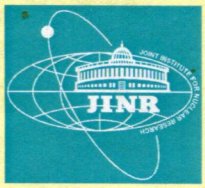
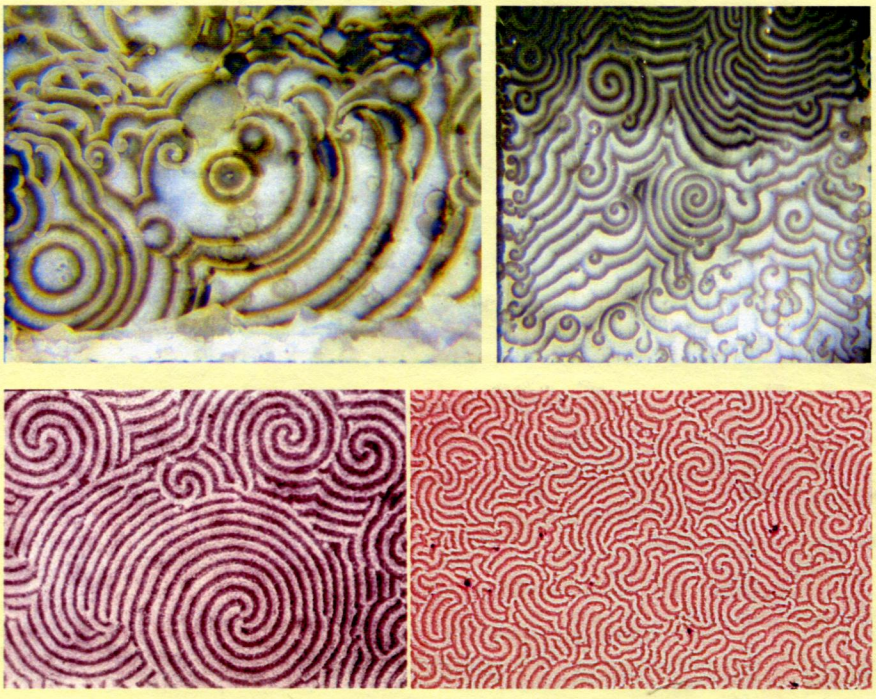
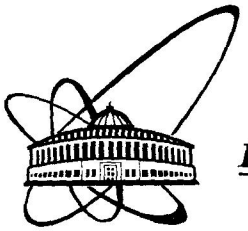


BLTP Bogoliubov Laboratory of Theoretical Physics

Nucleation Theory and Applications

Edited by Jürn W. P. Schmelzer
Gerd Röpke
Vyatcheslav B. Priezzhev





BLTP Bogoliubov Laboratory of Theoretical Physics

Nucleation Theory and Applications

Edited by Jürn W. P. Schmelzer
Gerd Röpke
Vyatcheslav B. Priezzhev

Dubna JINR 2008

УДК 536.42
ББК 22.317
N91

The contributions are reproduced directly from the originals presented by the Organizing Committee.

Nucleation Theory and Applications / Eds.: J. W. P. Schmelzer, G. Röpke, N91 V. B. Priezzhev. — Dubna: JINR, 2008. — XIII, 475 p.

ISBN 978-5-9530-0199-1

The present book consists of contributions directed to the analysis of first- and second-order phase transitions from both experimental and theoretical points of view. They have been presented and discussed in the course of the research workshops «Nucleation Theory and Applications» organized at the Bogoliubov Laboratory of Theoretical Physics of the Joint Institute for Nuclear Research in Dubna, Russia, in the period from 2006 to 2008. The volume of the proceedings supplements results published in three former conference proceedings in the years 1999, 2002 and 2005 also in Dubna and two monographs with overview lectures published by WILEY-VCH in 1999 and 2005. In the present proceedings, the spectrum of different topics includes experimental investigations of thermodynamic properties of matter (in thermodynamic equilibrium and non-equilibrium states including glasses), nucleation-growth phenomena and their theoretical interpretation, the theoretical analysis of the course of first- and second-order phase transitions, the discussion of principal problems of the thermodynamic description of clusters, molecular-dynamic analyses of phase equilibria and clustering phenomena, and a variety of applications.

Теория нуклеации и ее применения / Под ред. Ю. Шмельцера, Г. Рёпке, В. Б. Приезжева. — Дубна: ОИЯИ, 2008. — XIII, 475 с.

ISBN 978-5-9530-0199-1

В сборнике представлены результаты экспериментального и теоретического анализа фазовых превращений первого и второго рода, которые докладывались и обсуждались на рабочих совещаниях «Теория нуклеации и ее применения», проходивших в Лаборатории теоретической физики им. Н. Н. Боголюбова Объединенного института ядерных исследований в 2006–2008 гг. Эти результаты дополняют данные, опубликованные в трех предыдущих томах серии, вышедших в свет в 1999, 2002 и 2005 гг. в Дубне, и двух монографиях, изданных в 1999 и 2005 гг. издательством WILEY-VCH. Сборник состоит из 25 разделов, в которых отражены результаты экспериментального анализа свойств веществ (в термодинамически равновесных и неравновесных состояниях, включая стекла), процессов нуклеации и роста кластеров новых фаз и теоретическая интерпретация этих данных, общий теоретический анализ фазовых превращений первого и второго рода, обсуждаются принципиальные вопросы термодинамического описания кластеров, молекулярно-динамического анализа фазовых равновесий и процессов агрегации, а также рассматриваются разнообразные применения теории.

УДК 536.42
ББК 22.317

ISBN 978-5-9530-0199-1

© Joint Institute for Nuclear Research, 2008

Contents

1 **Introductory Remarks** 1

2 **Classical and Generalized Gibbs' Approaches and the Properties of Critical Clusters in Nucleation Theory**

Jürn W. P. Schmelzer

Institut für Physik, Universität Rostock, Universitätsplatz, 18051 Rostock, Germany 3

2.1 Introduction . . . 3
2.2 Generalized Gibbs' Approach and the Work of Critical Cluster Formation . . . 4
2.3 The Temperature of the Critical Clusters . . . 5
2.3.1 The Problem . . . 5
2.3.2 Results of MD-simulations . . . 7
2.3.3 Interpretation in Terms of the Generalized Gibbs' Approach . . . 7
2.4 Discussion . . . 9

3 **On the Thermodynamic Properties of Metastable Systems**

Vladimir G. Baidakov

Institute of Thermal Physics, Ural Branch of the Russian Academy of Sciences, 620016 Ekaterinburg, Amundsen Str. 106, Russia 11

3.1 Introduction . . . 11
3.2 Effect of Fluctuations on the Thermodynamic Properties of a System: General Considerations 11
3.3 Effect of Fluctuations on the Thermodynamic Properties of a System: An Example . . . 13
3.4 Discussion . . . 15

4 **Nanoscale Structure of the Liquid–Gas Interphase Surface and the Capillary Fluctuations**

Dmitry I. Zhukhovitskii

Joint Institute of High Temperatures, Russian Academy of Sciences, Izhorskaya 13/19, 125412 Moscow, Russia 17

4.1 Introduction . . . 17
4.2 Simulation Procedure . . . 19
4.3 Definition of the Cluster Surface . . . 21
4.3.1 Definition of a Bond . . . 21
4.3.2 Cluster Particles Classification . . . 22
4.3.3 Calculation of the Number of Bonds for a Cluster with Arbitrary Size . . . 25
4.4 Wave Number Fourier Spectrum of Surface Fuctuations . . . 26
4.4.1 Cluster Slice Spectra from MD Simulation . . . 26
4.4.2 Capillary Fluctuations of a Planar Liquid–Gas Interphase Surface . . . 29
4.4.3 Capillary Fluctuations of the Cluster Surface . . . 31
4.4.4 Other Estimates for the Surface Variance . . . 32
4.5 Frequency Fourier Spectrum . . . 34
4.6 Average Density Distribution . . . 36

4.7 Conclusions . . . 38

5 Method of Direct Numerical Solution for Simulation of Supersaturated Vapor Condensation
Naoum M. Kortsensteyn[1] and Arsenij K. Yastrebov[2]
[1] Krzhizhanovsky Power Engineering Institute, Leninskij pr. 19, 119991 Moscow, Russia
[2] Moscow Power Engineering Institute (Technical University), Krasnokazarmennaya ul. 14, 111250 Moscow, Russia **41**
5.1 Introduction . . . 41
5.2 Method of Direct Numerical Solution . . . 43
5.3 Formulation of the Relaxation Problem . . . 45
5.4 Results of Calculations and Discussion . . . 47
5.4.1 Free-molecular Regime of Droplet Growth . . . 47
5.4.2 Transitional Regime of Droplet Growth . . . 49
5.4.3 Dependence of the Saturation Pressure on Droplet Radius . . . 51
5.5 Conclusions . . . 54

6 On the Condensation-Ionization Instability in Aerosol Plasmas
Naoum M. Kortsensteyn and Eugene V. Samuilov
Krzhizhanovsky Power Engineering Institute, Leninskij pr. 19, 119991 Moscow, Russia **57**
6.1 Introduction . . . 57
6.2 Properties of Explosion Products . . . 58
6.3 Formation of Condensation Aerosol . . . 62
6.3.1 Schema of the Condensation Process . . . 62
6.3.2 Set of Equations . . . 62
6.3.3 Inclusion of Heterogeneous Condensation and Brownian Coagulation . . . 63
6.3.4 Calculation Results . . . 64
6.3.5 Effect of Non-Evaporated Droplets on the Process of Bulk Condensation . . . 65
6.3.6 Calculation of $n_d r_d$ and $n_d r_d^3 (g_{MgO})$ . . . 66
6.4 Ionisation of Condensation Aerosol . . . 67
6.4.1 Calculation of the Electron Concentration . . . 67
6.4.2 Inclusion of the Ionic Nucleation . . . 70
6.5 Conclusions . . . 71

7 Decay of Metastable States: Nucleation Initiated by Transitions of Already Formed Embryos
Victor B. Kurasov
St. Petersburg State University, Department Computational Physics, 198904 St. Petersburg, Petrodvoretz, Russia **73**
7.1 Introduction . . . 73
7.2 Qualitative Description . . . 73
7.3 Effective Source . . . 74
7.4 Secondary Nucleation . . . 75
7.5 Approximation for $S(x)$ . . . 76
7.6 Nucleation at Small and Intermediate D-Values . . . 77
7.7 Nucleation at Large D-Values . . . 78
7.8 Concluding Remarks . . . 79

8 Non-Steady Theory of Heat Effects at Droplet Diffusional Growth
Alexander P. Grinin, Gennady Yu. Gor, and Fedor M. Kuni
St. Petersburg State University, Institute of Physics, 198504 St. Petersburg, Petrodvorets, Ulyanovskaya st. 1, Russia **81**

8.1 Introduction 81
8.2 Non-steady Vapour Concentration Profile around the Droplet Growing in Diffusion Regime 82
8.3 Non-steady Temperature Profile around the Droplet Growing in Diffusion Regime 86
8.4 Approximation of High Density of the Liquid in the Droplet 88
8.5 Strong Display of Condensation Heat Release Effects 90
8.6 Weak Display of Condensation Heat Release Effects 92

9 Possible Mechanisms of Pattern Formation in Plasma Melting of Glasses: Coupling of Melting and Flow Processes, Oscillations, Rayleigh-Taylor and Convective Instabilities

Alexander L. Tseskis[1], *Naoum M. Kortsenstein*[2], *and Jürn W. P. Schmelzer*[3]

[1] *Am Weidenbusch 29, 51381 Leverkusen, Germany*

[2] *Krzhizhanovsky Power Engineering Institute, Leninskij Prospekt 19, 117927 Moscow, Russia*

[3] *Institute of Physics, University of Rostock, 18051 Rostock, Germany* 97

9.1 Introduction 97
9.2 Structure Formation in Coupled Melting and Flow 99
9.3 Structure Formation in Oscillating Fluids 99
9.4 The Rayleigh-Taylor Instability 100
9.4.1 Basic Mechanism 100
9.4.2 Rayleigh's Original Approach 102
9.4.3 Extensions of Rayleigh's Theory 103
9.4.4 Rayleigh-Taylor Instability and Waves on Fluid Surfaces 103
9.5 Diffusive Convection 105
9.6 Conclusions 108

10 Crystallization of Quartz Glasses

Victor K. Leko

OOO "Thermex", Srednij Prospekt 86, 199105 St. Petersburg, Russia 109

10.1 Introduction 109
10.2 Literature Review 112
10.3 Development of Experimental Techniques 122
10.4 Basic Phenomenological Features of Crystallization Processes 124
10.5 Influence of the Degree of Silica Reduction 128
10.6 Influence of Concentration of "Structural Water" 132
10.7 Influence of Fusion Penetration Degree of Quartz or Cristobalite Particles on Crystallization of Quartz Glasses 136
10.8 Influence of Surface Contamination on Crystallization Kinetics 139
10.9 Influence of the Composition of the Gaseous Medium on Crystallization of Quartz Glass . 141
10.9.1 Introductory Comments 141
10.9.2 On Crystallization in Dry Gas Media 141
10.9.3 Experiments on Crystallization in an Atmosphere Containing Water Vapor 143
10.9.4 Crystallization of Quartz Glasses in the Atmosphere of Gases in Equilibrium with the Melt 143
10.10 Influence of the Drawing Process on Crystallization of Tubes of Quartz Glasses 146
10.11 Discussion of the Results 151
10.11.1 Introductory Remarks 151
10.11.2 Influence of Surface Reactions on Crystallization 152
10.11.3 Relation between Crystallization Rate and Viscosity 155
10.12 Conclusions 162

11 Formation and Evolution of Bubbles in Silica Melts and Methods of Their Removal from the

Melt
Boris Z. Pevzner and Sergey V. Tarakanov
Laboratory of Glass Properties, St-Petersburg, Russia **167**
Part I: Experimental Data and Basic Mechanisms 167
11.1 Introduction 167
11.2 Sources of Bubbles in Silica Melt and in Silica Glass 168
11.2.1 Brief Information on the Technology of Silica Glass Production 168
11.2.2 Raw Materials as the Sources of Bubbles 169
11.2.3 The Furnace Atmosphere as a Source of Bubbles 171
11.2.4 Interaction of Heaters and Form-Shaping Equipment with the Melt as Source of Bubbles 172
11.2.5 Brief Report on the Concentrations of Impurities, Including Dissolved Gases, in Commercial Silica Glasses 173
11.2.6 Experimental Study of Formation and Evolution of Bubbles in Silica Melts 173
11.3 Physico-chemical Properties of Silica Melts Influencing the Formation and Evolution of Gas Bubbles 176
11.3.1 Surface Tension 176
11.3.2 Density 176
11.3.3 Viscosity 177
11.3.4 Solubility and Diffusion of Gases 178
11.4 Summary to Part I 186
Part II: Theoretical Consideration and Computer Simulation of the Process 187
11.5 Introduction to Part II 187
11.5.1 Main Stages of Fusion of Powdered Silica under Heating as well as the formation of the Bubble Structure 187
11.5.2 Selection of Parameters for the Temperature Dependence Equations that describe the Properties of the Silica Melt Affecting the Kinetics of the Process 188
11.6 Microrheological Model and Computer Simulation of the Process 189
11.6.1 The Microrheological Model of Sintering the Powder and Forming the Structure of a Porous Body 189
11.6.2 Influence of Some Technology Factors on Formation of Bubble Structure under Heating of Powdered Silica Glass: Computer Simulation of the Process 196
11.7 Summary to Part II 203
Part III: Mathematical Modeling and Computer Simulation of the Behavior of Gas-Filled Bubbles in Silica Melts 206
11.8 Introduction 206
11.9 Behavior of Isolated Bubbles 208
11.10 Behavior of Solitary Gas-Filled Bubbles under Mass Exchange with the Melt 209
11.11 Two-phase Approach to the Description of a Monodisperse Ensemble of Bubbles 211
11.12 Two-phase Approach to the Description of Polydisperse Ensembles of Bubbles 216
11.13 Diffusion of the Dissolved Gas in the Melt 219
11.14 Relative Motion of Bubbles in the Melt: Modification of the Mathematical Model 222
11.15 Flow of the Melt Governed by the Motion of the Bubbles: Complete System of Equations for Modeling of the Behavior of Gas-filled Bubble Ensembles in the Melt 226
11.16 Summary to Part III 229

12 Thermodynamics of Melting and the Formation of Glasses and Crystals
Hans-Jürgen Hoffmann
Technische Universität Berlin, Institute of Materials Science and Technology: Vitreous Materials, Englische Strasse 20, 10587 Berlin, Germany **235**

12.1 Introduction . . . 235
12.2 Analysis of the Enthalpy Functions of One-component Systems . . . 237
12.2.1 Theoretical Preliminaries . . . 237
12.2.2 Mono-atomic One-component Systems . . . 239
12.2.3 Multi-atomic One-component Systems . . . 242
12.3 Melting and the Glass Transformation . . . 242
12.4 Effects Occurring in the Glass Transformation Range . . . 244
12.5 What Makes Solids and Melts Expand? . . . 245
12.6 Modulus of Compression of the Chemical Elements . . . 250
12.7 Necessary Criteria for Glass Formation . . . 250
12.8 Possible Extension to Multi-component Systems . . . 253
12.9 Discussion . . . 254

13 Phase and Glass Forming Diagrams and Crystallization Behavior of the BaO - TiO_2 - B_2O_3 Stoichiometric Glass Ceramics

Rafael M. Hovhannisyan, Hovakim A. Alexanyan, Hovsep Shirinyan, Bella V. Grigoryan and Berta V. Petrosyan

Scientific-Production Enterprise of Material Science, 17 Charents street, 0025 Yerevan, Armenia 257
13.1 Introduction . . . 257
13.2 Experimental . . . 258
13.3 Results . . . 260
13.3.1 Glass Formation and Phase Diagrams . . . 260
13.3.2 Crystallization Behavior of Stoichiometric Compositions in the BaO-TiO_2-B_2O_3-system . . . 263
13.4 Discussion . . . 269
13.5 Conclusions . . . 270

14 Adiabatic Nucleation in Devitrifying and Non-Devitrifying Oxide Glasses

Erich Meyer and Vitorvani Soares

Instituto de Física da Universidade Federal do Rio de Janeiro, Bloco A - C.T., Cidade Universitária, 21945-970 Rio de Janeiro, Brazil 273
14.1 Introduction . . . 273
14.2 Basic Thermodynamics . . . 274
14.3 Nucleation . . . 275
14.4 Thermodynamics of the Nucleus . . . 276
14.5 Diffusion and Viscosity . . . 278
14.6 The Nucleation Frequency . . . 281
14.7 Comparison with Experimental Data . . . 281
14.8 Discussion and Conclusions . . . 282

15 Fluctuation Theory Applied to Water Vapor Nucleation

Norberto Helil Pasqua and Bernhard Joachim Mokross

Instituto de Física de São Carlos, Universidade de São Paulo, 13560-970, Caixa Postal 369, São Carlos-SP, Brazil 285
15.1 Introduction . . . 285
15.2 Nucleation Induced by Fluctuations: The Model . . . 286
15.3 Preliminary Results . . . 287
15.4 Conclusions and Application of Constant Pressure Ensemble to Fluctuation Theory . . . 288
15.5 Appendices . . . 289
15.5.1 Appendix A: Numerical Algorithm . . . 289

15.5.2 Appendix B: Experimental Procedure and Data Analysis 291

16 Glass as a Solid Non-equilibrium Phase under Negative Pressure

Leonid M. Landa, Scott Thomsen, and Richard Hulme

Guardian Industries Corporation, Science and Technology, 14511 Romine Road, Carleton, MI 48117, USA **295**

16.1 Introduction 295
16.2 Negative Pressure in a Glass-forming System 296
16.3 Excess Volume of Glass 296
16.4 Phase Transitions in the "Liquid → Glass" System 297
16.5 Absence of the Leap of Entropy in the Transition Point 299
16.6 Ehrenfest's Equation and Glass Transition of a Liquid 300
16.7 Sufficient Indicators of Negative Pressure 301
16.8 Conclusions 301

17 On the Interpretation of the Glass Transition in Terms of Fictive (Internal) Pressure and Fictive Temperature

Jürn W. P. Schmelzer [1] ***and Ivan Gutzow*** [2]

[1] ***Institut für Physik, Universität Rostock, 18051 Rostock, Germany***
[2] ***Rostislaw Kaischew Institute of Physical Chemistry, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*** **303**

17.1 Introduction 303
17.2 Basic Thermodynamic Equations 303
17.3 Thermodynamic Properties 305
17.4 Fictive (Internal) Pressure as the Structural Order Parameter 309
17.4.1 Definition and Consequences 309
17.4.2 Some Further Topics of Discussion 310
17.5 On Some Recent Attempts of Re-Introduction of Fictive Temperatures into the Thermodynamics of the Glassy State 313
17.6 Model-Independent Definition of Fictive (Internal) Pressure and Fictive Temperature . . . 315

18 Cluster Dynamics Simulation of Mixed Cu-Vacancy Clusters in Neutron-irradiated Fe-Cu Alloys

Alexander R. Gokhman [1] ***and Frank Bergner*** [2]

[1] ***South Ukraine Pedagogical University, Staroportofrankovskaya 26, 65020 Odessa, Ukraine***
[2] ***Forschungszentrum Dresden - Rossendorf, Postfach 510119, 01314 Dresden, Germany*** **319**

18.1 Introduction 319
18.2 Irradiation Conditions 320
18.3 Study of the Iron-Copper-Vacancy System in Neutron Irradiated Model Alloy B 320
18.4 Conclusion 325

19 Formation of Nano - Size Condensed States in Amorphous - Crystal Silicon Multi-Interface Structures

[1] ***V. P. Yefimov, A. S. Abyzov, A. N. Dovbnya, V. V. Slezov, A. V. Rybka, V. V. Zakutin, N. G. Reshetnyak, A. A. Blinkin, E. P. Bereznyak, V. S. Demin, V. P. Romasko,*** [2] ***Yu. E. Gordienko, S. V. Babychenko, and G. N. Bendeberya***

[1] ***National Science Centre, Kharkov Institute of Physics and Technology, Akademicheskaya 1, Kharkov, 61108, Ukraine***
[2] ***Kharkov National University of Radioelectronics, Lenin Avenue 14, Kharkov, 61166, Ukraine*** **327**

19.1 Introduction 327

19.2 Model of Lateral Amorphous-Crystal Structures in the (c-Si)-Semiconductor of p-Type . . 330
19.3 Influence of Dimensional Effects on the Optical and Electric Properties of the Interface Structures . . . 331
19.4 Irradiation Technique . . . 333
19.5 Investigation of Electric Parameters at the Surface of the Samples . . . 336
19.6 IR-absorption Spectra . . . 341
19.7 Conclusions . . . 341

20 Nonlinear Fast Relaxation of Coexisting Short and Lengthy Micelles
Mikhail S. Kshevetskiy and Alexander K. Shchekin
Department of Statistical Physics, St. Petersburg State University, Ulyanovskaya st. 1, Petrodvorets, 198 504 St. Petersburg, Russia **343**
20.1 Introduction . . . 343
20.2 Kinetic Equation of Micellization and Quasi-equilibrium Distributions . . . 344
20.3 Moment Equations for Short Micelles . . . 345
20.4 Moment Equations for Lengthy Micelles . . . 348
20.5 Solution of the Moment Equations for the Short Micelles . . . 350
20.6 Solution of the Moment Equations for the Lengthy Micelles . . . 351
20.7 Solution of the Moment Equations for Coexisting Short and Lengthy Micelles . . . 353
20.8 Conclusions . . . 354

21 Deliquescence and Efflorescence Barriers in Heterogeneous Nucleation in Undersaturated Vapor
Alexander K. Shchekin and Ilya V. Shabaev
Department of Statistical Physics, St. Petersburg State University, Ulyanovskaya st. 1, Petrodvorets, 198 504 St. Petersburg, Russia **357**
21.1 Introduction . . . 357
21.2 Two-dimensional Surface of the Work of Droplet Formation . . . 358
21.3 Well and Saddle Points of the Work of Droplet Formation at Partial Dissolution of the Nucleus 360
21.4 Stable and Unstable Variables of the Droplet State . . . 365

22 On Bose-Einstein Condensation in a Weakly Interacting Bose Gas
Alexander L. Tseskis
Am Weidenbusch 29, 51381 Leverkusen, Germany **369**
22.1 Introduction . . . 369
22.2 Critical Temperature and LEH at $D = 3$ . . . 370
22.3 BEC in a Non-ideal Weakly Interacting Bose Gas . . . 372
22.4 Conclusions . . . 376

23 On the Effect of Elastic Stresses on Crystallization Processes in Finite Domains
***Alexander S. Abyzov*[(1)], *Jürn W. P. Schmelzer*[(2)], *and Vladimir M. Fokin*[(3)]**
[(1)] ***National Science Center, Kharkov Institute of Physics and Technology, Academician Street 1, 61108 Kharkov, Ukraine***
[(2)] ***Institut für Physik, Universität Rostock, 18051 Rostock, Germany***
[(3)] ***Vavilov State Optical Institute, Russian Academy of Sciences, ul. Babushkina 36-1, 193 171 St. Petersburg, Russia*** **379**
23.1 Introduction . . . 379
23.2 Systems with Spherical Geometry: Basic Equations . . . 380
23.3 Determination of the Constants C_1 and C_2 for Different Cases . . . 380
23.3.1 Deformation of a Sphere . . . 380

23.3.2 Deformation of a Hollow Sphere (Mantle) . . . 381
23.4 Crystal Formation in the Center of a Finite Spherical Domain . . . 382
23.4.1 Basic Balance Equation . . . 382
23.4.2 Phase Formation at Moderate (Zero) External Pressure . . . 383
23.4.3 Phase Formation at Constant Values of the External Radius . . . 385
23.4.4 Account of Viscous Properties of the Matrix . . . 385
23.5 Crystallization of the Mantle of a Finite Spherical Domain . . . 388
23.5.1 Phase Formation at Moderate (Zero) External Pressure . . . 388
23.5.2 Phase Formation at Constant Value of the External Radius . . . 389
23.5.3 Shell Formation at Constant Values of the External Radius . . . 391
23.5.4 Account of Viscous Properties of the Matrix . . . 396
23.6 Discussion . . . 396

24 Atmospheric New Particle Formation by Heterogeneous Nucleation Revisited: Comments on Phenomenology and Genesis

Olaf Hellmuth[1], Jürn W. P. Schmelzer[2], Alexander K. Shchekin[3], Alexander S. Abyzov[4]

[1] Leibniz Institute for Tropospheric Research, 04318 Leipzig, Germany

[2] University Rostock, Institute of Physics, 18051 Rostock, Germany and Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics, 141 980 Dubna, Russia

[3] St. Petersburg State University, Department of Statistical Physics, 198 504 St. Petersburg, Russia

[4] Kharkov Institute of Physics and Technology, 61 108 Kharkov, Ukraine **399**

24.1 Motivation . . . 400
24.1.1 Impact of Aerosols on Biospheric and Geospheric Processes . . . 400
24.1.2 Relevance of Aerosol–Cloud Interactions . . . 401
24.2 Origin and Impact of Pre-existing Particulate Matter in the Atmosphere . . . 403
24.2.1 Mineral Dust . . . 403
24.2.2 Meteoric Dust . . . 405
24.3 Questions of Interest with Respect to Sulphate–Mineral Dust Interactions . . . 406
24.3.1 Deficits and Requirements . . . 406
24.3.2 Relevance of Heterogeneous Nucleation . . . 407
24.4 Heterogeneous Nucleation of Water Vapour and Sulphuric Acid Vapour in the Atmosphere 407
24.4.1 Origin of Sulphuric Acid Vapour . . . 407
24.4.2 Applicability of Classical Nucleation Theory . . . 409
24.4.3 CHNT-Expression for the Heterogeneous Nucleation Rate . . . 410
24.4.4 Kinetic Prefactor in the Nucleation Rate Expression . . . 411
24.4.5 Thermodynamic Part . . . 423
24.4.6 Hydrate Formation . . . 433
24.5 Example: Results of Nucleation Rate Calculations . . . 441
24.6 Conclusions . . . 446
24.7 Appendix: Thermodynamic Bulk Properties . . . 448
24.7.1 Saturation Vapour Pressure over a Flat Surface of the Pure Substance . . . 448
24.7.2 Liquid Phase Activity Coefficients . . . 448
24.7.3 Bulk Surface Tension . . . 448
24.7.4 Bulk Mass Density . . . 449

25 Appendices **455**
25.1 Programs of the Research Workshops 2006, 2007 and 2008 . . . 456
25.1.1 Research Workshop 2006 . . . 456
25.1.2 Research Workshop 2007 . . . 458
25.1.3 Research Workshop 2008 . . . 462

25.2 Content of the Proceedings *Nucleation Theory and Applications* 1997-99, 2000-02, and 2003-05 and of the Monograph *Nucleation Theory and Applications* with Overview Lectures Published by WILEY-VCH in 2005 465
25.3 Monographs Published or Accepted by WILEY-VCH for Publication Prepared by Participants of the Workshops 469
25.4 List of Participants 469