

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,
July 2002

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

Ristig, M.L.; Gernoth, K.A. (Eds.)

2003, XII, 196 p., Hardcover

ISBN: 978-3-540-44386-5