Computational Methods for Microstructure-Property Relationships

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Editors

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This book is dedicated to all those individuals whose discontent with the present state of knowledge and vision for the future make the research wheels turn

Preface

Design of and with materials plays an intrinsic role in today's challenging world of high performance structural components and applications. They constitute an integral part of comprehensive structural design, given the opportunity offered by optimal materials design for structural performance and life enhancement. These opportunities impose high demands on effective modeling and simulation methodologies to establish quantitative relations between the material microstructure and physical properties at different length scales. The rapid advances in computer and computational sciences enable sophisticated simulations that unravel the underpinnings of complex material microstructure on behavior. In concert with outstanding advances in experimental methods, these computational tools are increasingly able to enhance the fundamental understanding of microstructure–property relations, thus enabling materials and process design for improved performance and life.

The field of computational materials modeling transcends traditional disciplinary boundaries between mechanics, materials science, physics and chemistry, mathematics and computer science. In addition, it is creating a true synergy between experiments and modeling in terms of incorporation of physics, calibration, and validation. The results of these unified efforts at various scales are yielding unprecedented levels of rigor and accuracy in predictions of complicated phenomena that have previously eluded scientists and engineers. The role of microstructure on physical properties and performance is emerging as a quantitative discipline with broad and direct implications on material design.

This book "Computational Methods for Microstructure–Property Relationships" is an attempt to capture this rapid advancement at a period of time, with a glimpse of what is yet to come in this very dynamic emergent field of science and technology. It introduces state-of-the-art advances in computational modeling as well as experimental approaches for materials structure–property relations. Representing a body of collected works by well-known professionals in the field, it covers topics ranging from materials modeling principles with a multiscale perspective to materials design. It presents the current state of knowledge for a wide collection of research areas related to materials assessment in structures–materials interactions. The collection aims at establishing the necessity of a robust integrated computational mechanics and computational materials science framework,

together with an experimental validation protocol, that treats heterogeneous materials at microstructural and continuum scales. Selectively encompassing both computational mechanics and computational materials science disciplines, it offers an analysis of current techniques and selected topics important to industry researchers, such as deformation, creep,. and fatigue of primarily metallic materials. It emphasizes modeling at continuum and heterogeneous microstructural scales, e.g. crystalline or grain scales, validated with experimental observations. This book in intended for researchers in academia, industry, and government laboratories to understand the issues and challenges involved in predicting performance and failure in materials, with a focus on the engineering structure–materials interaction. Researchers, engineers, and professionals involved with predicting the performance and failure of materials are expected to find this book a valuable reference.

This book is topically divided into four essential parts. The first part deals with 3D image-based materials structure data collection and representation and microstructure builders for mechanical response simulations.

Chapter "Serial Sectioning Methods for Generating 3D Characterization Data of Grain-and Precipitate-Scale Microstructures" introduces serial-sectioning methods for 3D characterization of grain- and precipitate-scale microstructures. It focuses on the use of serial-sectioning methods and associated instrumentation as a means for collecting microstructural, crystallographic, and chemical data. Chapter "Digital Representation of Materials Grain Structure" discusses the state-of-the-art methods in the field of microstructure representation with focus on the following: data collection, feature identification, mesh generation, quantitative descriptors, and synthetic structure generation. Chapter "Multi-Scale Characterization and Domain Partitioning for Multi-Scale Analysis of Heterogeneous Materials" discusses the development of a multiscale characterization methodology leading to a microstructural morphology-based domain partitioning method for materials having nonuniform heterogeneous microstructure. The set of methods is intended to provide a concurrent multiscale analysis model with the initial computational domain that delineates regions of statistical homogeneity and heterogeneity. The method is intended as a preprocessor to multiscale analysis of mechanical behavior and damage of heterogeneous materials. Chapter "Coupling Microstructure Characterization with Microstructure Evolution" discusses the synergistic coupling of quantitative microstructure characterization via experimental imaging techniques, with computer simulations of microstructural evolution using the phase-field method. Having experimental images as inputs, the chapter describes uses of the phase-field method at different length scales to explore mechanisms of microstructural evolution, extract material parameters, conduct physics-based repairs of experimentally reconstructed microstructures, and evolve the microstructure for different time, temperature, stress, etc. regimes.

Part of this volume is devoted to materials constitutive laws and kinematical approaches, together with their coupling of material structure to responses via simulation codes. These are presented in next six chapters. Chapter "Representation of Materials Constitutive Responses in Finite Element Based Design Codes" surveys

FEM-based tools for simulating materials behavior and reviews the material models available in commercial codes. Chapter "Accounting for Microstructure in Large Deformation Models of Polycrystalline Metallic Materials" analyzes the influence of microstructure on large-strain mechanical behavior for metallic polycrystalline materials. Results of a macroscale continuum internal state variable-based model for tantalum are compared with those from a multiscale polycrystalline plasticity approach having explicit representation of the polycrystalline aggregate. In Chapter "Dislocation Mediated Continuum Plasticity: Case Studies on Modeling Scale Dependence, Scale-Invariance, and Directionality of Sharp Yield-Point", the authors discuss a field dislocation dynamics theory to account for the emergence of inhomogeneous dislocation distributions at mesoscopic length scales, as well as their coupling to initial and boundary conditions and consequences on mechanical behavior. Size effects and scale-invariant intermittency are interpreted through field dislocation dynamics. Anisotropy of strain hardening induced by the emergence of internal stress fields is also reviewed in this chapter. Chapter "Dislocation-Mediated Time-Dependent Deformation in Crystalline Solids" shows a methodology for incorporating the effects of slip gradients associated with intra-grain deformation heterogeneity in crystal-plasticity-based finite element simulation. The treatise quantifies the orientation dependence of the misorientation field in the polycrystalline microstructure and introduces a modification of the kinematic decomposition that accommodates distortions arising from the presence of a static dislocation distribution. Chapter "Modeling Heterogeneous Intra-Grain Deformations Using Finite Element Formulations" is a review of two crystal plasticity-based methodologies for the prediction of microstructure–property relations in polycrystalline aggregates. These include a mean-field, second-order viscoplastic self-consistent method and a Fast Fourier Transform-based full-field method. Numerical examples demonstrate that models like the FFT-based formulation can explicitly account for interaction between individual grains. Finally, chapter 11 discusses multiscale modeling of plastic deformation and strength in crystalline materials with emphasis on models and experiments below the grain level. Specifically, the chapter deals with experimental advances and theoretical models for characterizing dislocations at the subgrain level.

The third part introduces computational mechanics for time dependency of materials with links to fracture mechanics and multi-time scaling methods for fatigue in next three chapters. Chapter "Stochastic Upscaling for Inelastic Material Behavior from Limited Experimental Data" develops time-dependent plastic deformation and creep models for crystalline solids using dislocation-level mechanics. The theory uses microstructural information to develop broad quantitative mechanistic relationships that match the observed phenomenology. The discussion includes mobility-controlled systems, where dislocations move through the crystal under stress and interaction of dislocations with discrete obstacles for a range of alloys. Chapter "DDSim: Framework for Multiscale Structural Prognosis" introduces a prototype hierarchical computational simulation system called damage and durability simulator (DDSim) for prognosis of fatigue life of airframe components. While this prototype focuses on fatigue cracking, the framework can be extended to other

modes of damage. Chapter "Modeling Fatigue Crack Nucleation Using Crystal Plasticity Finite Element Simulations and Multi-Time Scaling" addresses two important aspects of predicting fatigue crack nucleation in polycrystalline alloys under dwell cyclic loading. The first is a microstructure-sensitive criterion for dwell fatigue crack initiation in polycrystalline titanium alloys, while the second part of this chapter discusses a wavelet transformation-based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations. The WATMUS algorithm significantly enhances the computational efficiency for fatigue life prediction.

Finally, the fourth part of this book deals with some additional emerging topics in the next three chapters. Chapter "Challenges Below the Grain Scale and Multiscale Models" examines selected experimental methods at different length scales that are important tools in building models for location specific design. While special experimental techniques are needed to probe the material at finer scales to assess the local behaviors, testing methods at all scales are discussed to demonstrate the breadth of experimental capability available at each scale of the material. A stochastic upscaling approach for strain-hardening plastic materials from limited experimental data based on random matrix theory is introduced in chapter "Emerging Methods for Matching Simulation and Experimental Scales". The uncertainty characterized by constitutive tangential matrices can be construed as a reflection, on the coarse scales, of fluctuations of the fine scale features from which constitutive matrices are constructed. Finally, chapter "Simulation-Assisted Design and Accelerated Insertion of Materials" introduces some emerging concepts for robust design of materials and challenges for the synthesis of modeling and simulation and materials design. The distinction between materials design and multiscale modeling is elucidated in this chapter with emphasis on top-down requirements on material structure and performance to meet product requirements.

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Microstructure–Property–Design Relationships in the Simulation Era: An Introduction

Dennis M. Dimiduk

Abstract Computational methods are affecting a paradigm change for using microstructure–property relationships within materials and structures engineering. This chapter examines the emergent use of quantitative computational tools for microstructure–property–design relationships, primarily for structural alloys. Three major phases are described as a historical "serial paradigm," current "integrated computational materials engineering" and, future "virtual materials systems" emerging from advances in multiscale materials modeling. The latter two phases bring unique demands for integrating microstructure representations, constitutive descriptions, numerical codes, and experimental methods. Importantly, these approaches are forcing a fundamental restructuring of materials data for structural engineering wherein data centers on a hierarchy of model parameterizations and validations, rather than the current application-specific design limits. Examining aspects of current research on microstructure-sensitive design tools for single-crystal turbine blades provides an accessible glimpse into future computational tools and their data requirements. Finally, brief descriptions set context and interrelationships for the remaining chapters of the book.

1 Microstructure–Property–Design Relationships and Structural Materials Engineering

Present-day advancements in microstructure–property relationships are coming about via computational methods. The efforts largely recognize that microstructure–property relationships evolve over a wide range of scales and that both technical and computational advances must occur for adequate representations of these

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relationships within predictive tools. However, many of these efforts fall short of full recognition that engineered materials are systems. What is needed is a computational methodology and framework for systems engineering of materials and the sciences that support such an approach. The systems engineering of materials within a simulation environment will provide advances to both the materials utilization and representations for usefully advancing quantitative microstructure–property relationships. To better understand what is needed from the computational framework, it is useful to briefly examine materials in present-day engineering.

About 100 years ago, a defining aspect of materials science and engineering (MSE) had its origin in the first microscopy studies of materials structure; yet, nearly a half-century would pass before their impact evolved into the MSE discipline (Smith 1988; Cahn 2001; Olson 1997). With the study of microstructure (including defect structure or statistical extrema), the materials engineer gained an important tool by which processes and properties are controlled. Microstructure–properties science was born and has expanded ever since. MSE now recognizes four major disciplines of practice that identify the unique character of the MSE field: processing–structure–properties–design, irrespective of the material type, class, or design application (see Fig. 1). However, unlike other mainstream engineering

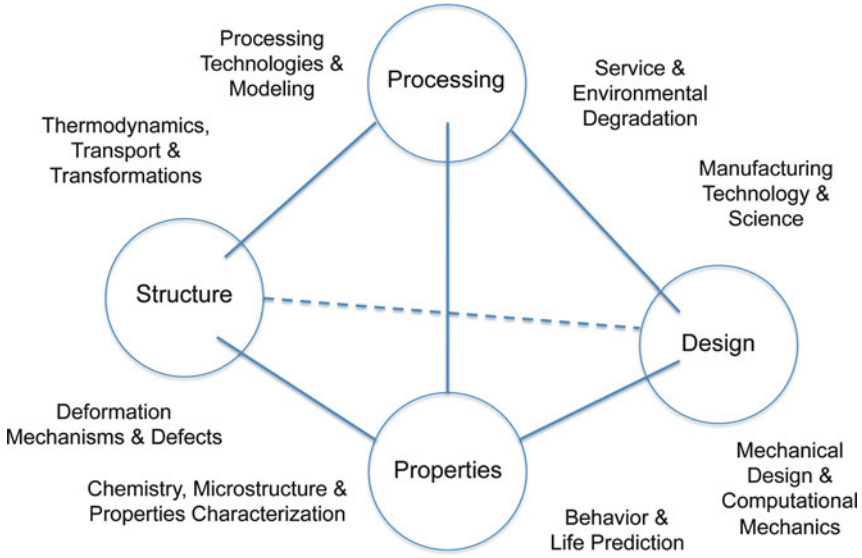

Fig. 1 The four defining disciplines of practice for materials science and engineering (MSE) represented as a tetrahedron. In this context, "Processing" refers to composition, synthesis, and processing in general. "Structure" refers to all aspects of microstructure, including both intrinsic and extrinsic defects from the atomic to macroscopic scales. "Properties" and "Design" refer to materials performance and behavior and, to engineering design rather than materials design, respectively. Selected examples of the types of studies and activities that tend to link the major disciplines are shown about the periphery of the figure

disciplines (e.g., civil, chemical, electrical, and mechanical) that largely came into existence as the quantitative frameworks for them emerged, the same cannot be said for MSE.

More broadly speaking, structural alloys tend to be defined from two different perspectives. Materials producers (and patent law) associate them with compositions of matter and the prescribed synthesis and process paths by which they are formed into engineered products. Alternatively, from a structures-design engineering perspective, materials are viewed as contextual databases containing representative measured values of property bounds, including statistical minima, as functions of selected variables, such as temperature or state of stress. These are often represented within models. The contextual aspect of those databases usually relates to specific application products and manufacturing processes. Additionally, the structures engineer also attributes the businesses and practices that make materials available as products to the materials engineering discipline. Historically, the metallurgist, ceramist or chemical engineer and, more recently the materials-scientist or engineer carried out the onerous task of melding these perspectives into unified activities and practices for safe and affordable structures. Within this engineering reality, the notion of microstructure–property relationships is only implicit at best. While both materials and process engineers and part designers recognize that structural materials have significant microstructural variations, there are few quantitative tools and standards that permit integration of that knowledge into the broad engineering process, especially in a predictive manner. Consequently, outside of the MSE community, processing–properties–design relationships (not including structure) are generally recognized via the "allowables" (i.e., distributions of property values including statistically defined minima) for using a material for a given design. For most of today's products, one typically defines an application and then seeks to define and document a processing specification through specific suppliers by which a selected composition of matter will reproducibly lead to properties (performance) for that application. Material microstructure descriptors, such as grain size (ASTM 2002), are only used as specifications of the material for process assurance.

For higher value engineered structures (e.g., a gas turbine engine disk), a database of processing–properties relationships typically develops in which the data are reduced to phenomenological constitutive laws that are linked to the application design process via finite element method simulations of the part configuration. With few exceptions, these constitutive relationships are assumed to hold over volumes of material that are essentially on the scale of the part (meter scale), even though every metallurgist or materials scientist understands that heterogeneities or defects that affect properties exist over many length scales from the full part to the atomic level. Clearly, there is a disconnection between MSE, and the broader engineering community as the notion of processing–structure–properties–design essentially does not exist beyond MSE.

This disconnection is a rational result of the fact that even after a century of development the quantitative links between processes and structure and, structure and properties, are insufficiently advanced to permit direct systems-oriented

optimization of materials and products (in "Simulation-Assisted Design and Accelerated Insertion of Materials" by McDowell and Backman). There is simply too much complexity associated with the kinetics of processes to quantitatively define the resulting microstructures within the equally complex hierarchy of length and timescales of the applications. For electronic materials, the length and timescales may be extremely small fractions of seconds and nanometer dimensions, while for structural composites they may be at the scale of the components and system dimensions (meters) over timeframes of years.

Fortunately, current advances in computing capabilities and MSE tools bring opportunities for not only expanding the quantitative basis for processing–structure–property–design relationships within simulation environments but also for redefining aspects of MSE within those simulation environments. In so doing, MSE becomes a quantitative engineering discipline for structural materials and several aspects of its relationship to other engineering disciplines will be redefined. Full recognition of this opportunity stems from considering aspects of the use of computer modeling and simulations along the evolutionary path of MSE.

2 Computational Materials Science for Microstructure

Computers and simulation were available essentially since the origins of MSE as a recognized discipline. Several phases of their use in MSE are linked to growth in computational capacity and databases. In the 1950s and 1960s, the computer was commonly used to model specific phenomena, usually within a mean-field, especially where numerical solutions to differential equations were necessary. From a materials engineering perspective, perhaps the best example of this is the computer calculation of phase diagrams or the "CalPhad" method that was well developed by the end of the 1960s (Kaufman and Bernstein 1970). During that period foundations were built for materials-oriented computer simulations that last to this day (see additional diverse examples such as computing diffraction contrast of transmission electron microscopy images (Head et al. 1973) and plasticity analysis for metal deformation (Mandel 1973; Kocks 1987) to name but two others. Importantly, even though the foundational sciences were known more than 40 years ago, neither the computational capacity nor the necessary databases were sufficiently developed for the CalPhad method to have significant engineering impact at that time for alloy or process development. Only about 10 years ago did the method begin to add value to engineered products and the practices of MSE. Today, after more than a decade of sustained development investments for engineering, CalPhad techniques are becoming a part of standard industrial methods (NMAB 2008; Backman et al. 2006).

A second phase in the maturation of materials computational methods occurred during the 1970s and 1980s through research in process modeling. Simulation codes evolved that are still in use today (ProCAST http, DEFORM http). These codes, based on continuum fields and state variables without treatments of microstructure, are essential to design engineering of aerospace and other industrial parts

and components. Also during this period, methods for solving a range of materials challenges from the electronic structure of materials to techniques for plasticity and stress analysis continued to advance (Hafner 2000; McDowell 2000). Methods for simulating plasticity under crystallographic constraint within the finite-element method gave new insights into behavior at the mesoscopic scale, including strain localization during crystal slip (Asaro 1983).

One could say that during the late 1970s through mid 1980s, computational materials science (CMS) came into its own as a discipline of study. Here, the term CMS refers to the activities of a widespread community of investigators that are developing simulation tools to represent unit mechanisms exhibited by materials. These include such techniques as electronic structure methods for selected material properties and thermodynamic quantities (Hafner 2000; van de Walle et al. 2002; Liu et al. 2006); empirical atomistic methods that offer insight into understanding dislocation core structures, surfaces and grain boundaries (Daw and Baskes 1984; Vitek 1985; Tschopp et al. 2008); dislocation dynamics methods (Devincre et al. 2001; Ghoniem et al. 2000); phase field methods and, many others. A good compendium of such methods may be found in the work edited by Yip (2005).

However, the majority of the CMS-based advances in understanding mechanisms of materials behavior had little or no impact on materials engineering. While the quantitative nature of simulated results improved, too frequently they lacked comprehensive context or sufficient accuracy for use in engineering design. The few applications of simulation-based methods to industrial-world microstructure–properties engineering tended to use simulation results to provide qualitative insight into existing engineering processes (see for example Dimiduk 1998); however, there were notable exceptions (Shercliff and Ashby 1990). There are numerous reasons for this, but obvious among them was insufficient computational capacity together with the integrated data available during that time.

Throughout the 1980s and 1990s, many materials simulation efforts were performed in relative isolation within the MSE, physics, mechanics, and chemistry communities having few linkages to engineering techniques or design tools. Unlike other engineering disciplines, one might suppose that the role of simulations within MSE was viewed as only interesting or important for understanding qualitative behavior trends since so little community-wide work was carried out to establish standard techniques and methods as foundations for industrial practice. Consequently, simulation-centric materials engineering methods continued to evolve in a piece-wise fashion within proprietary corporate communities. Throughout this period, there were few efforts outside of the process-modeling discipline that attempted to integrate mechanistic or heuristic knowledge within simulations to understand the microstructure–property relationships in engineered products, as a standard methodology of practice. Although some researchers recognized that the quantitative aspects of microstructure–property relationships were underdeveloped (Cedar 2000), CMS was often characterized as simply “applied quantum mechanics” (Bernholc 1999). During this period, CMS was essentially a “cottage industry” of models and modelers of and to itself (Dimiduk et al. 2004a).

During the mid and late 1990s, a few industry, government and academic leaders began to see the limiting aspects of this state of CMS (see for example Olson 1997; Christodoulou DARPA-AIM http; Fraser CAMM http). These leaders recognized that CMS approaches to materials modeling typically originated from the "bottom up" of the length and time scales and that such approaches rarely made an impact on the practices or efficiencies of design engineering, especially for structural materials. Further, there was recognition in the MSE community that significant computing capability was becoming sufficiently widespread that new approaches to simulation-based materials engineering should be attempted from the "top down." As a result, two notable new initiatives in computational-based materials engineering were initiated in the first year of the new millennium (NMAB 2008).

3 Integrated Computational Materials Engineering

3.1 Materials Readiness and the Evolving Microstructure–Properties–Design Paradigm

To best understand the uniqueness of the integrated computational materials engineering (ICME) approach and its impact on the practices associated with microstructure–properties–design relationships, it is useful to first understand the concepts of materials engineering readiness. Materials development and process engineering involves significant open-ended risk and cost. To manage and mitigate that risk, the MSE community adopted various frameworks for assessing readiness along the pathway toward product application. These frameworks are similar to ones used for other engineering but are tailored (especially within major manufacturing companies) to materials and processes disciplines. Figure 2 illustrates the highest-level structured "stage-gate" process that exists within most materials and processes practice. Typically, ten levels of readiness are defined and the progression of application-specific technologies through these levels occurs within well-defined engineering templates. These templates demand specific test data, cost assessments, manufacturing source qualification, etc. that gain fidelity *and scope* at each stage of development. This serially staged paradigm of materials and processes technology maturity to some degree reflects the learning curve that innately exists for anything new. Unfortunately, the expanding scope required at each step is a key limiter to this paradigm that adds significant risk, quite often cost, and certainly time.

Reviews of case studies of materials development that follow a serial paradigm have shown that it leads to serious challenges for materials development and limits the opportunities for coupling materials and process advancements within mainstream engineering design practice (NMAB 2008; NMAB 2004; Lipsitt et al. 2001; Dimiduk 2001; Dimiduk et al. 2003). The serial paradigm leads to what has been called the "valley-of-death" for new materials and processes. That valley exists for several reasons including funding gaps, long time requirements for experimental

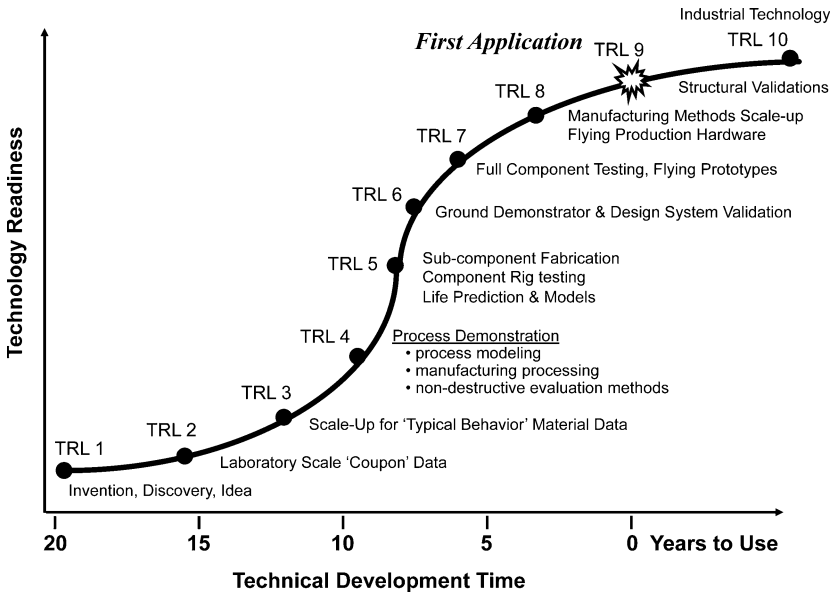

Fig. 2 General technology readiness levels (TRL) for materials. The ten stages of materials readiness are adopted from the broader engineering readiness metrics used for products and systems. Historically, achieving the transition from TRL 3 to TRL 5 is the most difficult step. The reason for this is that technical risks typically remain high at TRL 3; however, the financial outlays required to mitigate them also grow much more substantially at this stage by comparison to the lower levels. Better materials and processes simulation tools are needed throughout, but especially for risk mitigation through the TRL 3–5 maturity levels. For aerospace materials, evolutionary advances (such as modified alloy compositions within established applications) are known to require 7–12 years to reach first use. For more challenging completely new materials, such introducing ceramic composites or TiAl alloys in turbine engines, the time span for achieving fist-use readiness exceeded 26 and 36 years, respectively

or empirical iterations and, what may loosely be called a "point contact" interface between present-day design engineering and materials engineering.

To further illustrate this point of contact, Fig. 3 schematically depicts the broad engineering procedural steps that may be used to select the geometric configuration of a manufactured aerospace metal component. The figure also shows selected materials and processes procedural steps that are taken to assure appropriate microstructure–property relationships are maintained in the final product. Inspection of the figure reveals that the primary interface between the design process and the materials development process lies in the steps needed to assure that validated constitutive descriptions (or minima curves and allowables) are available for the design optimization procedures. Thus, within this schematic depiction, the interface between the communities is a point contact. This point of contact includes not only the constitutive laws that reside within component design codes, but also their empirical validation against databases that must sufficiently encompass the variations of microstructure–property relationships judged to be important to the specific

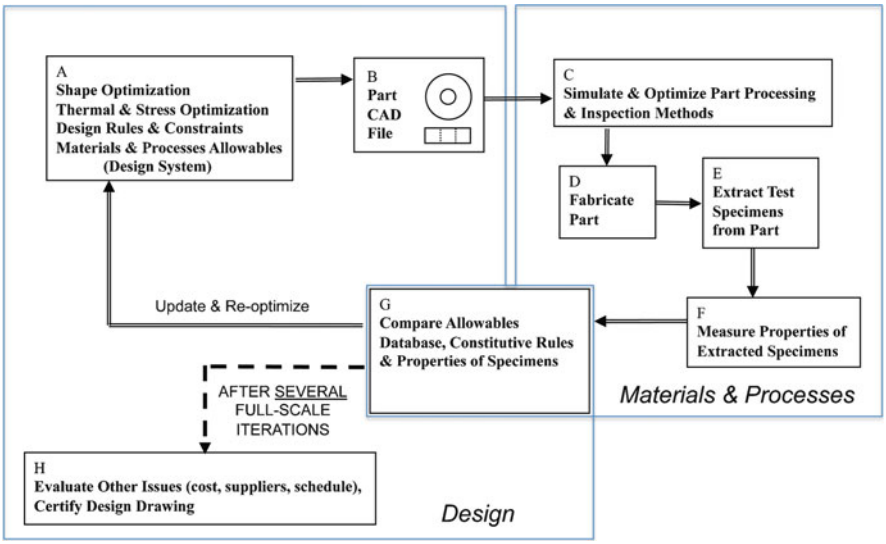

Fig. 3 Schematic representation of activities within today's experiment-intensive processing–properties–design serial paradigm for materials engineering. The methodology has no explicit consideration of microstructure. Microstructural effects are only implicitly considered when extracting specimens and as selected specifications for parts. Microstructural effects/variation is represented through expensive, time-consuming testing and multiple full-scale process and test iterations are usually required

design. Given that the allowables databases are produced from application-specific, full-scale development hardware, this serial approach inevitably leads to a conservative estimation of material performance and does so through a costly process.

Since part-specific and feature-specific microstructures and properties cannot be accounted for within the design system, the observed "worst-case" uncertainties are assigned to all parts at all locations (Christodoulou and Larsen 2004). Consequently, microstructure–property relationships are specified and controlled in the context of their application databases alone, usually via testing of full-scale prototype parts. However, further advancement in the design process demands a less conservative and more realistic, probabilistic approach (McClung et al. 2008; Millwater and Osborn 2006). That new demand is driving the MSE community toward developing predictive tools for location-specific properties that can be used within probabilistic design tools.

Herein lies one major hurdle for microstructure–properties sciences and materials development in general. As long as materials behavior can only be indirectly defined within the very specific contexts of their applications, via extensive testing of samples excised from full-scale prototypes that may not even directly capture the design or materials-limiting features of interest, materials development will always entail long development times and high costs. That fundamental limitation in the procedure for obtaining and representing materials performance data presently

places the whole of MSE into a unique domain that is outside of those of the other engineering disciplines. The time scales, cost structures and design tools are simply mismatched, while the risk is high. Today one develops empirical knowledge of materials response to chemistry and process iterations within the stage-gated templates described previously, such that learned practitioners of the engineering disciplines can support design judgments. Those judgments inevitably entail reasonable assurances to business managers that the financial investments in scale-up and advances in technology readiness are affordable within business plans and product timing. For the future, materials development needs to be achieved via a new materials-to-design paradigm. Essential to that paradigm is that the materials readiness structure (readiness templates) be re-cast to maximize the scope of readiness information at the earliest stages; then, to expand only their fidelity with added development investments and time. Fortunately, efforts toward building these are well underway.

3.2 Accelerated Insertion of Materials, Virtual Aluminum Castings, and the ICME Paradigm

Today, the computational tools that facilitate quantitative support for the development and investment judgments required for materials scale-up are just emerging. Examples of these exist within the ICME demonstration efforts that occurred during this decade (NMAB 2008). Essentially, the underlying concept behind the efforts is that having simulation tools for all aspects of new product and materials development will reduce development time while lowering costs and risks. Two notable examples of the ICME paradigm will now be discussed.

Within the aerospace sector, the Accelerated Insertion of Materials (AIM) program was sponsored by the US Defense Advanced Research Projects Agency (DARPA) and the United States Air Force, to examine and restructure the paradigms for metal and organic-composite materials development (NMAB 2008; Backman et al. 2006; Dimiduk et al. 2003, 2004a, b). Similarly, within the automotive sector, the Virtual Aluminum Castings (VAC) program was sponsored by Ford Motor Company (NMAB 2008; Allison et al. 2006). In the specific sense of microstructure–property relationships, the efforts showed that representing the microstructural aspects of materials (especially including kinetics and mechanical behavior), via models that are integrated within design-engineering optimization protocols and software, yields dividends to the product development cycle. Importantly, the case studies showed that even elementary theory and empirical models have a substantial positive impact on the design engineering process when fully integrated within a computational environment (NMAB 2008; Dimiduk et al. 2003). Somehow, that important payoff to engineering was missed by most of the CMS and MSE research communities and to this day is not developed as an integrated materials engineering standard practice. Also, when viewed from the perspectives of these demonstrations, there is now a clear justification for expanding the fidelity

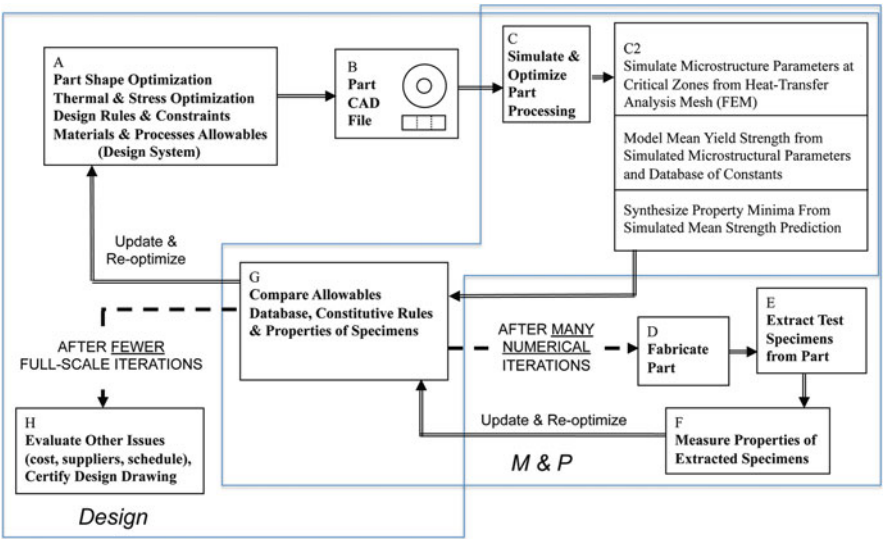

Fig. 4 Schematic representation of activities within ICME paradigm for materials engineering (see text for explanation). Methodology explicitly includes microstructural-based design via microstructure evolution within process models and, mechanical property models being applied to various regions of designed part. Including microstructure–property relationships via simulations means that the domains of design and materials engineering overlap much more significantly within ICME than within the historical paradigm for materials engineering. The ICME paradigm includes the early cases of explicitly using processing–structure–properties–design within closed-loop engineering frameworks

of microstructure–property representations and predictive capabilities and, also a somewhat general template for both focusing those developments and then integrating them into the product value stream as they occur.

The materials and processes development paradigm has changed with the evolution of ICME. Figure 4 shows a similar schematic as the one previously described in Fig. 3, but with modifications that reflect broad procedural changes brought about via the ICME approach as it was applied in the AIM program. Two aspects of the new procedure are noteworthy. First, as shown by the expanded activities associated with step "C2" (in the upper right-hand side of the figure), specific simulation tools focused on microstructure–property relationships enter into the development paradigm. Second, utilizing such tools fundamentally changes the experimental activity that currently takes place to empirically assure the manufactured products perform in the desired fashion. Rather than many full-scale synthesis and processing trials followed by sectioning and testing, many of the results of such efforts are now anticipated via simulations. Having models, even in empirical form, integrated with the design process permits iteration and optimization via design tools and minimizes the time-consuming and expensive procedures associated with full-scale prototype product development. Thus, the overlap between engineering design and MSE fields of practice has expanded. That expansion is the direct result of

using simulation tools to provide a more quantitative and structured description of the microstructure–property relationships of materials. A widespread acceptance by a peer group of engineers, systematic reductions in the types, cost and quantity of data needed and, the predictive nature or capabilities of the microstructure–properties relationship tools used within such a paradigm, are all direct measures of the quantitative advance of the field. Future advances in computational methods for microstructure–property relationships should be evaluated by those metrics.

3.3 The Evolving Needs for Materials Data

Another important aspect of the ICME paradigm for materials not explicitly shown in Fig. 4 was a significant aspect of the both AIM and VAC feasibility demonstrations. That aspect pertained to the development of models and the nature of experimental data. Within the historical processing–properties–design paradigm for materials, critical design data exists almost entirely in the form of measured mechanical properties obtained from production-scale hardware – again, having little explicit connection to microstructure. However, the ICME paradigm changes the structure and types of data that are essential to design. *Under the ICME approach, data must be associated with models and supported simulation codes*. Also, specific types of data are collected for the primary purpose of validating codes. That data often extends outside of the ranges typically associated with prototype parts and may be associated with certain pedigree-type materials and microstructures. Fortunately, just as simulation tools and models are becoming more advanced, test and evaluation procedures are becoming automated and miniaturized. Critical data can increasingly be measured from small-scale samples prepared to validate kinetics or mechanical behavior domains for models.

The last paragraph discusses points that are nontrivial and merit further comment. For example, the nature of data intrinsic to an expanding ICME paradigm is data associated with simulation tools and their validation. Those tools by their inherent architectures and operative material models define the data required for their use. In this respect, the ICME paradigm is in its infancy and aspects of data taxonomy and efficiencies must be developed for the purposes of supporting simulations. However, even from the initial case studies just described, the ICME paradigm suggests a different view of data and materials informatics than the one described by recent reports on the subject (Cebon and Ashby 2006; Arnold 2006). Those reports essentially describe higher-fidelity extensions of the classical MSE-design paradigm – a paradigm constrained by the empirical development of handbook materials allowables. Within that paradigm, the role of the computer is “passive” in that it primarily facilitates the organization of greater quantities of information. When data sets are sufficiently large and too complex for typical human interrogation, this paradigm may not exclude cases of the “blind discovery” of new relational knowledge (data mining) in a more “active” mode.

However, computational tools and simulation environments are beginning to synthesize data that may be fused with conventional empirical measurements (Liu et al. 2006; van de Walle et al. 2002). The practice is likely to spread far beyond its present use within alloy thermodynamics. Yet, there is little readiness for this within the old processing–properties–design paradigm and the practice is limited even within the current ICME paradigm. The MSE and design communities have a formidable task ahead of them to define appropriate data architectures and a taxonomy that will not only permit full "active" utilization of materials simulations in the design process but also maintain efficient certifiable engineering practices throughout the new simulation era. Within an emergent paradigm called here "virtual materials systems" that taxonomy and the actual data are facets of the substantially expanded and quantitative nature of microstructure–property relationships. Finally, the new ICME paradigm suggests that the materials allowables view of data will change to more effectively utilize the active power of materials simulations for "synthesizing" data and providing quantitative insights into materials response.

3.4 ICME: Lessons Learned

There is value to considering lessons learned from the initial case studies of AIM and VAC. The recent report by the US National Materials Advisory Board discusses some of these lessons (NMAB 2008), but a selected three global aspects are highlighted here. First, for the longer term, the contrasting primary attributes of engineering design and MSE must be bridged. For engineering design, those attributes include a simulation-centric community of practitioners, education structures that convey such practices, well developed and supported simulation tools that are integrated with heuristic data and, the expectation that many rapid-time-frame simulations will be carried out as a routine part of the design process. Conversely, the primary attributes of MSE in this regard currently include long lead times for experiment results within a data focused community of practitioners, an educational system that is just now grappling with an appropriate treatment of ICME and its tools, relatively few established and supported simulation codes that are still too separated from heuristic data and, a general expectation that when simulations are done they will commonly be characterized by relatively few large-scale simulations performed in a supercomputing environment. As aspects of the previous discussion and portions of this book support, the gap between these communities exists in no small part because of the still underdeveloped quantitative sciences and standards associated with materials microstructure–properties kinetics and mechanical behavior.

A second lesson contained in ICME is that the engineering design paradigm needs to evolve to explicitly include material heterogeneity within engineered parts (read microstructure–property–design relationships). In present day design practice, those aspects of heterogeneity not broadly included in databases or represented in analytical and simulation tools tend to be captured via heuristic rules that constrain the design process. For example, heterogeneities within materials lead to a