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Volume

22A

**Fundamentals of
Modeling for
Metals Processing**



The Materials
Information Society

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Fundamentals of Modeling for Metals Processing

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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 equilibria, 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 ($\text{kg} \times 10^3$) 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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Introduction to Fundamentals of Modeling for Metals Processing

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THE FORMULATION AND APPLICATION of modeling and simulation methods for metallic materials and manufacturing process design and development is rapidly increasing. Classic models that predict the behavior of metals under processing conditions are continuing to be used and enhanced with greater understanding of the mechanisms that control the evolution of microstructure, texture, and defects. New theories and associated mathematical models are being developed and applied to metallic alloy systems for existing and new processing methods. To complement empirical descriptions of material behavior during processing, so-called first-principles approaches, such as those based on atomistic and molecular dynamics calculations, are now being developed to provide fundamental understanding of the mechanisms that control observed behaviors of existing and emerging alloys, such as those for unique or highly demanding applications.

The recent development of the integrated computational materials engineering (ICME) discipline allows fundamental research to be linked to industrial applications (Ref 1). See the article "Integrated Computational Materials Engineering" in this Volume. The refinement of models and modeling methods results in greater capability and accuracy of metallurgical predictions, such as phase equilibria, microstructure, and subsequent mechanical properties. The ability to rapidly apply fundamental models to practical component design and manufacturing applications has spurred unprecedented collaboration between universities, research laboratories, software companies, and industrial users of modeling and simulation tools. The linkage of component design, alloy design, and component manufacture through modeling and simulation methods will allow for continued advancement in the area of alloy research, advanced process and equipment development, and enhanced component capability.

Modeling and simulation activities are increasing within the materials field as well as other science and engineering disciplines. Development, enhancement, and implementation

of computational modeling and analysis technologies to describe and predict physics-based processes are occurring globally within universities and research centers in nearly every country (Ref 2). In addition to increased collaboration between industry and academia, there are increased numbers of multinational collaborative efforts aimed at increasing the capabilities and state-of-the-art of material and process modeling. Fundamental understanding of metallic materials and processing is increasing rapidly and becoming available globally through these and other science and engineering efforts.

Volumes 22A and 22B of the *ASM Handbook* series describe the current state-of-the-art of modeling and simulation for metals processing. The present Volume (22A), *Fundamentals of Modeling for Metals Processing*, focuses on mathematical descriptions of the behavior of metallic materials during processing (and resultant properties) as well as process modeling per se. These models may be broadly characterized into three types on the basis of approach and mathematical expression utilized as being phenomenological (based primarily on direct observations/measurements), mechanistic/physics based, or a combination of the two.

Phenomenological and mechanistic models are also separated by application type, including materials models or process models. Materials models for metals can also be considered metallurgical process models, where grain growth, precipitation, recrystallization, or dislocation impedance are examples of processes within metals and alloys. Materials models describe how, for example, microstructure, crystallographic texture, and defects evolve as a function of local metallurgical process variables, including history and path dependences.

Process models, on the other hand, describe manufacturing processes that require understanding of external independent parameters and boundary conditions and provide information about macroscopic component changes and/or information for metallurgical process models. The nomenclature within this field, however, can cause some confusion, so it is

important to understand and clearly define the type of models being discussed.

Manufacturing process modeling addresses the integration of material behavior models with the description of specific processes (e.g., forging, investment casting), which typically include equipment/process characteristics and interface effects (such as heat transfer and friction). The equations describing the physical phenomena in material behavior models and/or their coupling with process models are often too complex for solution by analytical means, except under somewhat restrictive (albeit often insightful) conditions. This is usually the case for real-world industrial processes. In such cases, numerical simulation methods must be used to describe material behavior, process mechanics, and processing-structure-mechanical behavior relationships. Volume 22B, *Metals Process Simulation*, deals with the state-of-the-art of the simulation of specific materials processes, including associated input-data requirements.

Various major sections of this Volume summarize the fundamentals of materials modeling, including modeling of microstructure and texture evolution, modeling of damage and defect evolution, modeling of mechanical properties, and material-specific models for industrial alloys. This article provides a brief historical perspective, a classification of metallurgical processes that are discussed within this Volume, basic model development efforts, and an overview of the potential future directions for the modeling of metals processing.

Historical Perspective

Models of various forms have been developed nearly since the beginning of time. Models can be very simple, such as an "if/then" relationship, or extremely complex mathematical expressions with numerous parameters, some of which may be easily measured and well understood and others that are not physically observable or readily inferred. All models have one thing in common: They attempt to

provide improved understanding of the nature and the variables that influence and control the results of processes, whether a naturally occurring process or man-made. The study of processes leads to theories and subsequent models that can and are used to predict future applications of the studied process. Figure 1 shows a schematic flow path for the development of models that provide improved understanding of processes, where metallurgical or manufacturing process-based.

Models are developed due to need or curiosity. The drive to increase understanding of nature and metallurgical processes has provided a substantial foundation for materials and process modeling. For the most part, the development of material behavior and process models has been spearheaded by metallurgical and mechanical engineers, respectively. Over the last two decades, however, a great emphasis has been placed on the need for coupling material behavior and process models, leading to work that is truly interdisciplinary in nature.

Material behavior models for processing have evolved from ones that are largely empirical in nature to those that incorporate physics-based mechanisms. For example, work in the first half of the 20th century led to engineering (phenomenological) models of:

- Deformation and strain hardening, such as Schmid's law and the Hollomon equation
- Kinetics of recrystallization (such as the Avrami equation), grain growth (such as the Beck equation), and precipitation/phase transformation
- Ductility for solid-state processes

Similarly, phenomenological models of macrostructure evolution during solidification and evaporation during vapor processing were

developed for a number of alloy systems. For the most part, these phenomenological models were applicable only to the range of process parameters for which measurements had been made and hence were essentially methods of fitting experimental data. The development of a fundamental understanding of the mechanisms underlying these phenomena, such as dislocation glide/climb and diffusion, led to rudimentary physics-based models, such as those for the large-strain deformation of polycrystalline aggregates, phase transformations based on classical nucleation theory and diffusional growth, and grain growth, among others, in the 1940s to 1960s. Beginning in the 1980s, the incorporation of the fundamental concepts of thermodynamics and thermal physics (due to, for example, Gibbs, Ising, and others) led to a great expansion of mechanism-based models, such as those designed to predict phase equilibria (e.g., Calphad), recrystallization and grain growth (Monte Carlo and cellular-automaton techniques), and precipitation and solidification problems (e.g., phase-field methods). The successful implementation of these newer techniques was made possible by the advent of inexpensive computers and ever-increasing computing power beginning in the 1990s.

Modern process models have evolved from relatively simple analytical and numerical techniques. These include the slab, upper-bound, and slip-line field methods (for predicting loads/forming pressures during metal forming, for instance) and the solution of relatively simple partial-differential equations (for various heat flow, solidification, and diffusion problems) that evolved during the 1920s to 1980s. The development of mainframe, mini-, and then microcomputers and associated software beginning in the 1970s and 1980s led

to the ability to simulate much more complex processing problems, often based on finite-difference or finite-element numerical techniques. These latter approaches have also enabled the simulation of coupled phenomena, such as those involving simultaneous deformation/solidification, energy transport, and mass transport.

Classes of Material Behavior Models

Material behavior models can be grouped broadly into three classes: statistical, phenomenological, and mechanism based.

Statistical models typically require large amounts of experimental data to derive a mathematical relationship between independent/controlled process parameters and predictions of metallurgical process results. For example, linear regression analysis is often used to "fit" pairs or a series of data to determine relationships (Ref 4). This approach has pros and cons. One advantage is that data generated during the manufacture of components can often be used to generate models, but the available data often do not contain all of the required parameters. In other words, the data may mask second-order or confounding parameters, making difficult the establishment of statistical models that capture the fundamental relationships. Other disadvantages consist of not knowing a priori what metallurgical or processing parameters influence the specific results of a process, and the issue that not all metallurgical processes and relationships are linear. A specific type of statistical analysis, known as artificial neural-network (ANN) modeling, overcomes some of these drawbacks for the development of multivariable, nonlinear relationships, but this approach also requires large amounts of data (Ref 5). In addition, ANN, like other statistical approaches, suffers from not being able to predict results outside the range of data used for "training" the model. Since the physics of the metallurgical process being modeled are not known, extrapolating statistical-based models outside the parameter range in which they are trained is not advisable and can lead to errors and large deviations from reality if the physics of the process change are not captured within the model.

Phenomenological models typically rely on equations that define the relationship between process variables and resulting microstructure, properties, and so on. These types of models can be used to describe phenomena such as recrystallization, grain growth, and creep of metallic materials. For example, Avrami (sigmoidal-type) equations have been used frequently to fit observations of the kinetics of static (and dynamic) recrystallization and other phase transformations during metals processing (Ref 6–8). Such relationships quantify the nucleation and growth mechanisms that lead to an initial slow incubation period, followed by a rapid rate of increase in the

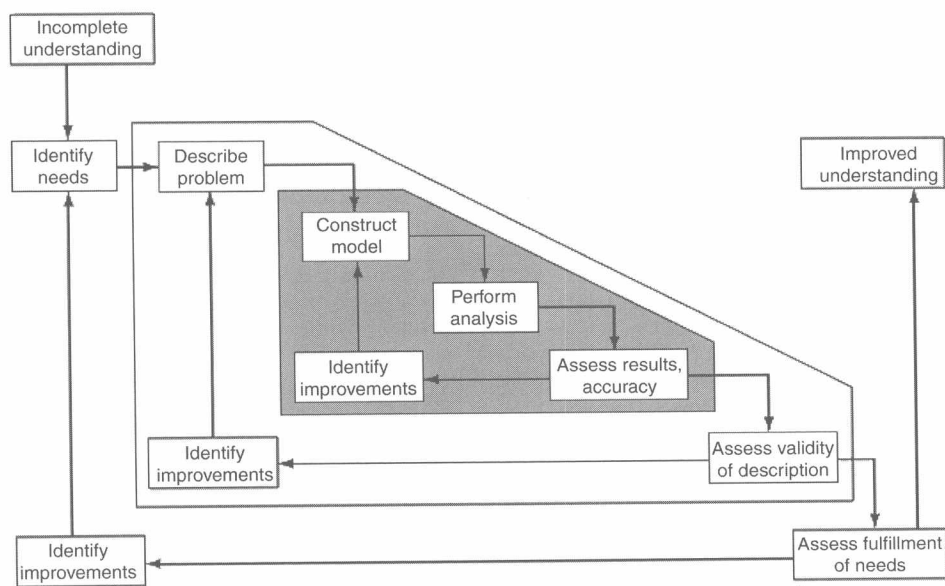


Fig. 1 Process flow for development of models to increase understanding of metallurgical and manufacturing processes. Source: Ref 3

recrystallized/transformed volume fraction, and then a final reduction in the rate of the process until the reaction or metallurgical process completes. Typical applications include the rate of decomposition of austenite in steels that underlie time-temperature-transformation and cooling-transformation diagrams (Ref 9). Similarly, Arrhenius rate-type equations are often used to describe the temperature dependence of metallurgical phenomena, such as the plastic flow of metals at high temperature (using the temperature-compensated strain rate, or Zener-Hollomon parameter), grain growth (Ref 10), and creep (using the Larson-Miller parameter) (Ref 11).

In phenomenological models, the underlying mechanism(s) that control the rate of the metallurgical process are often not known precisely nor explicitly incorporated. This type of modeling approach may also have several inherent limitations:

- Experimental data are often needed to establish or calibrate the relationship, even for mathematical expressions in which the form is known.
- If the mechanism controlling the process changes, the form of the fit assumed in the model may not be appropriate.

Mechanistic models are often called physics based due to their ability to include all of the relevant physical parameters that influence the outcome of a process to a high degree of fidelity. As such, mechanism-based models tend to be the most robust.

Examples of mechanistic models comprise phase-field approaches for microstructure evolution, such as solidification, grain growth, and solid-state precipitate growth. In each of these cases, the mechanisms that control the migration of grain or interface boundaries, such as bulk diffusion or interface reaction, and

suitable input parameters, such as grain/interface boundary energy, must be known (Ref 12, 13). An example of a mechanistic mechanical property relationship is the Hall-Petch model for yield strength as a function of grain size of single-phase alloys (Ref 14). This model relates the applied stress for plastic flow to the slip length within a grain and the stress concentration for slip transmission into neighboring grains. This simple model is effective and is readily used for metallurgical understanding of tensile property control and optimization (Ref 15). However, the grain size is not the only microstructural feature that can influence the yield strength. Additional models are required to describe contributions from solid-solution, precipitation/dispersion, and dislocation strengthening (strain hardening).

Mechanistic models do provide the ability to predict behavior outside the range for which they were developed, provided the controlling mechanism is unchanged. In some cases, the failure of a mechanism-based model to describe observations may provide the impetus for new fundamental understanding. For instance, such was the case for the discovery of microtwinning during creep of nickel-base superalloys (Ref 16). Existing mechanistic creep models did not accurately capture the behavior within a specific temperature-stress regime. After careful focused observations, the new mechanism was discovered. Figure 2 shows micrographic evidence of the new creep mechanism, microtwinning, within nickel-base superalloys.

This Volume contains articles on a range of metallurgical and materials processes. Table 1 lists the various formulations and mathematical methods to predict the relationships and interactions within metallurgical processes. Further development of modeling tools will continue to be seen in both mathematical expression and mathematical formulation for calculation of predictions.

Future Outlook

Modeling and simulation technology will continue to grow because it provides a means

to assess “what-if” scenarios and to conduct virtual experiments. Material behavior and process models provide useful information to both design and manufacturing engineers. Currently, industry is developing holistic component and product design approaches that include metallurgical and process models. In this regard, ICME provides a means of mathematically linking complex metallurgical processes to the mechanical design of components. ICME will be the prevailing method in the future for industry to design and optimize components, alloys, and manufacturing processes in a fully-coupled manner.

Another trend that is gaining momentum is the increasing interest of academic and research institutions in the development of fundamental material behavior and process models for the manufacture of metal products. This may be due to factors such as:

- Widespread availability of inexpensive computer hardware and software
- Limited mechanistic understanding of metallurgical phenomena under processing conditions for alloys of commercial importance and hence a strong technology pull from industry
- Increased use of modeling and simulation within industry develops a need for engineers and scientists with knowledge and background in this area
- Acceptance of modeling and simulation in general as a worthy research subject
- Application of modeling and simulation as a teaching method within multidisciplinary engineering fields
- Shift toward near-term investments and the concomitant reduction in research staff within many companies

Despite the reduction in modeling research within industry, the application of models in the commercial milieu is creating an increased demand for modeling tools, engineering analysis capabilities, and engineers that can apply modeling and simulation tools to industrial challenges. These needs are being addressed by academia in a very synergistic

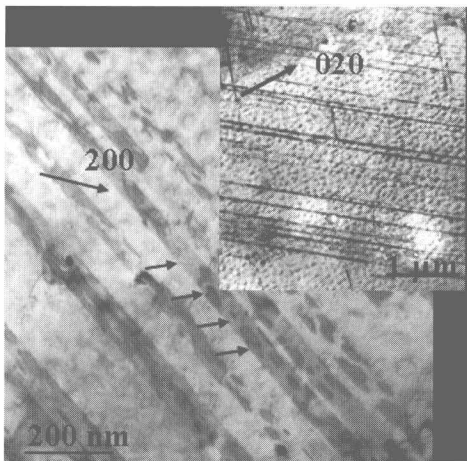


Fig. 2 Recent discovery of microtwins in nickel-base superalloys after creep deformation has led to further investigation and development of a model that describes this new mechanism. Courtesy of M. Mills, The Ohio State University

Table 1 Examples of mathematical modeling approach and applications for metals processing

| Tool | Typical application(s) |
|--|--|
| Slab, upper-bound, slip-line field models | Loads, metal flow, gross defects in bulk forming |
| Finite-element models deformation processes | Strain/metal flow, strain rate, temperature in deformation processes; powder consolidation |
| Finite-element/finite-difference models solidification processes | Fluid flow, solidification in solidification processes |
| Nucleation and growth models | Plethora of phase transformations, recrystallization, etc. |
| Crystal-plasticity models | Deformation-texture evolution |
| Cellular-automata models | Recrystallization, solidification microstructure |
| Phase-field models | Precipitation, grain growth, solidification microstructure |
| Monte Carlo models | Grain growth, recrystallization |
| Vertex models | Grain growth |
| Defect/failure models solid-state processes | Cavity nucleation, growth, coalescence; failure maps |
| Defect/failure models — solidification | Hot tearing, porosity |
| Constitutive equation models | Material behavior, metal flow |