institute.

For HMI, 2003 marked a further step on the road towards the new – *programme-oriented* – funding system of the Helmholtz Association. For our activities in the research field *Health*, it was the first year under the new funding. The Solar-Energy Division very successfully passed the evaluation of its proposed programmatic strategy for the coming five-year period. The Structural Research Division around our large-scale facilities had to prepare for its evaluation scheduled for April 2004.

We do sincerely hope that after the evaluation of the Structural Research years without evaluations of this kind will follow. It is essential that in the coming years doing science will again become the top priority of our work. Thanks to the very high motivation of all the staff at HMI and the guests and collaborators from outside 2003 was a very successful year, despite all the additional work load caused by the evaluations. This motivation is most gratefully appreciated.

2003 has seen the beginning of activities, which will secure the top position of HMI's research and the research opportunities for guests: reappointments have been prepared in the Solar-Energy Division – they should bear fruit in 2004; in the Structural-Research Division, the foundation was laid for the construction of a second neutron-guide hall – the prerequisite for the installation of two new neutron-scattering instruments, which will further strengthen the profile of our BENSC operation.

We are sure that the scientific results of 2003 and the strategic planning prepared for the evaluation constitute an excellent basis for further strengthening HMI's scientific programme and its standing in the community.

Thanks are not only due to the HMI staff for their excellent work, but 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.

Michael Steiner Scientific Director

