High-Pressure Crystallography

edited by

Andrzej Katrusiak
Faculty of Chemistry,
Adam Mickiewicz University, Poznań, Poland

and

Paul McMillan
Department of Chemistry,
University College London, United Kingdom

Kluwer Academic Publishers
Dordrecht / Boston / London

Published in cooperation with NATO Scientific Affairs Division
TABLE of CONTENTS

Preface
A. Katrusiak, P.F. McMillan ix-xi

1. HIGH PRESSURE CRYSTALLOGRAPHY: EXPERIMENTAL TECHNIQUES AND DATA ANALYSIS

High Pressure Diffraction from Good Powders, Poor Powders and Poor Single Crystals
M.I. McMahon 1

Some Practical Aspects of Studying Equations of State and Structural Phase Transitions at High Pressure
R.J. Angel 21

Structure Maps for Constrained Structures at High Pressures from Powder Diffraction
J.B. Parise 37

High-Pressure Single-Crystal Diffractometry with Laboratory X-Ray Sources
A. Katrusiak 57

Neutron Diffraction Studies of Ices and Ice Mixtures
J.S. Loveday 69

An Introduction to Diamond Anvil Cells and Loading Techniques
E. Soignard, P.F. McMillan 81

High-Pressure Crystallographic Experiments with a CCD Detector
A. Budzianowski, A. Katrusiak 101

From Phase Identification to Structure Solution: X-Ray Crystallography at High Pressures
W.A. Crichton, M. Mezouar 113

Synchrotron Radiation Study Using Large Volume Presses
O. Shimomura 131

Modulation and its Crystallographic Methodology
V. Petřiček, M. Dušek 139
2. THEORETICAL METHODS AND RESULTS, AND NEW METHODS FOR DATA ANALYSIS

Introduction to High Pressure Computational Crystallography
B. Winkler

Computational High Pressure Science
J.S. Tse

Theory of Minerals at High and Ultrahigh Pressures:
Structure, Properties, Dynamics, and Phase Transitions
A.R. Oganov

Equations of State and Thermophysical Properties of Solids Under Pressure
W.B. Holzapfel

Reverse Monte Carlo Modelling of Diffraction Data:
Structural studies of amorphous ices
L. Pusztai

3. COMPLEMENTARY HIGH-PRESSURE TECHNIQUES AND METHODS OF STRUCTURE DETERMINATION

X-Ray Absorption Spectroscopy under Extreme Conditions
J.P. Itie

Analysis of Localised Strains in Crystals by Convergent Beam Electron Diffraction
A. Armigliato, R. Balboni, A. Benedetti, S. Frabboni

Phase Transitions Studied by High-Pressure Dielectric Spectroscopy and Calorimetry
M. Szafranński

Electronic, Structural, and Magnetic Properties of Transition-Metal Insulators at Very High Pressures
M.P. Pasternak, G.Kh. Rozenberg, W.M. Xu, R.D. Taylor

Magnetic Properties of Crystals and their Studies at High-Pressure Conditions
I.N. Goncharenko

Correlation Between the Structure and Optical Properties of Perovskites at High Pressure
F. Rodriguez

Solid Phase Transformations under High Dynamic Pressures
S.S. Batsanov
4. APPLICATIONS OF HIGH PRESSURE CRYSTALLOGRAPHY

Crystallography and Solid State Chemistry at High Pressure
P.F. McMillan 367

High-Pressure Crystallography at Elevated Temperatures: Experimental Approach
L. Dubrovinsky, N. Dubrovinskaia 393

Synthesis of Superhard Phases: In Situ Studies
V.L. Solozhenko 411

Pressure Effects on Structural and Electronic Properties of Superconductors

Novel Hume-Rothery Phases in Simple Metals and Alloys under High Pressure
V.F. Degtyareva 447

High Pressure Crystal Chemistry: "Stuffed" Framework Structures at High-Pressure
N.L. Ross, R.T. Downs 457

The High Pressure Crystallography of Gas Hydrates
W.F. Kuhs 475

Molecules in Strained Environment
E.V. Boldyreva 495

General Description of Hydrogen-Bonded Solids at Varied Pressures and Temperatures
A. Katrusiak 513

Why Study Quasicrystals at High Pressures?
G. Krauss, W. Steurer 521

State of the Art and Prospects of Macromolecular X-Ray Crystallography at High Hydrostatic Pressure
R. Fourme, E. Girard, R. Kahn, I. Ascone, M. Mezouar, T. Lin, J.E. Johnson 527

Soft Materials and Biomaterials under Pressure
S.M. Gruner 543

AUTHORS INDEX 557
SUBJECT INDEX 559