Lecture Notes in Physics

Springer
Berlin
Heidelberg
New York
Barcelona
Hong Kong
London
Milan
Paris
Singapore
Tokyo

Physics and Astronomy ONLINE LIBRARY
http://www.springer.de/phys/

Editorial Policy

The series *Lecture Notes in Physics* (LNP), founded in 1969, reports new developments in physics research and teaching -- quickly, informally but with a high quality. Manuscripts to be considered for publication are topical volumes consisting of a limited number of contributions, carefully edited and closely related to each other. Each contribution should contain at least partly original and previously unpublished material, be written in a clear, pedagogical style and aimed at a broader readership, especially graduate students and nonspecialist researchers wishing to familiarize themselves with the topic concerned. For this reason, traditional proceedings cannot be considered for this series though volumes to appear in this series are often based on material presented at conferences, workshops and schools (in exceptional cases the original papers and/or those not included in the printed book may be added on an accompanying CD ROM, together with the abstracts of posters and other material suitable for publication, e.g. large tables, colour pictures, program codes, etc.).

Acceptance

A project can only be accepted tentatively for publication, by both the editorial board and the publisher, following thorough examination of the material submitted. The book proposal sent to the publisher should consist at least of a preliminary table of contents outlining the structure of the book together with abstracts of all contributions to be included.
Final acceptance is issued by the series editor in charge, in consultation with the publisher, only after receiving the complete manuscript. Final acceptance, possibly requiring minor corrections, usually follows the tentative acceptance unless the final manuscript differs significantly from expectations (project outline). In particular, the series editors are entitled to reject individual contributions if they do not meet the high quality standards of this series. The final manuscript must be camera-ready, and should include both an informative introduction and a sufficiently detailed subject index.

Contractual Aspects

Publication in LNP is free of charge. There is no formal contract, no royalties are paid, and no bulk orders are required, although special discounts are offered in this case. The volume editors receive jointly 30 free copies for their personal use and are entitled, as are the contributing authors, to purchase Springer books at a reduced rate. The publisher secures the copyright for each volume. As a rule, no reprints of individual contributions can be supplied.

Manuscript Submission

The manuscript in its final and approved version must be submitted in camera-ready form. The corresponding electronic source files are also required for the production process, in particular the online version. Technical assistance in compiling the final manuscript can be provided by the publisher's production editor(s), especially with regard to the publisher's own Latex macro package which has been specially designed for this series.

Online Version/ LNP Homepage

LNP homepage (list of available titles, aims and scope, editorial contacts etc.):
http://www.springer.de/phys/books/lnpp/

LNP online (abstracts, full-texts, subscriptions etc.):
http://link.springer.de/series/lnpp/

M. Ristig K. Gernoth (Eds.)

Particle Scattering, X-Ray Diffraction, and Microstructure of Solids and Liquids

Springer

Editors

Manfred L. Ristig
Universität zu Köln
Institut für Theoretische Physik
Zülpicher Strasse 77
50937 Köln, Germany

Klaus A. Gernoth
UMIST
Department of Physics
P. O. Box 88
Manchester M60 1QD, United Kingdom

Cover Picture: (see contribution by Götz Eckold in this volume)

Library of Congress Cataloging-in-Publication Data.
Particle scattering, X-ray diffraction, and microstructure of solids and liquids / M. Ristig, K. Gernoth (eds.).
p. cm. -- (Lecture notes in physics, ISSN 0075-8450 ; 610)
Includes bibliographical references.
ISBN 354044386X (acid-free paper)
1. Scattering (Physics) 2. X-rays--Diffraction. 3. Microstructure. I. Ristig, M. L. (Manfred L.) II. Gernoth, Klaus A. II Series.

QC794.6.S3 P37 2002
530.4'11--dc21
2002036559
ISSN 0075-8450
ISBN 3-540-44386-X Springer-Verlag Berlin Heidelberg New York

Springer-Verlag Berlin Heidelberg New York
a member of BertelsmannSpringer Science+Business Media GmbH

http://www.springer.de

Printed in Germany

Typesetting: Camera-ready by the authors/editor
Camera-data conversion by Steingraeber Satztechnik GmbH Heidelberg
Cover design: *design & production*, Heidelberg

Printed on acid-free paper
54/3141/du - 5 4 3 2 1 0

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 fourty 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,
July 2002

Manfred L. Ristig
Klaus A. Gernoth

List of Contributors

Prof. Michael P. Allen
University of Bristol,
H. H. Wills Physics Laboratory,
Royal Fort, Tyndall Avenue,
Bristol BCS8 1TL, UK
m.p.allen@bristol.ac.uk

Prof. Dr. Götz Eckold
Universität Göttingen,
Institut für Physikalische Chemie,
Tammanstr. 6,
37077 Göttingen, Germany
geckold@gwdg.de

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

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

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

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

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

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 BCS8 1TL, UK
m.p.allen@bristol.ac.uk

Aranzazu Maira-Vidal
C.S.I.C. / Instituto de Estructura de la Materia,
Dept. de Fisica Nuclear y Estadistica,
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-hereaus-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
kelisbi@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
fornasin@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 Fritsch
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 Schülke
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

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

Contents

Scattering from Condensed Matter: A Brief Introduction
Klaus A. Gernoth and Manfred L. Ristig 1

Scattering Studies of Condensed Helium Isotopes
Ralph O. Simmons 7

The One- and Two-Body Densities of Crystalline Matter and Bragg and Diffuse Scattering of Neutrons and X-Rays
Klaus A. Gernoth 43

Average Structure vs. Real Structure: Molecular Dynamics Studies of Silica
Martin H. Müser 75

Simulation and Theory of Inhomogeneous Liquid Crystals
Mike Allen 101

Disorder Diffuse Scattering of Crystals and Quasicrystals
Friedrich Frey 133

Inelastic Neutron Scattering from Structural Excitations
Götz Eckold 167