

Contents

1. Overview	1
<i>Klaus Bange, Wilfried Heimerl, Dieter Krause</i>	
1.1 The “Object”: Amorphous Material, Glass, and Glass Ceramics	2
1.2 Qualitative Relations of Properties with Composition and Structure	8
1.3 The Importance of the Chemical Composition	11
1.3.1 Methods and Strategies	12
1.3.2 Indirect Analysis	13
1.3.3 Direct Analysis	13
1.3.4 New Developments and Future Trends	15
1.4 Methods for Structure Determination	17
1.5 Analysis of Glass Defects	20
References	26
2. The Chemical Analysis of Glasses, Glass Ceramics, and Related Materials	29
2.1 Sampling and Sample Preparation	29
2.1.1 Mechanical Pretreatment Before Digestion <i>Lothar Meckel</i>	29
2.1.2 Methods of Decomposing Glasses and Glass Ceramics for Analysis <i>Lothar Meckel</i>	32
2.1.3 Methods of Preparing Samples for Analysis in the Solid State <i>Hartmut Müller, Bernd Valentin</i>	39
2.2 Methods for Digested (Wet) Samples <i>Lothar Meckel</i>	42
2.2.1 Gravimetric Methods	42
2.2.2 Volumetric Methods	43
2.2.3 Molecular Absorption Spectroscopy (MAS)	44
2.2.4 Atomic Absorption Spectroscopy (AAS)	45
2.2.5 Atomic Emission Spectroscopy (AES)	47
2.2.6 Infrared (IR) Detection and Measurement of the Thermal Conductivity	48
2.2.7 Mass Spectrometry	49

2.3	Methods for Direct Instrumental Analysis of Solid Samples	50
2.3.1	Inductively Coupled Mass Spectrometry with Laser Ablation System <i>Christine Strubel</i>	50
2.3.2	Electron Probe Microanalysis (EPMA) <i>Hartmut Müller</i>	52
2.3.3	X-Ray Fluorescence (XRF) Analysis <i>Bernd Valentin</i>	58
2.3.4	Special Applications of XRF in the Glass Industry <i>Bernd Valentin</i>	62
2.3.5	Laser-Induced Breakdown Spectroscopy (LIBS) <i>Lothar Meckel</i>	65
2.3.6	Gas-Analysis and Extraction Methods <i>Matthias Jäger</i>	66
2.4	Specific Examples and Results for Glass and Glass Ceramics	73
2.4.1	Qualitative and Quantitative Analysis of Major Components <i>Lothar Meckel, Hartmut Müller, Bernd Valentin</i>	73
2.4.2	Species Analysis <i>Ruth Effenberger</i>	94
2.4.3	Quantitative Analysis of Trace-Element Concentrations <i>Friedrich G.K. Baucke, Frank Dauth, Brigitte Leibecke, Lothar Meckel</i>	96
2.4.4	Quantitative Analysis of Water Content <i>Fritz W. Krämer, Rainer Haspel</i>	120
2.4.5	Quantitative Analysis of Gas Content <i>Fritz W. Krämer</i>	124
2.5	Analysis of Cullet, Dust, Sludge, and Waste Water <i>Lothar Meckel</i>	128
	References	131
3.	The Quasi-Static Structure of Oxide Glasses	141
3.1	How to Describe the Topological Structure of Glasses <i>Christian Schultz-Münzenberg</i>	141
3.1.1	The Concept of Atom-Specific Structure Elements (ASEs) for Oxide Glasses	143
3.1.2	Distribution of ASEs in Binary Silicate Glasses	149
3.2	Some Selected Methods of Determining ASEs <i>Christian Schultz-Münzenberg</i>	153
3.2.1	Mössbauer Spectroscopy	153
3.2.2	Photoelectron Spectroscopy (XPS)	159
3.2.3	X-Ray Absorption Spectroscopy (XAS)	163
3.2.4	Raman Spectroscopy	168

3.3	Quantitative Results for ASEs	
	<i>Christian Schultz-Münzenberg</i>	171
3.3.1	Binary Silicate Glasses	171
3.3.2	Sodium Aluminosilicate Glasses (NAS Glasses)	180
3.3.3	Sn and Sb in Sodium Silicate Glasses	188
3.4	NMR Investigation of the Structure of Glasses: Conventional	
	MAS NMR Experiments <i>Christian Jäger</i>	199
3.4.1	Advantages and Limitations of NMR	199
3.4.2	Results of Structural Studies of Glasses	200
3.5	Two-Dimensional NMR Investigation of the Structure	
	of Glasses: Novel Approaches <i>Christian Jäger</i>	208
3.5.1	Measurements of Q ^[n] Group Connectivities and	
	of Borate Units in Glasses	212
3.5.2	Measurement of Heterogroup Connectivities	
	(Structural Units with Different Central Atoms	217
3.5.3	Characterization of Oxygen Bonds in Glasses	
	with ¹⁷ O DAS and MQMAS NMR	222
3.5.4	Order Phenomena in Extruded Calcium	
	Phosphate Glasses	230
3.5.5	Summary and Outlook	232
3.6	Thermochemistry and Structure of Oxide Glasses	
	<i>Reinhard Conradt</i>	234
3.6.1	Thermodynamic Features of the Glassy State	235
3.6.2	Structural Aspects in the Thermodynamic Treatment	
	of Mixed Phases	238
3.6.3	Glasses as Medium Range Order (MRO) Mixtures	244
3.6.4	Quantitative Thermochemical Treatment of Glasses	
	and Glass Melts	253
3.7	How Can Computer Simulations Contribute to the	
	Understanding of the Static Structure of Glasses?	
	<i>Kurt Binder, Walter Kob</i>	257
3.7.1	The Molecular Dynamics Method	257
3.7.2	Basic Features of a Molecular Dynamics Program:	
	An Introduction for the Novice	258
3.7.3	A Case Study: Cooling-Rate Dependence of the	
	Structure of Amorphous SiO ₂	262
3.7.4	Concluding Remarks	267
3.8	Flow-Induced Anisotropies in Glasses and Glass Melts	
	<i>Rolf Brückner</i>	269
3.8.1	Birefringence and Internal Stresses	270
3.8.2	Birefringence by External Elastic Stresses or Strains	271
3.8.3	Birefringence by Flow Stresses or Deformation Rates	
	(Flow Birefringence)	272

3.8.4	Double-Phase Glasses and Glass Melts ($\eta > 10^7$ Pa.s).....	287
3.8.5	Optically “Anomalous” Anisotropic Glasses and Melts	292
	References	296
4.	Dynamics of the Glass Structure	315
4.1	Applying the Dynamics of the Structure to Tailor the Glass Properties <i>Ulrich Fotheringham</i>	315
4.1.1	The Original Tool Model, Derived with a Double-Well- Potential Consideration	315
4.1.2	Monitoring the Structural Dynamics via a Dynamic Measurement of the Specific Heat	319
4.1.3	The Tool–Narayanaswamy Model.....	329
4.1.4	Tailoring Two Exemplary Glass Properties	339
4.2	How Can Computer Simulations Contribute to the Understanding of the Dynamics of Glasses and Glass Melts? <i>Walter Kob, Kurt Binder</i>	346
4.2.1	Model and Details of the Simulation	347
4.2.2	Results.....	348
4.2.3	Conclusions.....	358
4.3	How Can Inelastic Neutron Scattering Contribute to the Understanding of the Dynamics of Glasses? <i>Ulrich Buchenau, Andreas Wischnewski</i>	359
4.3.1	Neutron Measurements.....	363
4.3.2	Data Analysis.....	365
4.3.3	Implications for Sound Wave Scattering	367
4.4	Titania-Activated Nucleation in Lithium–Aluminosilicate Glass Ceramics Investigated by Raman Spectroscopy <i>Rüdiger Sprengard</i>	368
4.4.1	Titanium Coordination in $\text{SiO}_2 \cdot n\text{LiAlO}_2$ Glass	369
4.4.2	Titanium Segregation from the Glass Network	373
4.4.3	Conclusion	380
4.5	Nucleation at Silicate Glass Surfaces <i>Stefan Reinsch, Ralf Müller</i>	381
4.5.1	Experimental Procedure	381
4.5.2	Surface Nucleation Kinetics.....	382
4.5.3	Surface Nucleation Sites.....	383
4.5.4	Benefit of a Tuneable Surface Nucleation Density	390
	References	394

5. Chemical Resistance and Corrosion, and Ion Release	401
5.1 Requirements for Different Glass Products <i>Wilfried Heimerl</i>	401
5.2 Determination Methods and Standards, and Specific Examples <i>Wilfried Heimerl</i>	402
5.3 Ionic Processes between Glasses and Solutions <i>Friedrich G.K. Baucke</i>	407
5.3.1 The Electrochemically Structured Interface Glass/Solution: Interfacial Equilibria	409
5.3.2 Interfacial Equilibria Under the Influence of Subsurface Concentration Gradients	412
5.3.3 Specific Reactions Between Glasses and Solutions: An Example	421
5.4 Development of Glasses with Improved Corrosion Resistance <i>Peter Brix</i>	424
5.4.1 Requirements Profile and Design	424
5.4.2 Chemical Stability	430
5.4.3 Coincidence, Trial and Error	435
5.5 Thermodynamics of Glass Corrosion <i>Reinhard Conradt</i>	438
5.5.1 Physical Boundary Conditions in Different Corrosion Scenarios	438
5.5.2 Discussion of Individual Corrosion Models	439
5.5.3 The Gibbs Free Energy of Hydration of Multi-Component Glasses	442
5.5.4 Surface and Subsurface Effects	446
5.5.5 Application of a Corrosion Model	447
References	449
6. Analysis and Diagnosis of Local Defects	453
6.1 Bubbles <i>Rudolf Feile, Adolf Götz, Fritz W. Krämer</i>	453
6.1.1 Analysis of Gaseous Inclusions	453
6.1.2 Bubble Defect Diagnosis	467
6.2 Knots, Striae, and Stones <i>Hartmut Müller</i>	470
6.3 Glass Interaction with AZS <i>Hartmut Müller</i>	474
6.4 Microphase Separation in Glasses <i>Werner Vogel</i>	479
6.4.1 Two-Phase Glasses and Functional Change of Microphases	480
6.4.2 Multiple Phase Separation	482

6.4.3	Droplet Agglomeration after Secondary Phase Separation	485
6.4.4	Shell Formation Around Microphases	487
6.4.5	Other Practical Significances of Phase Separation Processes in Glasses	489
6.4.6	Control of Phase Separation	492
6.4.7	General Conclusions on Immiscibility Behaviour and Microstructure	493
6.5	Metal Inclusions: Platinum <i>Joseph S. Hayden, Alexander J. Marker III</i>	493
6.5.1	Sources of Platinum	494
6.5.2	Phosphate Laser Glass Melting Experiments	494
6.5.3	Summary and Conclusions	496
6.6	Platinum Particle Detection in Phosphate Laser Glasses <i>John H. Campbell, James F. Kimmons, Sheldon Schwartz</i>	498
6.6.1	Basis for Platinum Particle Detection: Laser-Induced Damage	500
6.6.2	Description of the Pt-Inclusion Inspection System	507
6.6.3	Inclusion Test Specification and Procedures	510
6.6.4	Past System Operational Experience and Current Status	512
	References	513
	List of Contributing Authors	520
	Sources of Figures and Tables	521
	Index	525