ASM Handbook®

Volume 22A
Fundamentals of Modeling for Metals Processing

Prepared under the direction of the
ASM International Handbook Committee

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Materials Park, Ohio 44073-0002
www.asminternational.org

First printing, December 2009

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Library of Congress Cataloging-in-Publication Data

ASM International

ASM Handbook
Includes bibliographical references and indexes
Contents: v.1. Properties and selection—irons, steels, and high-performance alloys—v.2. Properties and selection—nonferrous alloys and special-purpose materials—[etc.]—v.22A. Fundamentals of Modeling for Metals Processing

1. Metals—Handbooks, manuals, etc. 2. Metal-work—Handbooks, manuals, etc. I. ASM International. Handbook Committee. II. Metals Handbook.
TA459.M43 1990 620.1'6 90-115
SAN: 204-7586

ISBN-13: 978-1-61503-001-9
ISBN-10: 1-61503-001-8

ASM International®
Materials Park, OH 44073-0002
www.asminternational.org

Printed in the United States of America

Multiple copy reprints of individual articles are available from Technical Department, ASM International.

Foreword

This Volume 22A, *Fundamentals of Modeling for Metals Processing*, represents an expansion of the Handbook series in response to the expressed needs of members of the modeling and simulation community.

ASM International is indebted to the Co-Editors, David Furrer and S. Lee Semiatin, who had the vision for a comprehensive presentation of modeling of metals processing. They moved this vision from inception to this unified collection of content in a remarkably short time, through tireless effort. They recruited world renowned modeling experts who contributed entirely new content. We are likewise indebted to the approximately 120 volunteer authors and reviewers who fulfilled their commitments, squeezing this time intensive activity into their lives busy with family, career, and community commitments.

While this Handbook serves as an organizing vehicle for acquiring modeling knowledge, ASM International is pleased to have the means to disseminate this outstanding source of information in forms most attractive and most readily available to its members and to the technical community.

Modeling is an important aspect of "everything material." One can model at the submicroscopic scale where atomic structure is predominant; at an intermediate, or mesoscale at which grain size/grain structure effects are important; and at the macroscopic, continuum level at which bulk properties are typically determined. Through ASM's strategic content development efforts, specific needs for high-quality materials modeling information are met. Further enhancement will be forthcoming as the Co-Editors complement this work with Volume 22B, *Metals Process Simulation*.

The need for modeling metallurgical behavior during processing has long been recognized and ASM has been a forum for exchange of these ideas. Through mechanistic and phenomenological approaches, solidification and deformation processes can be optimized, the resulting mechanical properties controlled, and defects minimized. As computing power has increased and its cost decreased, more sophisticated simulation of metallurgical processes has enabled material scientists and engineers to maintain competitive advantage over those not willing or able to change.

As an organization of material scientists and engineers, ASM International is pleased to offer this content to practitioners and students of modeling as they continue their exciting journey of tailoring materials and processes to meet future functional needs. This new Handbook, in its printed and electronic forms, also moves us closer to achieving a strategic objective that will shape our society for the next fifty years: to accumulate, review, and distribute comprehensive materials information and to become the global resource for quality materials information.

Roger Fabian
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Preface

Scientists and engineers have always been curious about cause and effect relationships within nature. This is also the case relative to metals and materials. The understanding of the physics of metals has greatly increased from the earliest days of the field of metallurgy. The discovery of mechanisms that influence and control the behavior of metals has spurred continued research and further discovery. Initial understanding and description of controlling mechanisms were substantially phenomenological, based on observations and perceived interactions of material and process variables on resultant metallic material microstructure, mechanical properties and behavior. The conversion of mechanistic relationships into mathematical expressions is now the field of materials modeling.

The development of models and modeling methods is now allowing more rapid discovery of new alloy systems with greater optimization and application potential. Models are being integrated into computational tools for design and simulation of component processing and manufacture. The successful application of models by industry is also resulting in further pull for even further development of models that are more accurate and predictive. The study of mechanisms that control the evolution and behavior of metallic materials is continuing today at an even more aggressive pace.

Mechanistic models that more accurately describe the physics of metallurgical processes, such as grain growth, precipitation, phase equlibria, strength and deformation as examples are of great interest and importance to science and industry alike. Greater understanding of the physics of metals to the atomistic level, along with increased computational power, has resulted in further discovery and growth in the field of modeling and simulation.

This Handbook provides a review of the models that support the understanding of metallic materials and their processing. An accompanying volume will provide details of the integration of these models into software tools to allow simulation of manufacturing processes. The distinctly different, but complementary fields of Modeling and Simulation are providing new and increased capabilities for metallic materials for components and systems. The future of the metals industry is moving toward an integrated computational materials engineering (ICME) approach as a result of the hard work and dedication of the individuals, teams and organizations that have and continue to provide the needed models and simulation tools that are capable of providing engineers with accurate predictive guidance and direction.

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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.

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