Preface

The chapters of this volume are based on invited reviews presented at the 257th WE-Heraeus-Seminar, which was devoted to the topic “Particle Scattering, X-Ray Diffraction, and Microstructure of Solids and Liquids.” The meeting was organized to foster communication between scientists in nominally different but actually closely related fields of modern basic and applied research. It brought together theorists and experimentalists from diverse subfields of condensed matter physics, physics of quantum solids, crystallography and materials science, physical chemistry, and computational physics. The workshop focused on recent progress in theoretical and experimental investigations and studies of the microstructure of solids and classical and quantum crystals and liquids. Such studies allow essential insights into the dynamics and properties of these states of matter.

The most fundamental physical quantities for qualitatively and quantitatively describing the spatial microstructure are the one-body and two-body densities or, more generally, the reduced density-matrix elements of the constituents. Associated with these quantities are the structure factors, the structure functions, and the momentum distributions. These are accessible, at least in principle, by experimental measurements. Elastic and inelastic scattering of neutrons, atoms, etc., and X-ray diffraction experiments are widely employed physical processes that yield detailed information on the one-body and two-body density-matrix elements. Theoretical and experimental results reflect directly the point-group and space-group symmetries of the various systems as well as the breaking of symmetries at phase transitions, the loss of symmetry elements in disordered crystals or quasicrystals and the static and dynamic correlations between and among the constituent particles which are induced by their mutual interactions. Present-day theoretical methods, such as Monte-Carlo techniques, molecular-dynamics simulations, and semi-analytical integral equations theories offer adequate tools to analyze such effects and thus open the way to a deeper understanding of the behavior of matter and a systematic design of novel materials.
The presentations ranged over a spectrum of fields:
- Physics of quantum solids
- Theory of perfect crystals
- Computational physics
- Physics of liquid crystals
- Materials science
- Physical chemistry

The seminar provided a forum in which about forty invited participants could evaluate the current status and development of the various branches of the application of scattering and diffraction. The setting of the meeting in the Physikzentrum Bad Honnef created a pleasant and productive atmosphere for fruitful discussions and exchange of experience and ideas. During the three days of the seminar twenty talks were presented by internationally recognized experts in their fields, coming from Europe and the United States. Six of the papers – extended to present more self-contained reviews – appear in this volume. The workshop included an evening talk on “Nikolaus von Cues and the Idea of Modern Natural Science,” that offered a glimpse on the thinking of an extraordinary personality of more than half a millenium ago.

The meeting was made possible by the generosity of the WE-Heraeus-Stiftung. We express our sincere gratitude to Dr. Ernst Dreisigacker and Mrs. Jutta Lang from the WE-Heraeus-Stiftung for their excellent efforts in the general organization of the seminar. We also wish to extend our thanks to the staff of the Physikzentrum and to all speakers and participants for their contributions to a pleasant and fruitful workshop.

We wish to dedicate this volume to honor our colleague Wolfram Prandl, who participated and lectured on “Diffraction, Spectroscopy, and Thermodynamics” two months before his untimely death.

Koeln and Manchester, 
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Manfred L. Ristig
Klaus A. Gernoth
List of Contributors

Dr. Khaled AbuQuasem
Universität zu Köln,
Institut für Theoretische Physik,
50937 Köln, Germany
kq@thp.uni-koeln.de

Prof. Michael P. Allen
University of Bristol,
H. H. Wills Physics Laboratory,
Royal Fort, Tyndall Avenue,
Bristol BS8 1TL, UK
m.p.allen@bristol.ac.uk

Aranzazu Maira-Vidal
C.S.I.C. / Instituto de Estructura de la Materia,
Dept. de Física Nuclear y Estadística,
c/Serrano 123,
28006 Madrid, Spain
amaira@foton0.iem.csic.es

Prof. Dr. Ladislav Bohatý
Universität zu Köln,
Institut für Kristallographie,
50674 Köln, Germany
ladislav.bohaty@uni-koeln.de

Prof. Dr. Hans Boysen
Ludwig-Maximilians-Universität München,
Institut für Kristallographie,
Am Coulombwall 1,
85748 Garching, Germany
boysen@lrz.uni-muenchen.de

Prof. Dr. Eberhard Burkel
Universität Rostock,
Fachbereich Physik, Neue Materialien,
August-Bebel-Str. 55,
18051 Rostock, Germany
burkel@physik1.uni-rostock.de

Prof. John W. Clark
Washington University,
Department of Physics,
St. Louis, MO 63130, USA
jwc@wuphys.wustl.edu

Prof. Dr. Siegfried Dietrich
Max-Planck-Institut für Metallforschung,
Heisenbergstr. 1,
70569 Stuttgart, Germany
dietrich@mf.mpg.de

Dr. Ernst Dreisigacker
Wilhelm- und Else-Heraeus-Stiftung,
Postfach 1553,
63405 Hanau, Germany
dreisigacker@we-heraeus-stiftung.de

Dipl.-Phys. Joachim Dzubiella
Universität Düsseldorf,
Institut für Theoretische Physik II,
Universitätsstr. 1,
40225 Düsseldorf, Germany
joachim@thphy.uni-duesseldorf.de
Prof. Dr. Götz Eckold
Universität Göttingen,
Institut für Physikalische Chemie,
Tammanstr. 6,
37077 Göttingen, Germany
geckold@gwdg.de

Dipl.-Phys. Kalid Elisbihani
Universität Göttingen,
Institut für Physikalische Chemie,
Tammanstr. 6,
37077 Göttingen, Germany
kelisi@gwdg.de

Dr. Damian J. J. Farnell
Ludwig-Maximilians-Universität München,
Institut für Theoretische Physik,
Theresienstr. 37/399,
80333 München, Germany
farnell@theorie.physik.uni-muenchen.de

Dr. Ricardo Fernandez-Perea
C.S.I.C. / Instituto de Estructura de la Materia,
Dept. de Fisica Nuclear y Estadistica,
c/Serrano 123,
28006 Madrid, Spain
ricardo@langran.iem.csic.es

Prof. Paolo Fornasini
Università di Trento,
Dipartimento di Fisica,
Via Sommarive 14,
38050 Povo (Trento), Italy
fornasini@science.unitn.it

Prof. Dr. Friedrich Frey
Ludwig-Maximilians-Universität München,
Institut für Kristallographie,
Theresienstr. 41,
80333 München, Germany
frey@yoda.kri.physik.uni-muenchen.de

Prof. Dr. Werner Freyland
Universität Karlsruhe,
Institut für Physikalische Chemie,
Kaiserstr. 12,
76131 Karlsruhe, Germany
Werner.Freyland@chemie.uni-karlsruhe.de

Prof. Dr. Jürgen Frisch
Universität Regensburg,
Institut für Theoretische Physik,
Universitätsstr. 31,
93040 Regensburg, Germany
juergen.fritsch@physik.uni-regensburg.de

Dr. Klaus A. Gernoth
UMIST, Department of Physics,
P.O. Box 88,
Manchester M60 1QD, UK
k.a.gernoth@umist.ac.uk

Dipl.-Phys. Holger M. Harreis
Universität Düsseldorf,
Institut für Theoretische Physik II,
Universitätsstr. 1,
40225 Düsseldorf, Germany
harreis@thphy.uni-duesseldorf.de

Dr. Sven E. Krüger
Universität Magdeburg,
Institut für Theoretische Physik,
Postfach 4120,
39016 Magdeburg, Germany
sven.krueger@physik.uni-magdeburg.de

Priv.-Doz. Dr. Karl Kürten
Universität Wien,
Institut für Experimentalphysik,
Boltzmanngasse 5,
1090 Wien, Austria
kuerten@ap.univie.ac.at

Priv.-Doz. Dr. Christos N. Likos
Universität Düsseldorf,
Institut für Theoretische Physik II,
Universitätsstr. 1,
40225 Düsseldorf, Germany
likos@thphy.uni-duesseldorf.de
Prof. Stephen W. Lovesey  
Rutherford Appleton Laboratory, 
ISIS Facility, Chilton, 
Oxfordshire OX11 OQX, UK  
s.w.lovesey@rl.ac.uk

Dr. Martin Müser  
Universität Mainz, 
Institut für Theoretische Physik, 
Staudinger Weg 7, 
55099 Mainz, Germany  
martin.mueser@uni-mainz.de

Dr. Francesco Pederiva  
Università di Trento, 
Dipartimento di Fisica, 
Via Sommarive 14, 
38050 Povo (Trento), Italy  
pederiva@science.unitn.it

Priv.-Doz. Dr. Wolf-Christian Pilgrim  
Universität Marburg, 
Institut für Physikalische Chemie, 
Hans-Meerwein-Strasse, 
35032 Marburg, Germany  
pilgrim@mailer.uni-marburg.de

Prof. Dr. Wolfram Prandl †  
Universität Tübingen, 
Institut für Kristallographie, 
Auf der Morgenstelle 10, 
72076 Tübingen, Germany  
wolfram.prandl@uni-tuebingen.de

Prof. Dr. Johannes Richter  
Universität Magdeburg, 
Institut für Theoretische Physik, 
Postfach 4120, 
39016 Magdeburg, Germany  
johannes.richter@physik.uni-magdeburg.de

Prof. Dr. Manfred L. Ristig  
Universität zu Köln, 
Institut für Theoretische Physik, 
50937 Köln, Germany  
ristig@thp.uni-koeln.de

Prof. Dr. Gert Röpke  
Universität Rostock, 
Fachbereich Physik, 
Universitätsplatz 1, 
18051 Rostock, Germany  
roepke@darss.mpg.uni-rostock.de

Prof. Dr. Hans-Eckhardt Schäfer  
Universität Stuttgart, 
Institut für Theoretische und Angewandte Physik, 
Pfaffenwaldring 57, 
70569 Stuttgart, Germany  
schaefer@itap.physik.uni-stuttgart.de

Dr. Petra Schiebel  
Universität Tübingen, 
Institut für Kristallographie, 
Auf der Morgenstelle 10, 
72076 Tübingen, Germany  
petra.schiebel@uni-tuebingen.de

Dipl.-Phys. Karin Schmalzl  
Universität Regensburg, 
Institut für Theoretische Physik, 
Universitätsstr. 31, 
93040 Regensburg, Germany  
karin.schmalzl@physik.uni-regensburg.de

Prof. Dr. Winfried Schüulke  
Universität Dortmund, 
Experimentelle Physik I, 
Otto-Hahn-Strasse, 
44221 Dortmund, Germany  
schuelke@physik.uni-dortmund.de

Dr. Hans G. Senger  
Universität zu Köln, 
Thomas-Institut, 
Universitätsstr. 22, 
50932 Köln, Germany  
CuSeng@uni-koeln.de
XII  List of Contributors

Prof. Ralph O. Simmons
University of Illinois,
Physics Department,
1110 West Green Street,
Urbana, IL 61801, USA
ros@uiuc.edu

Prof. Dr. Dieter Strauch
Universität Regensburg,
Institut für Theoretische Physik,
Universitätsstr. 31,
93040 Regensburg, Germany
dieter.strauch@physik.uni-regensburg.de

Dr. Yoshikazu Tanaka
RIKEN, Institute for Physical and
Chemical Research,
1-1-1, Kouto, Mikazuki, Sayo, Hyogo,
629-5158, Japan
ytanaka@postman.riken.go.jp

Dr. David N. Timms
University of Portsmouth,
Physics Department,
St. Michael’s Building,
Portsmouth PO1 2DT, UK
david.timms@port.ac.uk

Prof. Dr. Hans-Jürgen Weber
Universität Dortmund,
Institut für Physik,
Otto-Hahn-Str. 4,
44227 Dortmund, Germany
weberhj@fkp.physik.uni-dortmund.de

Prof. Dr. Roland Winter
Universität Dortmund,
Lehrstuhl für Physikalische Chemie,
Otto-Hahn-Str. 6,
44227 Dortmund, Germany
winter@steak.chemie.uni-dortmund.de

Prof. Dr. Helmuth Zimmermann
Universität Erlangen-Nürnberg,
Institut für Angewandte Physik,
Bismarckstr. 10,
91054 Erlangen, Germany
helmuth.zimmermann@krist.uni-erlangen.de
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