Foreword


Many of the sections in this Volume will be familiar to ASM Handbook users, as they have been covered extensively across the ASM Handbook series: phase diagrams, casting and solidification, forming, machining, powder metallurgy, joining, heat treatment, and design. This Volume interprets these subjects in the interdisciplinary context of modeling, simulation, and computational engineering.

The high cost of capital investment in manufacturing can be mitigated by modeling and simulating the options. The effects of processing on materials can be tested and understood through modeling. This Volume and its companion, Volume 22A, provide materials engineers and scientists with the information they need to understand the potential and advantages of modeling and simulation and to provide them with the tools they need to work with the modeling experts.

When the first ASM Handbook was published in 1923 by ASM International’s predecessor, the American Society for Steel Treaters, the computational tools of choice were a slide rule, paper, pencil, and data tables—all conveniently sized to slip into a lab coat pocket. Today, computational tools are almost entirely software based, although some handheld electronics are also conveniently sized to slip into a lab coat pocket. Many of the basic concerns between then and now are the same: how to control properties during processing, how to minimize waste, how to maintain quality, and so on. Additional contemporary concerns include automated manufacturing, new alloys, new applications such as aerospace and medical devices, environmental responsibility, tracking, and so on.

ASM International is indebted to co-editors David Furrer and S. Lee Semiatin for their vision and leadership in bringing Volumes 22A and 22B to completion. The many authors and reviewers who worked on these Volumes shared that vision. Unlike the subjects about which they wrote, a technical article cannot be modeled or simulated; it must take tangible form as text and images, and this Volume is the direct result of the contributors’ generosity in sharing their time and expertise.

That first ASM Handbook was published as a loose-leaf collection of data sheets assembled in a leather-bound binder. Today’s ASM Handbooks are available online, in hardcover, or as DVDs. Times have changed, and ASM International continues to provide the quality information that materials science professionals need to chart the course of the future for their industries.

Frederick J. Lisy
President
ASM International

Stanley C. Theobald
Managing Director
ASM International
Preface

Computer-aided engineering and design have substantially changed the way new products are developed and defined. The pencil and drafting table have long since been replaced by the mouse and computer monitor. To date, much of this engineering transformation has been limited to geometric design, or the form and fit of a component. Efforts are now ongoing to develop computer-based tools to assess the function of components under the intended final application conditions (i.e., temperature, environment, stress, and time).

There have been substantial efforts over the past 25 years to develop and implement computer-based models to simulate manufacturing processes and the evolution of microstructure and accompanying mechanical properties within component materials. The rate of change within this area of engineering has continued to increase with increasing industrial application benefits from the use of such engineering tools, accompanied by the reduced cost and increased speed of computing systems required to perform increasingly complex simulations.

Volumes 22A and 22B of the ASM Handbook series summarize models that describe the behavior of metallic materials under processing conditions and describe the development and application of simulation methods for a wide range of materials and manufacturing processes. Such information allows the sharing of best practices among diverse scientific, engineering, and manufacturing disciplines. Background information on fundamental modeling methods detailed in Volume 22A provides the user with a solid foundation of the underlying physics that support many industrial simulation software packages. The present Volume provides an overview of a number of specific metals processing simulation tools applicable in the metals manufacturing industry for a wide range of engineering materials.

All simulation tools require a variety of inputs. For example, details regarding material and process boundary conditions are critical to the success of any computer-based simulation. Thus, this Handbook also provides information regarding material and process boundary conditions that are applicable to manufacturing methods. Additionally, this Volume provides guidance regarding how to develop and assess required thermophysical material data for materials that have not been previously characterized, so practitioners of simulation software packages can effectively generate required material and manufacturing process databases to enable successful predictions for metals processing methods.

The benefits provided by integrated computational materials engineering include reduced component development time, enhanced optimization of component design (design for performance, design for manufacturing, and design for cost), and increased right-the-first-time manufacturing. These benefits have led to an overwhelming pull for materials and manufacturing process simulation integration with early stages of component design.

D.U. Furrer, FASM
Rolls-Royce Corporation

S.L. Semiatin, FASM
Air Force Research Laboratory
Policy on Units of Measure

By a resolution of its Board of Trustees, ASM International has adopted the practice of publishing data in both metric and customary U.S. units of measure. In preparing this Handbook, the editors have attempted to present data in metric units based primarily on Système International d'Unités (SI), with secondary mention of the corresponding values in customary U.S. units. The decision to use SI as the primary system of units was based on the aforementioned resolution of the Board of Trustees and the widespread use of metric units throughout the world.

For the most part, numerical engineering data in the text and in tables are presented in SI-based units with the customary U.S. equivalents in parentheses (text) or adjoining columns (tables). For example, pressure, stress, and strength are shown both in SI units, which are pascals (Pa) with a suitable prefix, and in customary U.S. units, which are pounds per square inch (psi). To save space, large values of psi have been converted to kips per square inch (ksi), where 1 ksi = 1000 psi. The metric tonne (kg $\times 10^3$) has sometimes been shown in megagrams (Mg). Some strictly scientific data are presented in SI units only.

To clarify some illustrations, only one set of units is presented on artwork. References in the accompanying text to data in the illustrations are presented in both SI-based and customary U.S. units. On graphs and charts, grids corresponding to SI-based units usually appear along the left and bottom edges. Where appropriate, corresponding customary U.S. units appear along the top and right edges.

Data pertaining to a specification published by a specification-writing group may be given in only the units used in that specification or in dual units, depending on the nature of the data. For example, the typical yield strength of steel sheet made to a specification written in customary U.S. units would be presented in dual units, but the sheet thickness specified in that specification might be presented only in inches.

Data obtained according to standardized test methods for which the standard recommends a particular system of units are presented in the units of that system. Wherever feasible, equivalent units are also presented. Some statistical data may also be presented in only the original units used in the analysis.

Conversions and rounding have been done in accordance with IEEE/ASTM SI-10, with attention given to the number of significant digits in the original data. For example, an annealing temperature of 1570 °F contains three significant digits. In this case, the equivalent temperature would be given as 855 °C; the exact conversion to 854.44 °C would not be appropriate. For an invariant physical phenomenon that occurs at a precise temperature (such as the melting of pure silver), it would be appropriate to report the temperature as 961.93 °C or 1763.5 °F. In some instances (especially in tables and data compilations), temperature values in °C and °F are alternatives rather than conversions.

The policy of units of measure in this Handbook contains several exceptions to strict conformance to IEEE/ASTM SI-10; in each instance, the exception has been made in an effort to improve the clarity of the Handbook. The most notable exception is the use of g/cm$^3$ rather than kg/m$^3$ as the unit of measure for density (mass per unit volume). SI practice requires that only one virgule (diagonal) appear in units formed by combination of several basic units. Therefore, all of the units preceding the virgule are in the numerator and all units following the virgule are in the denominator of the expression; no parentheses are required to prevent ambiguity.
Officers and Trustees of ASM International (2009–2010)

Frederick J. Lisy
President and Trustee
Orbital Research Incorporated

Mark F. Smith
Vice President and Trustee
Sandia National Laboratories

Paul L. Huber
Treasurer and Trustee
Seco/Warwick Corporation

Roger J. Fabian
Immediate Past President and Trustee
Bodycote Thermal Processing

Stanley C. Theobald
Managing Director and Secretary
ASM International

Members of the ASM Handbook Committee (2009–2010)

Kent L. Johnson
(Chair 2008–; Member 1999–)
Materials Engineering Inc.

Craig D. Clauser
(Vice Chair 2009–; Member 2005–)
Craig Clauser Engineering Consulting Incorporated

Larry D. Hanke
(Immediate Past Chair; Member 1994–)
Materials Evaluation and Engineering Inc.

Viola L. Acoff (2005–)
University of Alabama

Lichun Leigh Chen (2002–)
Technical Materials Incorporated

Sarup K. Chopra (2007–)
Consultant

Craig V. Darragh (1989–)
The Timken Company (ret.)

Jon L. Dossett (2006–)
Consultant

Alan P. Druschitz (2009–)
University of Alabama-Birmingham

David U. Furrer (2006–)
Rolls-Royce Corporation

Jeffrey A. Hawk (1997–)
National Energy Technology Laboratory

William L. Mankins (1989–)
Metallurgical Services Inc.

Joseph W. Newkirk (2005–)
Missouri University of Science and Technology

Robert P. O'Shea, Jr. (2008–)
Baker Engineering and Risk Consultants

Cory J. Padfield (2006–)
American Axle & Manufacturing

Mufit Akinc
Iowa State University

Richard I. Asfahani
United States Steel Corporation

Sunniva R. Collins
Swagelok

Robert J. Fulton
Hoeganaes Corporation (retired)

Richard Knight
Drexel University

Jon L. Johnson
AEP

Digby D. Macdonald
Penn State University

Charles A. Parker
Honeywell Aerospace

Jon D. Tirpak
ATI

[Student board representatives]

Joshua Holzhausen
University of Washington

Natasha Rajan
University of Alberta

Chairs of the ASM Handbook Committee

J.F. Harper
(1923–1926) (Member 1923–1926)

W.J. Merten
(1927–1930) (Member 1923–1933)

L.B. Case
(1931–1933) (Member 1927–1933)

C.H. Herty, Jr.
(1934–1936) (Member 1930–1936)

J.P. Gill
(1937) (Member 1934–1937)

R.L. Dowdell
(1938–1939) (Member 1935–1939)

G.V. Luerssen
(1943–1947) (Member 1942–1947)

J.B. Johnson
(1948–1951) (Member 1944–1951)

E.O. Dixon

N.E. Promisel

R.W.E. Leiter

D.J. Wright
(1964–1965) (Member 1959–1967)

J.D. Graham

W.A. Stadler

G.J. Shubat

R. Ward

G.N. Maniar

M.G.H. Wells

J.L. McCall

L.J. Korb

T.D. Cooper

D.D. Huffman

D.L. Olson

R.J. Austin

W.L. Mankins
(1994–1997) (Member 1989–)

M.M. Gauthier

C.V. Darragh
(1999–2002) (Member 1989–)

Henry E. Fairman

Jeffrey A. Hawk
(2004–2006) (Member 1997–)

Larry D. Hanke
(2006–2008) (Member 1994–)

Kent L. Johnson
(2008–2010) (Member 1999–)
Authors and Contributors

John Agren  
Royal Institute of Technology, Stockholm, Sweden

Seokyoung Ahn  
The University of Texas-Pan American

Janet K. Allen  
University of Oklahoma

Taylan Altan  
The Ohio State University

Sudarsanam Suresh Babu  
The Ohio State University

C. C. Bampton  
Pratt & Whitney Rocketdyne

Jeff J. Bernath  
Edison Welding Institute Incorporated

Bernard Billia  
Aix-Marseille Université, France

Robert Brooks  
National Physical Laboratory, UK

Dennis J. Buchanan  
University of Dayton Research Institute

W.S. Cao  
CompuTherm LLC

Y.A. Chang  
University of Wisconsin

Anil Chaudhary  
Applied Optimization Inc.

S.L. Chen  
CompuTherm LLC

Suk Hwan Chung  
Hyundai Steel Co, South Korea

Seong-Taek Chung  
CetaTech, Inc.

Anders Engström  
Thermo-Calc Software AB, Stockholm, Sweden

Hans J. Fecht  
Ulm University, Germany

Chris Fischer  
Scientific Forming Technologies Corporation

D. U. Furrer  
Rolls-Royce Corporation

Ch.-A. Gandin  
Centre de Mise en Forme des Matériaux, Sophia Antipolis, France

Randall M. German  
San Diego State University

Somnath Ghosh  
The Ohio State University

Robert Goetz  
Rolls-Royce Corporation

Vassily Goloveshkin  
Moscow State University of Instrument Engineering and Computer Sciences (MGUPI)

G. Gottstein  
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany

Jianzheng Guo  
ESI US R&D

Samuel Hallström  
Thermo-Calc Software AB, Stockholm, Sweden

A. Jacot  
Ecole Polytechnique Fédérale de Lausanne, Switzerland

JongTae Jinn  
Scientific Forming Technologies Corporation

D. Kammer  
Northwestern University

Kanchan M. Kelkar  
Innovative Research Inc.

Pat Koch  
Engineous Software

M. V. Kral  
University of Canterbury, New Zealand

Matthew John M. Krane  
Purdue University

Howard Kuhn  
University of Pittsburgh

Young-Sam Kwon  
CetaTech, Inc.

Peter D. Lee  
Department of Materials, Imperial College, London, U.K

Guoji Li  
Scientific Forming Technologies Corporation

Ming Li  
Alcoa Technical Center

Kong Ma  
Rolls-Royce Corporation

Paul Mason  
Thermo-Calc Software Inc., Stockholm, Sweden

Ramesh S. Minisandram  
ATI Allvac

Alec Mitchell  
University of British Columbia

D. A. Molodov  
Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Germany

Seong Jin Park  
Mississippi State University

Suhas V. Patankar  
Innovative Research Inc.

Ashish D. Patel  
Carpenter Technologies

Michael Preuss  
Manchester University, UK

Peter J. Quested  
National Physical Laboratory, UK

A. D. Rollett  
Carnegie Mellon University

Yiming Rong  
Worcester Polytechnic Institute

D. J. Rowenhorst  
US Naval Research Laboratory

Valery Rudnev  
Inductoheat Incorporated

Victor Samarov  
Syntercet PM

Mark Samonds  
ESI US R&D

N. Saunders  
Thermotech / Sente Software Ltd., UK

S. L. Semiatin  
Air Force Research Laboratory

L. S. Shvindlerman  
Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Richard D. Sisson, Jr.  
Worcester Polytechnic Institute
Reviewers

Taylan Altan
The Ohio State University

Egbert Baake
Leibniz Universität Hannover

L. Battezzati
Università di Torino

Michel Bellet
Centre de Mise en Forme des Matériaux, Sophia Antipolis, France

Hongbo Cao
General Electric Global Research Center

Qing Chen
Thermo-Calc Software AB, Stockholm, Sweden

Jon Dantzig
University of Illinois at Urbana-Champaign

Uwe Diekmann
Metatech GmbH

Rollie Dutton
Air Force Research Laboratory

D.U. Furrer
Rolls-Royce Corporation

Martin E. Glicksman
University of Florida

Janez Grum
University Of Ljubljana

Jianzheng Guo
ESI US R&D

Larry Hanke
Materials Evaluation and Engineering Inc

Jeffrey Hawk
U.S. Department of Energy

Edmond Ilia
Metaldyne

Richard Johnson

Ursula Kattner
National Institute of Standards and Technology

Leijun Li
Utah State University

Daan Maijer
University of British Columbia

William Mankins
Metallurgical Services Incorporated

David McDowell
Georgia Institute of Technology

Tugrul Ozel
Rutgers University

S.L. Semiatin
Air Force Research Laboratory

Brian Thomas
University of Illinois at Urbana-Champaign

Ray Walker
Keystone Synergistic Enterprises, Inc.

Michael West
South Dakota School of Mines and Technology

John Wooten
CalRAM, Inc
Contents

Input Data for Simulations ............................................ 1

Introduction to Metals Process Simulation

* D.U. Furrer and S.L. Semiatin ................................. 3

Metals Process Simulation ........................................ 3

Thermophysical Properties of Liquids and Solidification

Microstructure Characteristics—Benchmark Data Generated
in Microgravity

* Hans J. Fecht and Bernard Billia .............................. 8

Casting and Solidification Processing from the Melt .... 8

Materials Processing in Space .................................. 10

Conclusion and Perspectives ..................................... 14

Thermophysical Properties

* Juan J. Valencia and Peter N. Quested ..................... 18

Sources and Availability of Reliable Data .................... 18

Limitations and Warning on the Use of Data ............... 18

Methods to Determine Thermophysical Properties ........ 18

Specific Heat Capacity and Enthalpy of Transformation .... 19

Enthalpy of Melting, Solidus and Liquidus Temperatures .... 20

Coefficient of Thermal Expansion .............................. 20

Density .................................................................. 22

Surface Tension ..................................................... 23

Viscosity .................................................................. 24

Electrical and Thermal Conductivity ......................... 25

Emissivity .................................................................. 25

Typical Thermophysical Properties Ranges of Some

Cast Alloys .................................................................. 28

Summary ..................................................................... 28

Measurement of Thermophysical Properties at High Temperatures

for Liquid, Semisolid, and Solid Commercial Alloys

* Peter Quested and Robert Brooks ............................ 33

Measurement Methods .............................................. 33

Thermal Conductivity/Thermal Diffusivity ................. 36

Density .................................................................. 37

Viscosity .................................................................. 38

Summary ..................................................................... 40

Measurement and Interpretation of Flow Stress Data for the

Simulation of Metal-Forming Processes

* S.L. Semiatin and T. Altan ...................................... 46

Tension Test .............................................................. 46

Uniaxial Compression Test ......................................... 47

Ring Test .................................................................. 50

Plane-Strain Compression Test ................................... 51

Torsion Test .............................................................. 51

Split-Hopkinson Bar Test .......................................... 52

Indentation Tests ....................................................... 52

Effect of Deformation Heating on Flow Stress ............ 53

Fitting of Flow-Stress Data .......................................... 53

Metallurgical Considerations at Hot Working Temperatures 53

Grain-Boundary Energy and Mobility

* G. Gottstein, D.A. Molodov, and L.S. Shvindlerman ....... 67

Grain-Boundary Energy .............................................. 67

Grain-Boundary Mobility .......................................... 74

Texture Measurement and Analysis

* A.D. Rollett .......................................................... 92

Guide for Nonexperts ............................................... 92

Pole Figure Measurement ........................................... 92

Electron Backscatter Diffraction .................................... 97

Types or Classes of Materials ........................................ 98

Summary ..................................................................... 98

Three-Dimensional Microstructure Representation

* G. Spanos, D.J. Rowenhorst, M.V. Kral, P.W. Voorhees, and D. Kammer ................................. 100

Three-Dimensional Characterization Methods ................ 100

Serial Sectioning by Mechanical Material-Removal Methods ......................................................... 101

Segmentation ............................................................. 103

Focused Ion Beam Tomography ................................... 107

Simulations—Inputting and Using 3-D Data .................. 109

Simulation of Phase Diagrams and Transformations .............. 115

Commercial Alloy Phase Diagrams and Their Industrial Applications

* F. Zhang, Y. Yang, W.S. Cao, S.L. Chen, K.S. Wu, and Y.A. Chang ........................................ 117

Industrial Applications ............................................... 117

Integration with Kinetic and Microstructural Evolution Models .......................................................... 122

Limitations of the CALPHAD Approach .................... 128

Conclusion ............................................................... 129

The Application of Thermodynamic and Material Property

Modeling to Process Simulation of Industrial Alloys

* N. Saunders .......................................................... 132

Calculation of Phase Equilibria in Multicomponent Alloys ................. 132

Application of CALPHAD Calculations to Industrial Alloys ............. 135

Extending CALPHAD Methods to Model General Material Properties ........................................... 138

Summary and Observations for the Future ..................... 150

Simulation of Solidification ........................................... 155

Modeling of Transport Phenomena during Solidification Processes

* Matthew John M. Krane ......................................... 157

Conservation Equations for Transport Phenomena ........... 157

Examples of Model Results ......................................... 161

Summary ..................................................................... 166

Modeling of Casting and Solidification Processes

* Jianzheng Guo and Mark Samonds .......................... 168

Computational Thermodynamics ................................. 168

Thermophysical Properties ........................................ 170

Fundamentals of the Modeling of Solidification Processes 171

Microstructure Simulation .......................................... 173

Defect Prediction ......................................................... 178

Examples of Modeling Applied in Casting Industries ... 185

Conclusions .............................................................. 191

Computational Analysis of the Vacuum Arc Remelting (VAR) and Electroslag Remelting (ESR) Processes

* Kanchan M. Kelkar, Suhas V. Patankar, Alec Mitchell, Runesh S. Minisandram, and Ashish D. Patel ........................................ 196

Process Description and Physical Phenomena .................. 196

Computational Modeling of Remelting Processes ............ 197