

# Integral Materials Modeling

Towards Physics-Based Through-Process Models

*Edited by*  
*Günter Gottstein*



WILEY-VCH Verlag GmbH & Co. KGaA



**Integral Materials Modeling**

*Edited by*

*Günter Gottstein*

## 1807–2007 Knowledge for Generations

Each generation has its unique needs and aspirations. When Charles Wiley first opened his small printing shop in lower Manhattan in 1807, it was a generation of boundless potential searching for an identity. And we were there, helping to define a new American literary tradition. Over half a century later, in the midst of the Second Industrial Revolution, it was a generation focused on building the future. Once again, we were there, supplying the critical scientific, technical, and engineering knowledge that helped frame the world. Throughout the 20th Century, and into the new millennium, nations began to reach out beyond their own borders and a new international community was born. Wiley was there, expanding its operations around the world to enable a global exchange of ideas, opinions, and know-how.

For 200 years, Wiley has been an integral part of each generation's journey, enabling the flow of information and understanding necessary to meet their needs and fulfill their aspirations. Today, bold new technologies are changing the way we live and learn. Wiley will be there, providing you the must-have knowledge you need to imagine new worlds, new possibilities, and new opportunities.

Generations come and go, but you can always count on Wiley to provide you the knowledge you need, when and where you need it!



*William J. Pesce*  
President and Chief Executive Officer



*Peter Booth Wiley*  
Chairman of the Board

# Integral Materials Modeling

Towards Physics-Based Through-Process Models

*Edited by*  
*Günter Gottstein*



WILEY-VCH Verlag GmbH & Co. KGaA

#### The Editor

**Prof. Dr. Günter Gottstein**

Institut für Metallkunde und  
Metallphysik der RWTH Aachen  
Kopernikusstrasse 14  
52074 Aachen  
Germany

■ All books published by Wiley-VCH are carefully produced. Nevertheless, authors, editors, and publisher do not warrant the information contained in these books, including this book, to be free of errors. Readers are advised to keep in mind that statements, data, illustrations, procedural details or other items may inadvertently be inaccurate.

#### Library of Congress Card No.: applied for British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library

#### Bibliographic information published by the Deutsche Nationalbibliothek

Die Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at <http://dnb.d-nb.de>

© 2007 WILEY-VCH Verlag GmbH & Co.  
KGaA, Weinheim

All rights reserved (including those of translation into other languages). No part of this book may be reproduced in any form – by photoprinting, microfilm, or any other means – nor transmitted or translated into a machine language without written permission from the publishers. Registered names, trademarks, etc. used in this book, even when not specifically marked as such, are not to be considered unprotected by law.

Printed in the Federal Republic of Germany  
Printed on acid-free paper

**Typesetting** Asco Typesetters, Hong Kong  
**Printing** betz-druck GmbH, Darmstadt  
**Bookbinding** Litges & Dopf Buchbinderei GmbH, Heppenheim  
**Wiley Bicentennial Logo** Richard J. Pacifico

ISBN 978-3-527-31711-0

## Contents

	<b>List of Contributors</b>	XV
<b>1</b>	<b>Introduction</b>	<b>1</b>
	<i>G. Gottstein</i>	
<b>2</b>	<b>Integral Materials Modeling</b>	<b>5</b>
	<i>G. Gottstein</i>	
	Abstract	5
2.1	Introduction	5
2.2	The Collaborative Research Center on “Integral Materials Modeling”	9
2.3	Through-Process Modeling	12
2.4	Outlook	13
	<i>References</i>	15
<b>3</b>	<b>Aluminum Through-Process Modeling: From Casting to Cup Drawing (TP C6)</b>	<b>17</b>
	<i>L. Neumann, R. Kopp, G. Hirt, E. Jannot, G. Gottstein, B. Hallstedt, J. M. Schneider, B. Pustal, and A. Bührig-Polaczek</i>	
	Abstract	17
3.1	Introduction	17
3.2	Casting and Solidification	18
3.2.1	The Casting Alloys	18
3.2.1.1	Casting	18
3.2.2	Simulation of the Casting Process	19
3.2.2.1	Thermodynamic Description of the Model Alloy	19
3.2.2.2	Simulation of Grain Nucleation and Growth Using a Multiphase Flow and Solidification Model	20
3.2.2.3	Simulation of Phase Fractions, Dendrite Arm Spacing, and Concentration Profiles Using a Microsegregation Model	21
3.3	Homogenization	23
3.3.1	Homogenization of Alloy AA3104	23
3.3.2	Simulation Methods	25

3.3.2.1	DICTRA Calculations	25
3.3.2.2	ClaNG Model	26
3.3.3	Experimental Procedure	26
3.3.4	Comparison between Experimental and Simulation Results	26
3.3.4.1	Primary Phases	26
3.3.4.2	Solute Concentrations	26
3.3.4.3	Dispersoid Precipitation	27
3.4	Hot and Cold Rolling	28
3.4.1	Flow Stress Modeling	28
3.4.2	Texture Simulation	28
3.4.3	Recrystallization	28
3.5	Cup Drawing	29
3.5.1	Anisotropy Update	29
3.5.2	Results	30
3.6	Conclusions and Outlook	31
	<i>References</i>	32

#### **4 From Casting to Product Properties: Modeling the Process Chain of Steels (TP C7)** 33

*U. Prah, W. Bleck, A.-P. Hollands, D. Senk, X. Li, G. Hirt, R. Kopp, V. Pavlyk, and U. Dilthey*

	Abstract	33
4.1	Introduction	33
4.2	Continuous Casting Simulation	35
4.3	Hot Rolling Simulation	36
4.4	Simulation of Phase Transformation	38
4.4.1	Physical Modeling of Isothermal Proeutectoid Ferrite Transformation	38
4.4.2	Semiempirical Modeling of Phase Transformation	39
4.5	Simulation of Mechanical Properties	40
4.6	Welding Simulation	42
4.7	Application	44
4.8	Summary	46
	<i>References</i>	47

#### **5 Status of Through-Process Simulation for Coated Gas Turbine Components (TP C8)** 49

*R. Herzog, N. Warnken, I. Steinbach, B. Hallstedt, C. Walter, J. Müller, D. Hajas, E. Münstermann, J.M. Schneider, R. Nickel, D. Parkot, K. Bobzin, E. Lugscheider, P. Bednarz, O. Trunova, and L. Singheiser*

	Abstract	49
5.1	Introduction	49
5.2	Solidification and Heat Treatment of the Nickel-Based Superalloy	51
5.3	CVD Processing of an Alumina Interdiffusion Barrier	54



5.4	Magnetron Sputter Process of NiCoCrAlY Corrosion-Protective Coating	55
5.5	Atmospheric Plasma Spraying of Ceramic TBC	56
5.6	Stress Response and Crack Formation at the Bond Coat/TBC Interface During Cyclic Thermal Loading	57
5.7	Conclusions	60
	<i>References</i>	60
<b>6</b>	<b>Deformation Behavior of a Plastic Pipe Fitting (TP C9)</b>	<b>63</b>
	<i>W. Michaeli, E. Schmachtenberg, M. Brinkmann, M. Bussmann, and B. Renner</i>	
	Abstract	63
6.1	Introduction	63
6.2	Aims and Procedure	64
6.3	Calculation of Local Inner Part Properties Using Extended Process Simulation	65
6.3.1	Developed Software	65
6.3.2	Temperature Field Calculation	66
6.3.3	Calculation of Inner Properties	67
6.3.4	Procedure of Simulating Inner Properties	69
6.4	Integration of Inner Properties into Structural Analysis	70
6.5	Conclusions and Perspectives	72
	<i>References</i>	72
<b>7</b>	<b>Modeling of Flow Processes During Solidification (TP A1)</b>	<b>75</b>
	<i>M. Bussmann, B. Renner, W. Michaeli, B. Pustal, A. Bührig-Polaczek, V. Pavlyk, O. Mokrov, and U. Dilthey</i>	
	Abstract	75
7.1	Introduction	75
7.1.1	Aluminum Cup	76
7.1.2	Plastics Pipe Fitting	77
7.1.3	Steel Profile	77
7.2	Software Development	78
7.2.1	Aluminum Cup	78
7.2.2	Plastics Pipe Fitting	79
7.2.3	Steel Profile	80
7.3	Experiments and Results	80
7.3.1	Aluminum Cup	80
7.3.2	Plastics Pipe Fitting	81
7.3.3	Steel Profile	82
7.4	Discussion	83
7.4.1	Aluminum Cup	83
7.4.2	Plastics Pipe Fitting	83
7.4.3	Steel Profile	84
	<i>References</i>	85

**8 Microstructure Modeling During Solidification of Castings (TP A2) 87**

*B. Pustal, A. Bührig-Polaczek, N. Warnken, I. Steinbach, M. Bussmann,  
B. Renner, W. Michaeli, A.-P. Hollands, D. Senk, C. Walter,  
B. Hallstedt, and J. M. Schneider*

	Abstract	87
8.1	Introduction	87
8.2	Experiments	88
8.2.1	Turbine Blade	88
8.2.2	Aluminum Cup	89
8.2.3	Plastics Pipe Fitting	90
8.2.4	Steel Profile	91
8.3	Models	92
8.3.1	Turbine Blade	92
8.3.2	Aluminum Cup	92
8.3.3	Plastics Pipe Fitting	92
8.3.4	Steel Profile	93
8.4	Simulations and Results	94
8.4.1	Turbine Blade	94
8.4.2	Aluminum Cup	95
8.4.3	Plastics Pipe Fitting	96
8.4.4	Steel Profile	97
8.5	Summary	98
8.5.1	Turbine Blade	98
8.5.2	Aluminum Cup	99
8.5.3	Plastics Pipe Fitting	99
8.5.4	Steel Profile	99
	<i>References</i>	100

**9 Coating of Turbine Blades (TP A3) 103**

*B. Hallstedt, J. Müller, D. Hajas, E. Münstermann, J.M. Schneider,  
R. Nickel, D. Parkot, K. Bobzin, and E. Lugscheider*

	Abstract	103
9.1	Introduction	103
9.2	Modeling and Simulation of Al <sub>2</sub> O <sub>3</sub> Chemical Vapor Deposition	103
9.3	Modeling and Simulation of the Magnetron Sputter Process	107
9.4	Modeling and Simulation of Atmospheric Plasma Spraying and Thermal Barrier Coating Characterization	110
9.4.1	Plasma Torch/Plasma Free Jet Simulation	110
9.4.2	Powder Particles Characteristics	112
9.4.3	Coating Formation Simulation	113
9.4.4	APS Coating Properties/Homogenization Methods	119
	<i>References</i>	122

<b>10</b>	<b>Hot and Cold Rolling of Aluminum Sheet (TP B1)</b>	<b>125</b>
	<i>L. Neumann, R. Kopp, G. Hirt, M. Crumbach, C. Schäfer, V. Mohles, and G. Gottstein</i>	
	Abstract	125
10.1	Introduction	125
10.2	Hot and Cold Rolling of Aluminum	126
10.2.1	Three-Internal-Variable Model (3IVM)	126
10.2.2	Full Constraints Taylor Texture Model	127
10.2.3	Grain Interaction Texture (GIA) Model	128
10.2.4	Recrystallization Nucleation (ReNuc)	128
10.2.5	Statistical Recrystallization Texture Model (StART)	129
10.2.6	Coupling GIA and 3IVM	129
10.2.7	Through-Process Model (TPM)	129
10.2.8	Texture Predictions	130
10.2.9	Hot Rolling	131
10.2.10	Cold Rolling	131
10.3	Database “StoRaDat” and Interfaces	133
10.4	Conclusions and Outlook	136
	<i>References</i>	136
<b>11</b>	<b>Modeling of the Hot Rolling Process of a C45 Steel (TP B1)</b>	<b>139</b>
	<i>X. Li, R. Kopp, G. Hirt, B. Zeislmair, and W. Bleck</i>	
	Abstract	139
11.1	Introduction	139
11.2	Experimental Procedure	140
11.2.1	Casting and Rolling in One Heat	140
11.2.2	Determination of Flow Curves	141
11.3	Modeling of the Hot Rolling Process	142
11.3.1	Phenomenological Modeling of the Grain Size Development During Hot Rolling	142
11.3.2	Modeling Precipitation During Hot Rolling	143
11.3.3	Microstructure Simulation of the Hot Rolling Process	144
11.4	Summary	147
	<i>References</i>	148
<b>12</b>	<b>Simulation of Phase Changes During Thermal Treatments of Various Metal Alloys (TP B2)</b>	<b>149</b>
	<i>M. Schneider, E. Jannot, V. Mohles, G. Gottstein, C. Walter, B. Hallstedt, J. M. Schneider, N. Warnken, I. Steinbach, F. Gerdemann, U. Prahl, and W. Bleck</i>	
	Abstract	149
12.1	Introduction	149

12.2	Aluminum Sheet AA3104: Precipitation Kinetics and Solute Distribution During Homogenization	150
12.2.1	Challenge	150
12.2.2	DICTRA Calculations	151
12.2.3	Statistical Precipitation Model: ClaNG	151
12.2.4	Evolution of the Primary Phases	152
12.2.5	Precipitation of Dispersoids	153
12.2.6	Conclusion on Al Sheet AA3104	153
12.3	Turbine Blades: Ni-Base Superalloys	154
12.3.1	Challenge	154
12.3.2	Simulation Models and Experiments	154
12.3.3	Results	155
12.4	C45 and S460 Steel: Isothermal Phase Transformation and Austenite Conditioning	157
12.4.1	Challenge	157
12.4.2	Simulation Models and Experiments	157
12.4.3	Results	158
	<i>References</i>	159
<b>13</b>	<b>Deep Drawing Properties of Aluminum Sheet (TP C6)</b>	<b>161</b>
	<i>L. Neumann, R. Kopp, G. Hirt, M. Crumbach, and G. Gottstein</i>	
	Abstract	161
13.1	Introduction	161
13.2	Modeling Setup for Prediction of Texture-Induced Anisotropy	162
13.2.1	Interfacing Texture to Plastic Anisotropy	162
13.2.2	Orthotropic Viscous Flow Approach	163
13.2.3	Update of the Yield Locus	164
13.3	Results and Discussion	165
13.4	Conclusions and Outlook	167
	<i>References</i>	167
<b>14</b>	<b>Simulation of Stress Response to Cyclic Thermal Loading in Thermal Barrier Composites for Gas Turbines (TP C8)</b>	<b>169</b>
	<i>R. Herzog, P. Bednarz, E. Trunova, and L. Singheiser</i>	
	Abstract	169
14.1	Introduction	169
14.2	Experimental	170
14.3	Finite Element Simulation	172
14.3.1	Mesh and Boundary Conditions	172
14.3.2	Material Data and Bond Coat Oxidation	172
14.3.3	Load Parameters	173
14.3.4	Simulated Stress Response	174
14.4	Conclusions	178
	<i>References</i>	179

<b>15</b>	<b>Through-Process Multiscale Models for the Prediction of Recrystallization Textures</b>	<b>181</b>
	<i>D. Raabe</i>	
	Abstract	181
15.1	Introduction to Recrystallization Models for Process Simulation	181
15.2	Models for Predicting Recrystallization Textures with Discretization of Space and Time	183
15.2.1	Introduction	183
15.2.2	Cellular Automaton Models of Recrystallization	183
15.2.3	Potts Monte Carlo Models of Recrystallization	189
15.3	Statistical Models for Predicting Recrystallization Textures	191
15.3.1	The Sebald–Gottstein Model	191
15.3.2	A New Texture Component-Based Avrami Model	192
15.4	Input to Recrystallization Models for Texture Prediction	194
15.4.1	Incorporation of Stored Deformation Energy into Recrystallization Models	194
15.4.2	Grain Boundary Input Parameters into Recrystallization Models for Texture Prediction	195
	<i>References</i>	195
<b>16</b>	<b>Analytic Interatomic Potentials for Atomic-Scale Simulations of Metals and Metal Compounds: A Brief Overview</b>	<b>197</b>
	<i>K. Albe, P. Erhart, and M. Müller</i>	
	Abstract	197
16.1	Introduction	197
16.2	Overview of Established Potential Schemes	198
16.3	Analytic Bond-Order Potentials (BOP)	202
16.4	Concluding Remarks	204
	<i>References</i>	205
<b>17</b>	<b>Selected Problems of Phase-Field Modeling in Materials Science</b>	<b>207</b>
	<i>H. Emmerich and R. Siquieri</i>	
	Abstract	207
17.1	Introduction to Phase-Field Modeling in Materials Science	207
17.2	Overview on Recent Issues in the Further Development of Phase-Field Modeling	209
17.2.1	Evolution of Nanostructures in Condensed Matter Systems	210
17.2.2	Dynamics in Soft-Matter Systems at the Micro- and Nanoscale	210
17.3	“Quantitative Phase-Field Simulations” of Nucleation and Growth in Peritectic Material Systems	211
17.3.1	A Quantitative Phase-Field Model for Peritectic Growth Taking Into Account Hydrodynamic Convection in the Molten Phase	213

17.3.2	Investigating Heterogeneous Nucleation in Peritectic Materials via the Phase-Field Method	215
17.4	Conclusions and Outlook	217
	<i>References</i>	217
<b>18</b>	<b>Prediction of Microstructure and Microporosity Development in Aluminum Gravity Casting Processes</b>	<b>219</b>
	<i>M. Schneider, W. Schaefer, G. Mazourkevitch, M. Wessén, I.L. Svensson, S. Seifeddine, J. Olsson, C. Beckermann, and K. Carlson</i>	
	Abstract	219
18.1	Introduction	219
18.2	Microstructure Modeling	220
18.3	Microporosity Modeling	222
18.4	Results and Discussion	225
18.4.1	Microstructure and Properties	225
18.4.2	Microporosity	228
18.5	Conclusions	230
	<i>References</i>	231
<b>19</b>	<b>Enhanced 3D Injection Molding Simulation by Implementing Applied Crystallization Models</b>	<b>233</b>
	<i>M. Thornagel</i>	
	Abstract	233
19.1	Introduction	233
19.2	Current Situation and Motivation	234
19.3	Implementation of Crystallization Models Into 3D-SIGMA	236
19.4	Crystallization Results: Parameter Study	238
19.5	Conclusions	242
	<i>References</i>	242
<b>20</b>	<b>Modeling Shearing of <math>\gamma'</math> in Ni-Based Superalloys</b>	<b>243</b>
	<i>C. Shen, J. Li, M.J. Mills, and Y. Wang</i>	
	Abstract	243
20.1	Introduction	243
20.2	Method	244
20.2.1	Dislocation and Stacking Fault Modeling	244
20.2.2	Calculation of Activation Energy	245
20.3	Results	246
20.3.1	Nucleation of SISF from APB	246
20.3.2	Nucleation of SESF from CSF	249
20.4	Summary	251
	<i>References</i>	251

<b>21</b>	<b>Minimal Free Energy Density of Annealed Polycrystals</b>	<b>253</b>
	<i>M. E. Glicksman and P. R. Rios</i>	
	Abstract	253
21.1	Introduction	253
21.2	Construction and Properties of ANHs	255
21.3	Assessing Network Partitioning: Isoperimetric Quotient and Dimensionless Energy Cost	258
21.4	Conclusions	262
	<i>References</i>	263
<b>22</b>	<b>Modeling Dynamic Grain Growth and its Consequences</b>	<b>265</b>
	<i>P. S. Bate</i>	
	Abstract	265
22.1	Introduction	265
22.2	Mechanical Behavior in Superplasticity	266
22.3	Dynamic Grain Growth	268
22.4	Microstructural Modeling of Dynamic Grain Growth	270
22.5	Conclusion	272
	<i>References</i>	274
<b>23</b>	<b>Modeling of Severe Plastic Deformation: Evolution of Microstructure, Texture, and Strength</b>	<b>275</b>
	<i>Y. Estrin</i>	
	Abstract	275
23.1	Introduction	275
23.2	Fundamentals of the Model	276
23.3	Application of the Model to the ECAP Process	279
23.4	Conclusion	283
	<i>References</i>	283
	<b>Subject Index</b>	<b>285</b>





## List of Contributors

**G. Gottstein, E. Jannot, C. Schäfer,  
V. Mohles, M. Schneider**

Institut für Metallkunde und  
Metallphysik  
Rheinisch-Westfälische  
Technische Hochschule Aachen  
52056 Aachen  
Germany

**A. Bührig-Polaczek, B. Pustal**

Gießerei-Institut  
RWTH Aachen  
52056 Aachen  
Germany

**W. Michaeli, E. Schmachtenberg,  
M. Brinkmann, M. Bussmann,  
B. Renner**

Institut für Kunststoffverarbeitung  
Rheinisch-Westfälische  
Technische Hochschule Aachen  
52056 Aachen  
Germany

**J. M. Schneider, B. Hallstedt, C.  
Walter, J. Müller, D. Hajas,  
E. Münstermann**

Institut für Werkstoffchemie  
Rheinisch-Westfälische  
Technische Hochschule Aachen  
52056 Aachen  
Germany

**G. Hirt, L. Neumann, R. Kopp, X. Li**

Institut für Bildsame Formgebung  
Rheinisch-Westfälische Technische  
Hochschule Aachen  
52056 Aachen  
Germany

**W. Bleck, U. Prah, A.-P. Hollands,  
D. Senk, B. Zeislmaier, F. Gerdemann**

Institut für Eisenhüttenkunde  
Rheinisch-Westfälische Technische  
Hochschule Aachen  
52056 Aachen  
Germany

**V. Pavlyk, U. Dilthey, O. Mokrov**

Institut für Schweißtechnik und  
Fügetechnik  
Rheinisch-Westfälische Technische  
Hochschule Aachen  
52062 Aachen  
Germany

**W. Bleck**

Institut für Eisenhüttenkunde  
Rheinisch-Westfälische Technische  
Hochschule Aachen  
52056 Aachen  
Germany

**H. Emmerich, R. Siquieri**

Institut für Gesteinshüttenkunde  
Lehr- und Forschungsgebiet  
Modellbildung in der  
Werkstofftechnik  
Rheinisch-Westfälische  
Technische Hochschule Aachen  
52064 Aachen  
Germany

**R. Nickel, D. Parkot, K. Bobzin,  
E. Lugscheider**

Institut für Oberflächentechnik  
Rheinisch-Westfälische  
Technische Hochschule Aachen  
52062 Aachen  
Germany

**L. Singheiser, R. Herzog,  
P. Bednarz, O. Trunova**

Institut für Werkstoffe und  
Verfahren der Energietechnik 2  
Forschungszentrum Jülich GmbH  
Leo-Brandt-Strasse  
52428 Jülich  
Germany

**K. Albe, P. Erhart, M. Müller**

Institut für Materialwissenschaft  
Technische Universität Darmstadt  
Petersenstrasse 23  
64287 Darmstadt  
Germany

**P. S. Bate**

School of Materials  
University of Manchester  
Grosvenor Street  
Manchester M1 7HS  
United Kingdom

**Y. Estrin**

Institut für Werkstoffkunde und  
Werkstofftechnik  
Technische Universität Clausthal  
Agricolastrasse 6  
38678 Clausthal-Zellerfeld  
Germany

**M. E. Glicksman**

Materials Science & Engineering  
Department  
Rensselaer Polytechnic Institute  
Troy, NY 12180-3590  
USA

**D. Raabe**

Max-Planck-Institut für Eisenforschung  
Max-Planck-Strasse 1  
40237 Düsseldorf  
Germany

**M. Schneider, W. Schaefer,**

**G. Mazourkevitch**

MAGMA Gießereitechnologie GmbH  
Kackertstrasse 11  
52072 Aachen  
Germany

**Y. Wang, C. Shen, J. Li, M. J. Mills**

Department of Materials Science and  
Engineering  
Ohio State University  
2041 College Road  
Columbus, Ohio 43210  
USA

**M. Thornagel**

SIGMA Engineering GmbH  
Kackertstrasse 11  
52072 Aachen  
Germany

***I. Steinbach, N. Warnken***

ACCESS e. V.  
Intzestrassse 5  
52072 Aachen  
Germany

***M. Crumbach***

Novelis Technology AG  
Badische Bahnhofstrasse 16  
8212 Neuhausen  
Switzerland

***M. Wessen, I. L. Svensson,***

***S. Seifeddine, J. Olsson***

Division Component Technology  
Jököping University  
55111 Jönköping  
Sweden

***C. Beckermann, K. Carlson***

University of Iowa  
Department of Mechanical and  
Industrial Engineering  
Iowa City, IA 52242-1527  
USA

***P. R. Rios***

Universidade Federal Fluminense  
Escola de Engenharia Industrial  
Metalúrgica  
de Volta Redonda  
Avenida dos Trabalhadores, 420  
Volta Redonda, 27255-125  
Brazil



## 1

**Introduction**

This book comprises the proceedings of the final symposium of the Collaborative Research Center (SFB 370) of the Deutsche Forschungsgemeinschaft on “Integral Materials Modeling” which took place in Aachen, Germany, on December 1–2, 2005. It is composed of the final reports of the projects and complementary manuscripts of renowned scientists in the field of materials modeling, covering a broad range of current simulation activities.

The projects are identified by their project numbers in their title. The manuscripts are organized such that after a list of persons involved in the SFB 370 the final through-process modeling exercises (group C) are introduced by the reports on supporting process and materials models (groups A and B) and complemented by the invited contributions. The first article on “Integral Materials Modeling” gives an introduction into the philosophy, history, and structure of the collaborative research center.

With the final symposium the SFB officially ended but its core topic was continued in a transfer program of the Deutsche Forschungsgemeinschaft (TFB 63) on “Industrially Relevant Modeling Tools”.

As a chairman of the collaborative research center on “Integral Materials Modeling” (SFB 370) I would like to express my sincere gratitude to my colleagues for their continuous support and encouragement. As a university professor it was my great pleasure to see the interest and engagement of the young doctoral students in the research program, their fascination by the scientific challenge, and their natural openness to interdisciplinary cooperation, discussion, and information exchange. Last but not least my thanks go to the review panels for their valuable advice and the Deutsche Forschungsgemeinschaft which not only funded the collaborative research center for 12 years but also offered unbureaucratic support.

*Günter Gottstein*  
Chairman, SFB 370  
Aachen, December 2006



**Collaborative Research Center (SFB 370) of the Deutsche Forschungsgemeinschaft  
on “Integral Materials Modeling” (1994–2005)**

**Board**

Prof. Dr. G. Gottstein, IMM  
Prof. Dr.-Ing. U. Diltthey, ISF  
Prof. Dr.-Ing. R. Kopp, IBF  
Prof. Dr.-Ing. G. Hirt, IBF

**Members**

Prof. Dr.-Ing. W. Bleck, IEHK	Prof. Dr.-Ing. D. Neuschütz, LTH
Prof. Dr.-Ing. K. Bobzin, IOT	Prof. Dr.-Ing. H. Nickel, FZ Jülich
Prof. Dr.-Ing. A. Bührig-Polaczek, GI	Dr. S. Rex, ACCESS
Prof. Dr.-Ing. W. Dahl, IEHK	Prof. Dr.-Ing. P.R. Sahm, GI
Prof. Dr.-Ing. E. El-Magd, IWK	Prof. Dr.-Ing. E. Schmachtenberg, IKV
Prof. Dr.-Ing. S. Engler, GI	Prof. Dr.-Ing. J. Schneider, MCh
Prof. Dr.-Ing. O. Knotek, IWK	Prof. Dr.-Ing. D.G. Senk, IEHK
Prof. Dr.-Ing. E. Lugscheider, LNWW	Prof. Dr.-Ing. L. Singheiser, FZ Jülich
Prof. Dr.-Ing. W. Michaeli, IWK	

**SFB-Managing Director at RWTH Aachen**

Dr. P. van den Brincken

**Guest Members**

Dr.-Ing. N. Aretz, Stuttgart  
Dr.-Ing. M. Keller, Duisburg  
Dr.-Ing. U. Lotter, Duisburg  
Dr. A. Ludwig, Leoben  
Dr.-Ing. L. Löchte, Bonn  
Prof. Dr. J. Vehoff, Saarbrücken

**Reviewers**

Prof. Dr.-Ing. D. Aurich, Berlin  
Prof. Dr.-Ing. H. Biermann, Freiberg  
Prof. Dr.-Ing. U. Draugelates, Clausthal  
Prof. Dr. J. Estrin, Clausthal  
Dr. F.J. Floßdorf, Düsseldorf  
Dr. A. Kamp, Dortmund  
Prof. Dr.-Ing. R. Kawalla, Freiberg  
Prof. Dr.-Ing. D. Munz, Karlsruhe  
Prof. Dr. P. Neumann, Düsseldorf

Dr. H. Pircher, Duisburg  
Prof. Dr.-Ing. H. Potente, Paderborn  
Dr. H. Riedel, Freiburg  
Prof. Dr. S. Schmauder, Stuttgart  
Prof. Dr.-Ing. R.F. Singer, Erlangen  
Prof. Dr.-Ing. H.D. Steffens, Dortmund  
Prof. Dr.-Ing. M. Wagner, Stuttgart  
Prof. Dr. E. Werner, München

**DFG-Correspondents (DFG-Senate Committee Members)**

Prof. Dr. H. Eschrig, Dresden  
Prof. Dr. W. Schulze, München  
Prof. Dr.-Ing. E. Ramm, Stuttgart  
Prof. Dr. H. Vahrenkamp, Freiburg  
Prof. Dr.-Ing. D. Löhe, Karlsruhe  
Prof. Dr. M. Reddehase, Mainz  
Prof. Dr. S. Müller, Leipzig

**DFG-Program Monitors**

Mr. T. Leppien  
Mrs. Dr. G. Retz-Schmidt  
Mrs. Dr. H. Hildebrandt  
Dr. J. Kunze

**DFG-Expert Advisors**

Dr.-Ing. J. Tobolski  
Dr.-Ing. F. Fischer  
Dr.-Ing. B. Jahnen





## 2

# Integral Materials Modeling

*G. Gottstein*

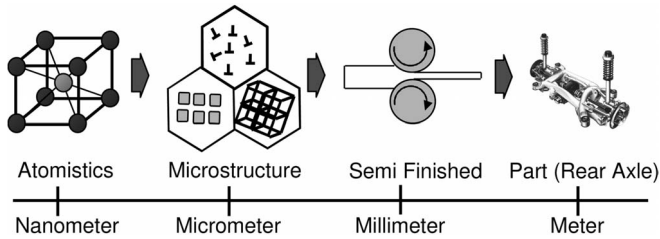
### Abstract

This chapter reviews the historical background of computational materials science and introduces the scientific concept of “integral materials modeling”. The objectives of the collaborative research center on this topic are formulated and an overview is given on the structure development and achievements of the research program.

### 2.1

#### Introduction

One of the ultimate dreams of materials science is the theoretical design of new materials. It would save tremendous costs that are currently invested in alloy development, e.g. for operating expensive pilot plants and conducting comprehensive materials testing, and in view of the fact that even today it takes more than 15 years before a new material eventually sees the market. That there is still need for research to develop new metallic materials although they have been successfully processed for more than 5000 years is not due to the large number of potential alloys that can be produced in multicomponent alloys out of 92 elements or even 70 elements with metallic character. On the contrary, if the properties of these alloys would only reflect the property mix of their components, it would be easy with current computer power to predict the properties of virtually any potential alloy system. However, the properties of a material do not reflect the properties of the constituent elements, rather the properties of a material are controlled by the spatial distribution of elements and crystal defects, which is also referred to as microstructure. The microstructure comprises phase distribution, elemental distribution, orientation distribution, as well as crystal defects like grain boundaries, dislocations, and point defects. What is more, the microstructure is seriously affected by materials processing. In essence, the properties of a material are not given by a superposition of elemental properties, but by a complex function of



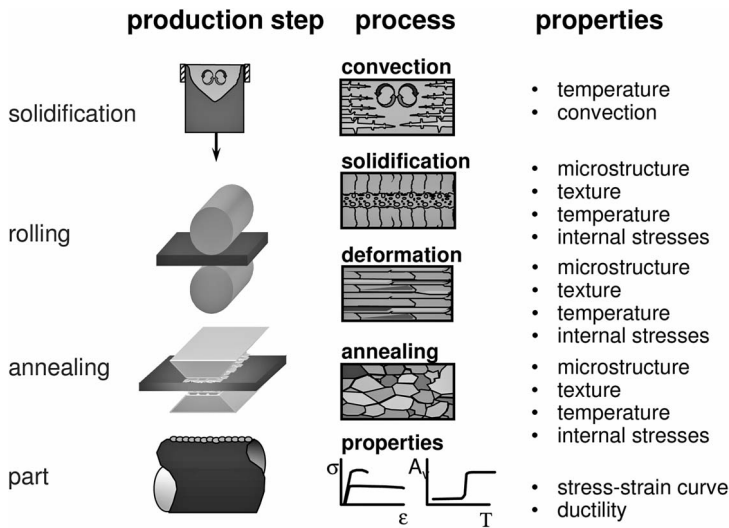
**Fig. 2.1** The scale problem of materials modeling: the macroscopic properties are defined by the microstructure which develops by atomic mechanisms.

its chemical composition and its processing history, and there is a virtually infinite number of possible microstructures and, therefore, of material properties. This is good news for alloy development since material properties can be changed by processing at constant chemistry in a wide range but it is a nightmare for materials modeling that aims at predicting material properties from the knowledge of materials chemistry and processing, and it appears hopeless to design computational strategies for optimization of materials chemistry and processing for a given desired property spectrum.

As a result, it is practically impossible to establish relations between materials properties and both processing parameters and the overall chemistry. This is because of the fact that the processing conditions are not the state variables of materials properties even though that would be desirable for the materials engineer who is used to formulate the properties of a product in terms of the engineering control parameters. Processing–property relationship may be most desirable for engineering practice, but unfortunately this approach cannot be successful. It is common in materials engineering to establish correlations between material properties and processing conditions. These correlations, however, are not equations of state for the material, and thus liable to fail when the chemistry or processing parameters are changed.

The only correct way to formulate equations of state for the terminal properties of a processed material is in terms of microstructure development during processing because the microstructure constitutes the state variable of the material. In fact, the microstructure is a fingerprint of the processing history of a material and determines the current properties of a material. That is why geologists hope to derive the history of rocks from today’s microstructure to understand the formation of the Earth’s crust. Consequently, the very problem of property predictions is to adequately quantify a microstructure and, in particular, to establish microstructure–property relationships. This requires an understanding of the controlling microstructural elements and the microscopic processes that determine a specific property.

An adequate characterization of the microstructure requires knowledge of the atomistic arrangement in a material. Therefore, a deeper physical understanding

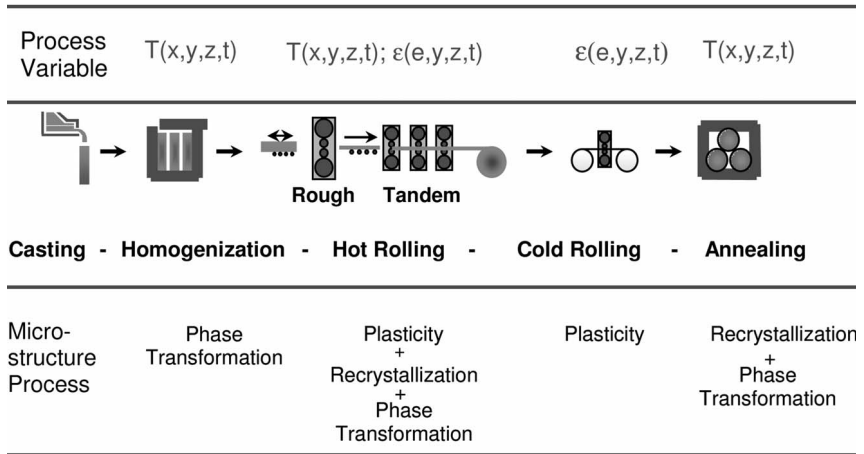


**Fig. 2.2** During conventional processing of a metallic material to the final product (here a welded tube) the microstructure changes during each processing step.

of material properties and phenomena could only be developed after the discovery of X-rays and their application to crystallography in the beginning of the 20th century. This engendered an understanding of material behavior on the basis of its atomistic arrangements and atomistic transport processes. Application of X-ray diffraction and spectroscopy complemented much later by electron and neutron diffraction and spectroscopy revealed the importance of nanoscale configurations, notably the crystal structure, crystal defects, and nanoscale chemistry, in terms of solute distribution and dispersion of second phases, for an interpretation of material properties. In fact, materials science in the 20th century was essentially dedicated to an understanding of microstructure evolution and a formulation of microstructure–property relationships.

From this research it became clear, however, that there are only a few although complex physical processes that impact the microstructure of a bulk metallic material. The mechanisms of these processes have been the subject of investigations for many years, and the outcome of this research constitutes the foundations and concepts of modern materials science.

In essence, there are three major processes that affect the microstructure of a material, namely phase transformations, plastic deformation, and restoration processes like recovery, recrystallization, and grain growth. These processes and their impact on microstructure are complex in detail and interdependent in a highly nonlinear fashion. Their thermodynamics, kinetics, and atomic mechanisms have been subject of numerous investigations over the past 50 years, which have substantiated that microstructural evolution is strongly related to the properties



**Fig. 2.3** For simulation of microstructure evolution the microstructure processes have to be interfaced to the process variables; here for sheet fabrication of an aluminum alloy.

and behavior of crystal defects: deformation of crystals proceeds by the generation, motion, interaction, and storage of dislocations; phase transformations are controlled by diffusion, the fundamental atomic transport mechanism; and recrystallization and grain growth involve the motion of grain boundaries.

These three microstructural processes affect each other, e.g. precipitation of a second phase hinders dislocation and grain boundary motion and, therefore, influences hardening during crystal plasticity and softening by recrystallization and grain growth. A major complication for the mathematical treatment of these processes is the local inhomogeneity that is introduced or even imposed by processing, e.g. fluctuation of composition, segregation of elements, deformation inhomogeneities, etc.

The theoretical foundations that govern the thermodynamics and kinetics of these processes have been developed during the past 50 years [1–4]. The respective equations of motion and equations of state for these processes are generally formulated in terms of partial differential equations. An analytical solution of these equations was in the vast majority of cases beyond reach, even impossible. Even 20 years ago such mathematical problems could be solved only by experts for very special cases. This situation changed dramatically with the advent of powerful computers, which could be utilized to solve numerically these difficult equations. With the increasingly powerful computers at hand to everybody nowadays, virtually every scientist can tackle these mathematical problems by utilizing sophisticated software. Moreover, the availability of high-performance computers has engendered novel computational techniques to address microstructural changes and thus the option to simulate microstructural evolution on the computer [5].

While the simulation of microstructure evolution constitutes a remarkable progress in computational materials science it does not yet solve the engineering problem to predict the properties of a material. Since the microstructure controls materials properties but is affected by each processing step, the prediction of terminal material properties or the behavior of a part under service conditions requires one to follow microstructural evolution along the entire processing chain, i.e. conventionally from the liquid state to the final product. To simulate this on the computer, it is necessary to connect the microstructural evolution to the processing parameters, which essentially means to subject each microstructural volume element to a temporal change of strain and temperature. In engineering applications this temperature and strain history of a material is typically computed by finite element (FE) approaches. On the other hand, the results of an FE simulation depend on the current properties of a material; hence microstructural evolution along the processing history and the local processing parameters, strain and temperature, are interdependent. In essence, both approaches, processing in terms of FE codes and microstructure in terms of physics-based microstructure evolution codes, have to be connected and interfaced in space and time. This means accounting for local and temporal changes of chemical composition, segregation, defect densities, etc., under changing boundary conditions. Therefore, it also requires advanced interface tools and sophisticated numerical techniques to solve the respective sets of mathematical equations and places a substantial demand on computing power.

## 2.2

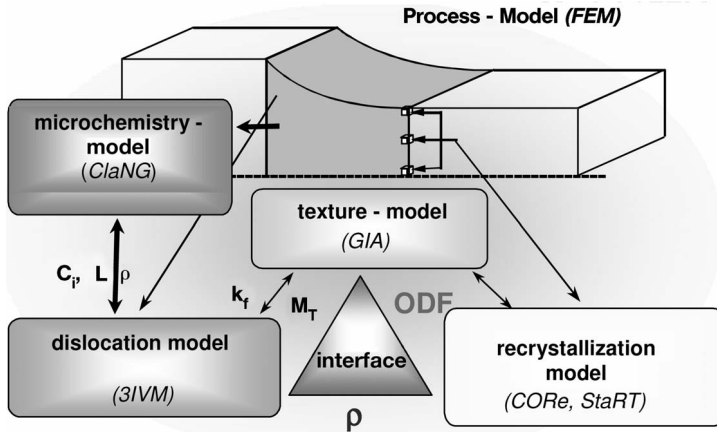
### The Collaborative Research Center on “Integral Materials Modeling”

In 1994 the collaborative research center on “Integral Materials Modeling” (SFB 370) of the Deutsche Forschungsgemeinschaft set out to tackle this problem and to develop strategies and techniques to predict terminal material properties from the knowledge of material chemistry and processing conditions. Since each processing step affects the microstructure, the microstructure evolution through the entire processing chain had to be traced to determine the final microstructure at the end of the processing chain in order to predict the properties associated with it. This though-process modeling approach on a physics-based microstructure definition was subject of research for a variety of materials and their processing. Two fundamental processing stages (A and B) were distinguished, which characterized virtually all materials fabrication procedures (Fig. 2.4):

- (A) Generation of the solid state from the liquid phase (solidification) or gas phase (condensation).
- (B) Processing of the solid by mechanical and thermal treatment.

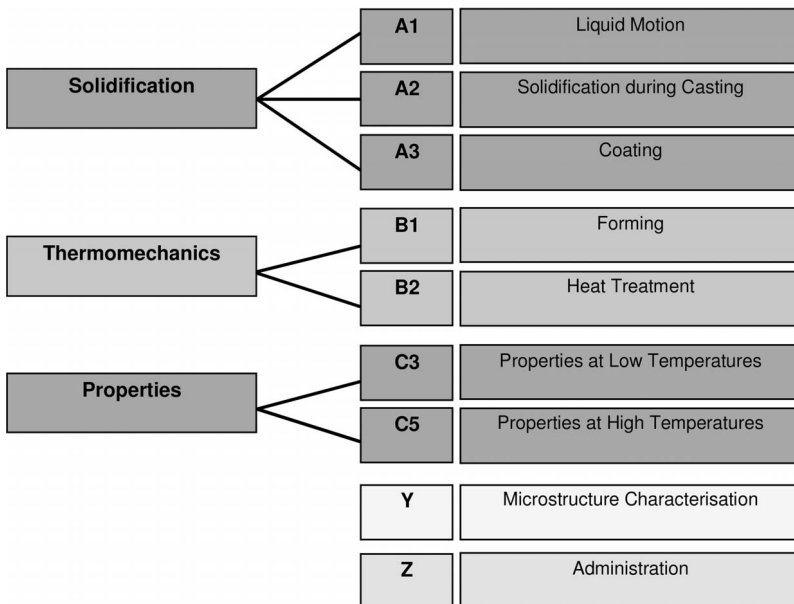
They determined the properties of the product which constituted stage C:

- (C) Determination of the specific properties of interest for a processed product.



**Fig. 2.4** Coupling of microstructure and processing by interfacing FEM and physics-based microstructure models. For each volume element the microstructural information has to be updated in every time step.

Depending on the specific product considered these processing stages can be connected in various ways (Fig. 2.5). For a net shape cast metallic part or an injection molded polymer, stage A directly connects to stage C. Stage A itself may be subdivided in to several steps, e.g. if a cast part is coated. A homogenization anneal



**Fig. 2.5** Topical structure of the collaborative research center (SFB 370) "Integral Materials Modeling" of the Deutsche Forschungsgemeinschaft.