

Table of Contents

Preface

The Role of Munich in X-Ray Crystallography and the Development of Powder Diffraction H. Jagodzinski	1
Indexing of Powder Diffraction Patterns D. Louër	17
Quo Vadis Quantitative Powder Diffraction Phase Analysis J. Fiala	27
Automated Multicomponent Phase Identification using Fuzzy Sets and Inverted Data Base Search C. Brandt, H. Rozendaal, T. Blaffert and S. Bates	35
XRD as a Tool in Phase-Diagram Imaging W. Lengauer and P. Ettmayer	41
Ambiguities in the Interpretation of Powder Patterns R.X. Fischer and E. Tillmanns	47
Detectability of Phases in Protective Magnetite Thin Film Samples V. Novosel Radovic, N. Nenadic and F. Safar	53
Depth Distribution of Phase Content Reconstruction in Thin Films X-Ray Diffractometry L.G. Shabelnikov	61
Quantitative Phase Analysis of Textured Materials H.G. Brokmeier	67
X-Ray Diffraction Line Profiles due to Real Polycrystals P. Klimanek	73
Quality of Unravelling of Experimental Diffraction Patterns with Artificially Varied Overlap E.J. Sonneveld, R. Delhez, T.H. de Keijser and E.J. Mittemeijer	85
PC-Profile Analysis of Peak Clusters in Angle and Energy Dispersive Powder Diffractometry C. Höffner, G. Will and F. Elf	91
Desummation of Mixed Powder Diffraction Lines A. Benabad-Sidky, G. Caboche, M.T. Mesnier and J.C. Niepce	99
A Method for Data Reduction and Optimal Experimental Design in XPD G. Querner, J. Bergmann and W. Blau	107
The Method of Synthesizing the Function of the Diffraction Maximum Shape. The Possibility of Applying it for Structural Refinement V.A. Kogan and M.F. Kupriyanov	113
A Correction for Truncation of Powder Diffraction Line Profiles A.C. Vermeulen, R. Delhez, T.H. de Keijser and E.J. Mittemeijer	119
Comparison of Single- and Multiple-Peak Methods for the Determination of Crystallite Size and Lattice Strain using Pseudo-Voigt Functions N. Zotov	125
X-Ray Powder Diffraction Data Reduction by Integrating the Wilson and the Warren-Averbach Theories G. Berti	131
Simulation of Diffraction Patterns from Small Bimetallic Crystals with Concentration Gradient J. Pielaszek and J. Barczynska	139
X-Ray Stress Analysis J.M. Sprauel and L. Castex	143
Influence of PSI- and OMEGA-Tilting on X-Ray Stress Analysis S. Fischer, E. Houtman and H.R. Maier	153
Non-Destructive Stress Measurement with Depth Resolution M. Härting and G. Fritsch	159

Determination of the Misfit and Layer Thickness of Monocrystalline Epitaxial Layers by Means of High-Resolution X-Ray Diffraction H.-. Brühl and H. Rhan	165
Preferred Orientation in Powder Diffraction H.J. Bunge	169
Texture Analysis of Multi-Phase Materials by Neutron Diffraction H.G. Brokmeier	179
Extinction in Texture Analysis A. Mücklich and P. Klimanek	185
Method of Scanning of Reciprocal Space of Axial Textures and its Applications to Structural Investigations G.A. Krinari and Z.J. Halitov	191
On the Use of Rietveld Refinements for Structural Studies P.-. Werner	197
The Two-Step-Method and its Applications in Crystallographic Problems G. Will	207
Sign Determination from Powder Diffraction Data of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ W. Limper, W. Prandl and T. Wroblewski	221
Fourier Maps Obtained from Powder Diffraction Data - Applications Beyond Pure Illustration S. Jantsch, J. Ihringer, W. Prandl and H. Ritter	227
Influence of Crystallite Size and Microstrain on Structure Refinement P. Scardi, L. Lutterotti, R. Di Maggio and P. Maistrelli	233
Crystal Size Dependent Anisotropic Line Broadening in Rietveld X-Ray Analysis R. Millini, G. Perego and S. Brückner	239
A Theta-Dependent Error Present in Powder Data of Highly Absorbing Materials: A Surface Roughness Effect? N. Masciocchi, H. Toraya and W. Parrish	245
Qualitative XRPD Analysis System V. Pivoriunas	251
Qualitative X-Ray Phase Analysis on the Basis of the Calculated Standards A.V. Chichagov	257
Program Package COMPHYS for IBM PC M.S. Nakhmanson	263
Solution of Nontraditional Problems Based upon PDF-2 M.S. Nakhmanson	267
Database for Qualitative X-Ray Diffraction Phase Analysis of Natural Materials E.K. Vasil'ev	271
GUFI-WYRIET: An Integrated PC Powder Pattern Analysis Package J. Schneider and R.E. Dinnebier	277
MRIA - A Program for a Full Profile Analysis of Powder Neutron-Diffraction Time-of-Flight (Direct and Fourier) Spectra V.B. Zlokazov and V.V. Chernyshev	283
Numerical Refinement of Lattice Parameters: Monoclinic Case W. Paszkowicz	289
Thermal Coefficient of Expansion (TCE)-Program for Calculation of TCE's for Single Crystals of all Systems R.A. Dilanyan, B.Z. Narymbetov and L.A. Novomlinski	295
Database for the Structural Problems of High Temperature Superconductors E.A. Gamazova and L.A. Novomlinski	299
PULPLOT - A PC Routine for the Graphic Representation and Superimposition of X-Ray Powder Diffraction Patterns W. Lengauer	303
New Instrumentation in Powder Diffraction J. Ihringer	307
A Powder Diffractometer for Large-Sized Specimens A.A. Evgrafov, A.P. Kokko, P.P. Bolshakov, A.L. Bunin, A.D. Plotnikov and S.Y. Betsofen	317

The Quantitative Powder Diffractometer, QPD J. Ladell, W.N. Schreiner and B.L. Greenberg	323
Imaging the Focus of a Microfocus X-Ray Source with Zone Plates A. Krutzenbichler and G. Fritsch	329
Fluid Cooled Rotating Anode Without Mechanical Feedthrough of the Anode Axis to the Vacuum J. Ihringer	335
Diffractometer with a Curved PSD for Analysis of Polycrystalline Microsamples D.A. Goganov, O.I. Ageev and B.M. Reizis	339
X-Ray Diffractometric Sensors in Commercial Production Y.S. Grigoriev and A.A. Evgrafov	343
New Detectors in X-Ray Diffraction P.A. Tucker	349
Highly Stable Position-Sensitive Detectors for Powder Diffractometry O.I. Ageev, D.A. Goganov, S.M. Goutkevich, I.B. Klochkova and E.K. Ovchinnikov	357
The INEL X-Ray Position Sensitive Detector: A Study of D-Spacing Accuracy and Exposure Time P. Deniard, M. Evain, J.M. Barbet and R. Brec	363
A Two-Dimensional CCD-Based Detector for X-Ray Radiation F. Elf, G. Will and S. Weisgerber	371
Analyser and P.S.D.: Energy Resolution Improvement S. Megtert, D. Dallé and D. Petermann	377
Physical Principles of X-Ray Storage Phosphors H. von Seggern	383
Silicon Pin Photodiodes as Detectors with High Dynamical Range for X-Rays B. Lengeler, U. Dedek, C. Storb, W. Weber and M. Schuster	389
A High Resolution Gas Electroluminescent Detector for X-Ray Structure Analysis D.A. Goganov and A.A. Schultz	395
The Application of a Proportional-Scintillation-Detector in X-Ray Diffractometry K. Richter, D. Meyer, J. Linz, K. Moras and W. Blau	399
Autoradiographic Image Enhancement of Debye-Scherrer Patterns B.I. Reznik, V.D. Rusov, M.U. Semenov and V.I. Petrashevich	405
Energy Dispersive XRPD at High Pressure L. Gerward	409
X-Ray Diffractometer for High Pressure and Low Temperatures H. Karzel, U. Potzel, W. Potzel, J. Moser, C. Schäfer, M. Steiner, M. Peter, A. Kratzer and G.M. Kalvius	419
First Experiments with a Newly Developed High-Pressure/High-Temperature Cell for Neutron Powder Diffraction K. Fütterer, W. Depmeier, J. Strobel and T. Vogt	427
Low- and High-Temperature Accessories for the D500 Powder Diffractometer M. Behr, F.D. Scherberich and T. Hahn	433
A New Attachment for Non-Ambient X-Ray Powder Diffraction Studies in Various Atmospheres K. Richter, B. Peplinski and P. Doppler	439
A Furnace for X-Ray Powder Diffraction with Synchrotron Radiation H. Arnold	445
Powder Diffraction using Synchrotron Radiation M. Hart	447
The Use of Debye Scherrer Geometry for High Resolution Powder Diffraction R.J. Cernik and G. Bushnell-Wye	455
A New Beauty for Adone: A High Resolution Powder Diffractometer for Synchrotron Radiation Experiments E. Burattini, G. Cappuccio, P. Maistrelli and S. Simeoni	463
Depth Profiling in Thin Films by Grazing Incidence Diffraction using Synchrotron Radiation T. Wroblewski	469

A New High Resolution Neutron Powder Diffractometer at the Brookhaven High Flux Beam Reactor	
L. Passell, S. Bar-Ziv, D.W. Gardner, D.E. Cox and J.D. Axe	475
A New Neutron-Multi-Detector Diffractometer at the Rossendorf-Reactor	
G. Merz, G. Försterling, V.A. Trunov and V.A. Ulyanov	481
Status and Horizons of Time-Resolved Neutron Scattering at the Pulsed Reactor IBR-2	
G.M. Mironova	487
Characterization of Epitaxial Thin Films by X-Ray Diffraction	
A. Segmüller	493
Glory and Misery of the Structure Analysis of Thin Polycrystalline Films	
V. Valvoda	503
Applied Crystallography in Advanced Ceramics	
R.L. Snyder	513
Neutron Powder Diffraction and Oxide Superconductors	
A.W. Hewat	529
Elucidation of Deformation and Recovery Mechanism in Nickel-Base Alloy 600 by X-Ray Rocking Curve Measurements	
S. Weissmann, W.E. Mayo and C.F. Lo	539
X-Ray Determination of the Martensite Structure in Fe-Ni Base Aged Alloys	
V.V. Kokorin and O.M. Shevchenko	545
Changing of the Crystalline Structure of Martensite of High-Nickel Steel at Low Temperature	
V.I. Bondar and V.E. Danil'chenko	551
X-Ray Examination of the Ribbon, Prepared by the High Speed Solidification of the Fe-Ni-Co-Ti Alloy	
V.A. Chernenko, M.Y. Hamarnik and L.E. Kozlova	557
X-Ray Diffraction Studies of Secondary Hardening in CrMoV Hot Working Tool Steels	
C. Herrmann and D. Naundorf	561
X-Ray Study of Annealing Process of Au₃Cu, AuCu and AuCu₃ at 270° C in Air	
J. Janczak and R. Kubiak	567
XRD Studies on Atomic Ordering of Ni-Cr Based Alloys	
A. Marucco	575
Structure of Electrodeposited Cu-Cd Alloys After Annealing	
E. Łągiewka and L. Pająk	581
In Situ Study of Ag Electrode in Contact with a Solid Oxide Electrolyte	
A.V. Ziborov, L.M. Plyasova and O.A. Mar'ina	589
Structure and Thermal Diffusion in Al/Fe Thin Films and Multilayers	
M.F. Ravet, J.F. Bobo, P. Frechard, O. Lenoble and M. Piecuch	595
On Character and Nature of Size Changes in the Lattice Parameters of Small Metal Particles	
M.Y. Gamarnik	601
Structure of Nanocrystalline Soft-Magnetic Materials	
N. Mattern	607
Application of Grazing Incidence for the Investigation of the High Temperature Corrosion of Steel	
N. Eisenreich, W. Engel, V. Kolarik, M. Juez-Lorenzo and A. Rehfeldt-Oskierski	613
High Temperature Corrosion Kinetics using a Fast X-Ray Diffraction Method	
V. Kolarik, M. Juez-Lorenzo, N. Eisenreich and W. Engel	617
Powder Diffraction Investigation of γ - ϵ and γ - ϵ' Transformations in an Fe-Mn-C Alloy	
B.I. Nikolin, V.I. Bondar and A.Y. Babkevich	623
Crystal Structure of Intermediate Phases in Binary B-Metal Alloys Induced by High Pressure	
V.F. Degtyareva	629
Neutron- and X-Ray Powder Investigation of the Zintl Phases NaTl and LiAl at Temperatures up to 900K	
M. Tadin, J. Schneider, H. Boysen and F. Frey	635
A High-Pressure X-Ray Diffraction Study of UAs_{0.6}Se_{0.4}	
L. Gerward, J. Staun Olsen, U. Benedict and H. Luo	643

XRD Characterization of Sputtered Mo and W Thin Films J.L.C. Daams, T.J. Vink, M.A.J. Somers and A.G. Dirks	647
Texture and Lattice Strain Determination of Molybdenum Thin Films Deposited by D.C. Magnetron Sputtering P. Gergaud, P. Bosland, J.J. Bacmann and J.L. Lebrun	653
Stress Analysis by X-Ray Diffraction. The Effect of Cementation on the Surface Distribution of Residual Stresses in Alloy Steels L.E. Depero, P. Bonzi and M. Zocchi	659
Neutron Diffraction Study of Sintering of Aluminium Oxide B.F. Palosz, H. Boysen and T. Vogt	665
Solid Way Synthesis of Barium Aluminate. High Temperature X-Rays Diffraction Study of Intermediary Compounds L. Perier-Camby, A.M. Vernay and G.P. Thomes	671
Solving X-Ray Powder Pattern Problems Dealing With Layer Structures in the Field of Calcium Aluminum Hydroxi Salts H. Pöllmann	679
X-Ray and Neutron Powder Investigations of Pure and Yttrium Doped CeO₂ at Temperatures up to 1600 K K. Berber, U. Martin, Z. Mursic, J. Schneider, H. Boysen and F. Frey	685
Phase Studies in the System Chromium-Manganese-Titanium Oxide at Different Oxygen Partial Pressures A. Naoumidis, H.A. Schulze and C. García-Rosales	691
X-Ray Diffraction of CuS₂ under High Pressure H. Hüpen, G. Will, C. Höffner and F. Elf	697
Influence of Nd-Substitution on the Orthorhombic/Rhombohedral Phase Transition of LaGaO₃ T. Berthold and B. Jobst	703
A Temperature-Resolved X-Ray Powder Diffraction Study of the Decomposition of Three Metal Hydroxide Nitrates M₅(OH)₈(NO₃)₂·2L (M=Cd,Zn; L=H₂O, NH₃) P. Bénard, J.-. Auffrédic and D. Louër	709
X-Ray Study of Crystallization Kinetics and Phase Transformations of Zinc- and Cadmium Diphosphide Films A.U. Sheleg, V.A. Denis, E.M. Zub and L.S. Unyarkha	715
The High-Temperature Phase of Zeolite Sr-rho Contracts Appreciably Compared with its Low-Temperature Form A. Bieniok and W.H. Baur	721
The Using of Multiphase Rietveld Refinement in Quantitative Analysis J. Maixner and M. Hušák	727
Process-Optimization in Large-Scale Production of Mn-Zn-Ferrites using Powder Diffraction A. Meden, V. Kaucic and A. Zivic	733
Rietveld Analysis and Quantitative Analysis of Ettringite Formed by Hydration of Lignite Gasification Ash W. Schmitz, B. Heide and P. Schreiter	739
Quantitative X-Ray Diffraction Rietveld Analysis of Low Temperature Coal Ashes M. Bellotto and C. Cristiani	745
The Calcite-Gypsum Conversion in Mortar Joints of Railroad Tunnels - An X-Ray Study B. Baumgartner, E. Wölfel, W. Mann and M. Betzler	751
The Analysis of Urinary Calculi by X-Ray Diffraction and IR-Spectroscopy D. Krausová, J. Kameníček and V. Bekárek	757
Powder Profile Refinement of a Commensurately Modulated Aluminate Sodalite W. Depmeier and A. Yamamoto	763
Phase Transitions of the Aluminate Sodalite CAW J.W. Strobel, W. Paulus and W. Depmeier	769
Crystal and Magnetic Structure of the Magnetically Modulated Spinel Zn_{1-x}Ga_{2x/3}Cr₂Se₄ Where (X=0.0, 0.1, 0.2, 0.3, 0.5) H. Rej, A. Bombik, J. Kusz, A. Oles, M. Pinod and J. Warczewski	771

Spinel Cation Distribution from Powder X-Ray Diffraction. Data Comparison with External-Field ^{57}Fe Mössbauer Spectroscopy at 4.2 K	
P.M.A. de Bakker, E. De Grave, D. Gryffroy, R.E. Vandenberghe and P. Moens	777
A Neutron Diffraction Study of some Spinel Compounds Containing Octahedral Ni and Mn at a 1:3 Ratio	
D. Gryffroy, R.E. Vandenberghe and E. Legrand	785
Symmetry of the Ferroelectric Phases of the Pyrochlore $\text{Cd}_2\text{Nb}_2\text{O}_7$ - A Study using a Very High Resolution Powder Diffractometer at a Synchrotron Radiation Source	
A. Küster, J. Ihringer, W. Limper, T. Wroblewski and W. Prandl	791
Production and Characterization of Thin Ferroelectric Lead Zirconate Titanate Films	
R. Bruchhaus, B. Jobst, H. Huber and D. Pitzer	797
Structural Data of the Monoclinic High-Temperature G-Form of $\text{La}_2\text{Si}_2\text{O}_7$ from X-Ray Powder Diffraction	
O. Greis, H.G. Bossemeyer, P. Greil, B. Breidenstein and A. Haase	803
X-Ray Powder Diffraction Study of Francolite by the Rietveld Method	
B. Perdikatis	809
An X-Ray Powder Diffraction Study on Calcium-Lead Hydroxyapatites	
A. Bigi, M. Gandolfi, M. Gazzano, A. Ripamonti, N. Roveri and S.A. Thomas	815
Rietveld Studies of the Aluminium-Iron Substitution in Synthetic Goethite	
J.-. Hazemann, J.F. Béar and A. Manceau	821
Powder X-Ray Diffraction Study of Topotactic Lithium Exchange in Manganese (III) Arsenate Hydrate	
M.G. Aranda, J.P. Attfield and S. Bruque	827
Refinement of the Crystal Structure of $\text{Pb}_2\text{HP}_3\text{O}_{10}$ by Rietveld Analysis	
G. Walther, R. Seydel and H. Worzala	833
Ab Initio Structure Determination of $\text{Zr}(\text{OH})_2(\text{NO}_3)_2 \cdot 5\text{H}_2\text{O}$ from X-Ray Powder Diffraction Data	
P. Bénard, M. Louër and D. Louër	839
Characterization of the Natural Zeolite Gonnardite. Structure Analysis of Natural and Cation Exchanged Species by the Rietveld Method	
G. Artioli and M.R. Torres Salvador	845
Luminescence Properties and X-Ray Diffraction Line Analysis of LaOBr:Tb	
H. Wulff and U. Sasum	851
Texture Analysis of Evaporate Polycrystalline $\text{Zn}_x\text{Cd}_{1-x}\text{S}$ Thin Films	
H. Dittrich, R. Schäffler and H.-. Schock	857
The Phase Composition of ZnO Ceramic Filters for the Desulfurization of Coal Gases in Dependence on their Preparation and the p,t Conditions	
U. Steinike, H.-. Hennig, K. Jancke, K.-. Redlich, N. Jentzsch and C. Möcklinghoff	863
Temperature Expansion in $(\text{La},\text{Sr})(\text{Mn},\text{Co})\text{O}_3$-Cathode Materials for Solid Oxide Fuel Cells	
A. Iberl, H. von Philipsborn, M. Schiessl, E. Ivers-Tiffée, W. Wersing and G. Zorn	869
Characterization of Oxygen-Electrode/Electrolyte Interface Reactions in Solid Oxide Fuel Cells by X-Ray Diffraction Measurements	
E. Ivers-Tiffée, B. Jobst, I. Kraus, R. Schachtner and M. Schiessl	875
Thermal Behaviour of Molecular Sieves (SAPO-11/AlPO-11 Type) Investigated by Synchrotron Radiation X-Ray Diffraction (SRXD)	
F. Neissendorfer, E. Jahn, S.N. Gusenko and M.A. Sheromov	883
Hydrogen Loss and Interdiffusion in Amorphous Si/SiC Multilayers	
G. Zorn, J. Kolodzey, H. Göbel, T. Fischer, P. Hanesch and R. Schwarz	887
Observation of Annealing Effects in Ti/TiN-Diffusion Barriers using High-Temperature X-Ray Diffraction	
G. Zorn and H. Joswig	893
Structure of TiN Thin Film Grains in Dependence on their Crystallographic Orientation	
V. Valvoda, R. Cerný, R. Kužel, M. Blomberg and M. Merisalo	903
Heat-Treated NiO and Changes of Microstructural Parameters	
S. Pocev, B. Marina and S. Bogoevski	909
X-Ray Determination of Characteristics of Finely Dispersed Supports and Supported Catalysts	
E.M. Moroz, V.A. Ushakov and S.V. Bogdanov	915

Indexing of New Superconducting Oxide Powder Patterns J. Hauck, B. Bischof, N. Dockal, E. Droste, C. Feiburg, H. Hindriks, S. Ipta, F. Klumpe, K. Mika and A. Preikschat	919
Stoichiometry and Temperature Dependence of $\text{YBa}_2\text{Cu}_3\text{O}_x$ Structure Parameters G. Försterling, I.V. Golosovsky and W. Plakhty	927
Temperature Dependence of the Lattice Constants of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ U. Wachtel, M.G. Gorskaja, S.K. Filatow, P. Paufler, W. Schmitz and W. Reichelt	935
Growth of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ Thin Films on R-Plane Sapphire (0112) Using Yttria Stabilized Zirconia (YSZ) Buffer Layers K. Hradil, H. Schmidt, W. Hösler, W. Wersing, F. Frey, B. Jobst and G. Zorn	941
X-Ray Absorption and Reflection in Materials Science B. Lengeler	947
Some Sample Preparation Methods for Powder Diffraction at Neste Oy H. Oesterholm and J. Vilhunen	959
Characterization of Gels and Thin Gel Films by X-Ray Diffraction Methods T. Gerber, B. Himmel, U. Buttler, H. Bürger and U. Bräutigam	965
Transmission Electron Microscopy: An Important Technique for the Determination of the Crystal Structure of Modulated High-T_c Superconductors O. Eibl, H. Budin, P. Pongratz and P. Skalicky	971