

Models, Databases, and Simulation Tools Needed for the Realization of Integrated Computational Materials Engineering

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INTRODUCTION

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THE INDICATIONS OF SUCCESS EXIST

It would be hard to argue against the fact that Integrated Computational Materials Engineering (ICME) is a fast growing discipline within material science and engineering. A quick scan of the proceedings from conferences such as Aeromat, Material Science and Technology, and the TMS Annual Meeting clearly shows it. What began a few years ago as one symposium has grown into multiple ICME related symposia at each of these conferences. As encouraging as the number of symposia being offered is the attendance at the symposia. For example, one of the ICME symposia at MS&T '10, the symposium in which this book is based, had five sessions which culminated in a panel discussion that was standing room only. In addition to the large, annual materials science and engineering conferences, smaller 1 to 2-day conferences/workshops sponsored by government agencies (e.g. AFRL and NIST) on specific aspects of ICME and by universities promoting their ICME work are regularly offered. And arguably the most significant news with regards to ICME and conferences is the July 2011 First World Congress on ICME. This five day TMS sponsored conference, specifically focused on ICME with an international advisory board of ICME leaders, shows how far ICME has spread across the globe.

Evidence for the growth of ICME can also be found in Academia. The University Materials Council (UMC) is composed of department heads for material science and engineering from major U.S. and Canadian universities. Meeting twice a year to share best practices in order to strengthen both the engineering content [1] and the educational process, the UMC's agenda for their Spring 2010 meeting was dedicated to ICME [2]. This meeting was held in response to the growing awareness that the universities play a major role in the success of ICME and therefore need to develop ICME curriculum in order to meet that need. To aid educators in the development of ICME courses, NSF is funding a "Summer School" on ICME to be held at the University of Michigan in 2011 [3]. Northwestern University recently announced a MS Certificate Program in ICME [4]. Course work for this certificate begins in the Fall of 2011.

Other signs that ICME is growing comes from the formation of ICME initiatives from work that did not start off with ICME in mind. One of the committees in ASM International is the Materials Properties Database Committee (MPDC). In the 2010 meeting of the MPDC, based on a study by ASM, the committee decided that it would create an ICME sub-committee in order to determine how ASM can meet the growing needs of the ICME community [5]. In 1999, the Air Force Research Laboratory (AFRL) created a consortium, the Metals Affordability Initiative (MAI), with members from both industry and government with a goal of reducing the cost and time to market of producing metal parts for aerospace applications [6]. Recently, AFRL and the other

members of the MAI consortium realized that ICME is a critical technology and should be a focus in order to realize the original MAI goals [7].

THE REALIZATION FOR SUCCESS IS IN WORK

While there is clear indication that ICME is growing, the realization for the successful implementation of ICME in daily work of researchers and engineers in industry and academia is still lacking. The MS&T 2010 ICME symposium was developed with this in mind. The goal of the symposium, “Tools, Models, Databases and Simulation Tools Developed and Needed to Realize the Vision of Integrated Computational Materials Engineering,” was two fold 1) capture the state of the art work in ICME and 2) provide an opportunity for ICME leaders to present and discuss current gaps and barriers holding ICME back from being a realized success. The conference symposium was divided into 5 sessions: one on *Informatics and Infrastructure*; two on *Material Models and Simulation Tools*; one on *Experimentation and Integration of Models*; and the final session consisting of a panel discussion on *Barriers to ICME and How to Overcome Them*. While this book contains approximately half of all the papers presented at the symposium, these representative papers have been organized into three sections in order to capture the overlap in topics and to avoid unnecessary divisions. The three sections are:

- Current State of ICME
- Database and Infrastructure Needed to Enable ICME
- Current Work and Models in ICME

The goal in this division was to first introduce the reader to a broad overview of the current state of ICME and then narrow down to specific needs and work that are going on in ICME. To varying degrees, each paper addressed the current gaps and barriers that currently exist in the topic that the authors were assigned to write about.

Current State of ICME

This section begins with a paper by Drs. Rani Sullivan and Steven Arnold. In this paper, they survey and review recent work being done in the field of Multiscale Modeling (MM). In doing so, they attempt to categorize work, clarify terminology (even to the point of introducing a new computational strategy descriptor, i.e., synergistic), summaries advantages and disadvantages of atomistic, micromechanics, and macromechanics multiscale approaches, establish the relatedness of MM with ICME, and lastly identify issues from MM that will help the ICME community do their work. This overview provides the reader with a good perspective of numerous issues that will be addressed in the chapters to follow.

Giving hope that ICME not only will produce real world value in the future but that this field already is producing real results today, Drs. Charles Kuehmann and Greg Olson document the success that they are having in implementing ICME techniques in the computational design of new materials and in the qualification of materials. Both the computational design of new materials and the computational qualification of a material are key goals for ICME. They, however, warn that ICME can only produce real practical results when engineering is as valued (i.e. “funded) as much as science is. They propose the creation of a National Engineering Foundation similar to and complementary with the National Science Foundation.

Agreeing with Drs. Kuehmann and Olson on the need for ICME to be rooted in engineering, Dr. David McDowell expands on the topic of the barriers that must be overcome for ICME to succeed. He looks at these barriers from the perspective of industry, government funding

agencies and academia. One of his key points is that ICME can only succeed when those involved realize the multidisciplinary nature of ICME and should not be regarded merely as a subset of material science and engineering.

Dr. George Spanos describes his view on how ICME will succeed when the four foundational groups all participate and work together. Dr. Spanos, like Dr. McDowell, recognizes the key role that industry, government and academia play but Dr. Spanos adds a new group, the professional societies. Coming from a government agency and now as the Technical Director at TMS, he understands very well what key role that often forgotten group, the professional society (e.g., AMS and TMS), can play in the development of ICME.

This section closes with a broad yet detailed paper on the current state of ICME in relationship to the aerospace propulsion industry. In their paper, Drs. Brad Cowles, Dan Backman and Rollie Dutton provide an assessment of the current state of specific areas within ICME that are currently employed and then go on to discuss barriers. Some of the areas described as barriers and challenges are topics within what is typically considered the domain of ICME but other challenges and barriers come from the culture in which science and engineering take place (e.g. Intellectual Property and Export Control issues). While these barriers may seem daunting, the authors close with their strategy on how ICME can be successfully implemented.

Database and Infrastructure Needed to Enable ICME

The next section covers the topic of database and infrastructure (often called “cyber-infrastructure”). Just as the transportation infrastructure is essential for the flow of commerce, the cyber-infrastructure is the road on which materials information for ICME flows and resides. The fundamental role of the ICME infrastructure in general and databases specifically play is recognized in the landmark ICME publication by the National Academy of Engineers in 2008 [8].

An aspect of the ICME infrastructure that will make it easier for people doing ICME to exchange data from one model or database to another is the development of standard format (or protocol) for data exchange. Dr. Tim Austin, et al., describe the benefits and need of having standards-compliant formats for the exchange of materials test data. They provide an example in which they have successfully demonstrated the feasibility of standards-compliant data formats in the area of materials test data. While no one will deny the benefits of having a standard format for data exchange, their work is an encouragement that such an endeavor is possible.

Building on his many years of work in materials informatics, Dr. Krishna Rajan shows how important it is to use the discipline of informatics when building a database. Calling the classification and organization of data using the discipline of informatics “ontology engineering”, Dr. Rajan effectively demonstrates how building a database based on ontology engineering principles can transform a database from merely a source of data to a means of learning and knowledge.

On the surface, a materials properties database may seem simply like a fancy means of storing, retrieving and distributing materials data; something akin to an electronic file cabinet. If that is what a materials database is and can be, the vision described in Dr. Rajan’s paper could never be realized. But Drs. Will Marsden, David Cebon and Elizabeth Cope show that an effective ICME materials database must allow the data inside a database to be seamlessly accessible by analysis tools. The database then must allow the results from the analysis to be read back into the database and stored with all the associated metadata while keeping track of their associations. While they did not specifically discuss integrating the database with an informatics tool as

described by Dr. Rajan, the basic concept of interoperability described by them make such an integration possible.

Current Work and Models in ICME

Dr. Chandler Becker's paper heads up the last (and largest) section of the book with her work on atomistic simulation and the role it plays in ICME. Dr. Becker begins with an overview of one of the goals of ICME, Materials by Design, then discusses the current atomistic work and ends with challenges that face the use of atomistic simulation in ICME. Her paper clearly show that while there are issues that need to be addressed in the use of atomistic simulation in ICME, the potential is there to make it a worthwhile pursuit.

The rest of the six papers in this section deal in some way with multiscale modeling. The first paper is by Dr. Geroge Gazonas, et al., which describes the modeling work that the Army Research Laboratory is doing on aluminum oxynitride (AlON). In their work, Dr. Gazonas, et al., describes both their experimental observations and the computational modeling work in order to show the feasibility of an ICME approach to modeling materials.

Although, Drs. Becker and Gazonas mention the benefit and use of ICME for the design of materials, the next two papers (one by Drs. Samit Roy and Abilash Nair and the other by Dr. Tom Lacy, et al.) discuss another benefit (albeit for different material systems); namely the ability to predict properties using the methodology provided by ICME. Using thermoplastic nanocomposites as an example, Dr. Roy proposes using a concurrent modeling approach to understand the strengthening mechanism in this material system. With this knowledge on hand, the goal is to be able to predict material properties. In similar fashion, Dr. Lacy, et al., show how using molecular dynamic simulations can result in data that can be used to feed NASA's composite failure analysis code (ImMAC). While all acknowledge that there are gaps and barriers, both papers move us forward in realizing how using ICME methodology in general and molecular dynamic simulation specifically can help us reduce the cost of the trial-and-error approach to materials characterization.

With the assumption (one based on the classic diagram by Olsen [9] and seen in many variations throughout this book) that ICME is inherently multiscale with reference to space and time, Drs. Mark Tschopp, Kiran Solanki and Mark Horstemeyer argue that a more generalized framework is needed in order to quantify the connection from one length scale to another. To argue their case, they focus on the relationship between interatomic potential to grain boundary structure and then to grain boundary properties.

Dr. Serge Kruch describes his work on multiscale modeling of composites, including elasto-viscoplasticity and damage, from the scale of the fiber and matrix constituents to that of a composite structural component. Contrast is drawn between the hierarchical approach, wherein homogenized constitutive equations are developed based on micromechanics prior to structural analysis, and the integrated approach (referred to as "synergistic" in Sullivan and Arnold's contribution), wherein micromechanics modeling is conducted during the structural analysis at each material point. Using the Transformation Field Analysis (TFA) micromechanics method with application to a SiC/Ti composite, it is shown that it is possible to achieve comparable accuracy with the hierarchical approach while saving significant computational time compared to the integrate (synergistic) approach.

Drs. Brett Bednarcyk and Steven Arnold conclude the body of the book with their general multiscale modeling framework for composites that has been implemented as a NASA developed software tool called ImMAC. Here, the synergistic approach to multiscale modeling of

composites (from the constituent to structural scale) is used, however, by using the efficient Generalized Method of Cells (GMC) micromechanics model, required computational time remains reasonably short. Two applications are presented; a SiC/Ti composite with viscoplasticity and damage, and a woven PMC with plasticity. These authors also argue that, for an analysis to truly qualify as multiscale modeling, three levels of scale (with two scale transitions) must be considered. Otherwise, if a two-scale analysis is considered to be multiscale, almost all structural analyses would qualify.

CONCLUSIONS

The breadth of the topics discussed in the book is a small taste of the wide number of topics that ICME as a discipline encompasses and the inter-disciplinary nature of ICME. The depth to which some of the authors in this book covered their subject matter is an example of the need for specialists in ICME. For ICME to succeed, scientist working in their areas of specialties will need to understand the role they play in ICME in order for the engineering of products using ICME to become a reality. And those working to make the vision of ICME a reality will need to understand the broad number of disciplines that ICME encompasses in order to ensure that ICME succeeds. This book ends with three over arching suggestions that the editors of this book believe are needed to make ICME successful.

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AN ANNOTATIVE REVIEW OF MULTISCALE MODELING AND ITS APPLICATION TO SCALES INHERENT IN THE FIELD OF ICME

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ABSTRACT

In order to obtain a general understanding of the rich and diverse research being conducted in the area of multiscale modeling (MM), an overview is conducted with a special focus on composite materials. The objective is to glean both qualitative and quantitative information with regards to MM efforts with intentions of revealing some issues that may enable the field of Integrated Computational Materials Engineering (ICME) as well as providing a starting point for specialists and non-specialists in the area of MM with regards to a variety of classifications.

INTRODUCTION

Multiscale Modeling (MM) is defined as the field of solving physical problems which have important features at multiple scales, particularly multiple spatial and (or) temporal scales. This definition encompasses the basic materials science paradigm shown in Olsen's [1] classic diagram, see overlapping ellipses in Figure 1. From this figure one immediately sees the interconnection of scales and their cause/effect relationship, e.g., processing conditions produce a particular microstructure from which properties are obtained, which then dictate a specific structural performance. Note that the evolution of line type in the insert (dotted to dashed to solid line) is purposely included to visually suggest to the reader the level of maturity/understanding (from immature, semi-mature, mature, respectively) of modeling at each level of scale. Furthermore, the figure demonstrates the importance of understanding the input and output at each scale in order to determine meaningful properties that are ultimately required by a structural analyst. Similarly, the experiments (whether virtual or laboratory) performed at each level can be viewed either as exploration or characterization experiments used to obtain the necessary model parameters operating at the present and/or next

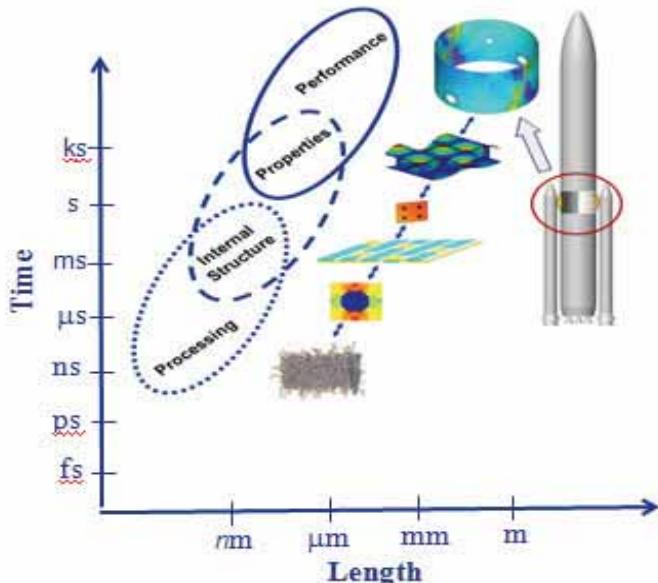


Figure 1 Schematic illustrating the multiple spatial and temporal scales active during material and structural design

higher level or be used to validate the modeling methods employed to transition from the lower level to the given level.

To get a general picture of multiscale modeling (MM) activity, the growth in the number of archival journal articles on MM of composite materials from 1989 to 2010 is noted and shown in Figure 2. The rapid rise of research in the area of MM (see curve (a)) is obviously due to the remarkable increase in computational power as shown in the inset figure (d). However, even with current computational power, only a limited volume of total atoms (approximately one cubic micron) have been modeled [2, 3].

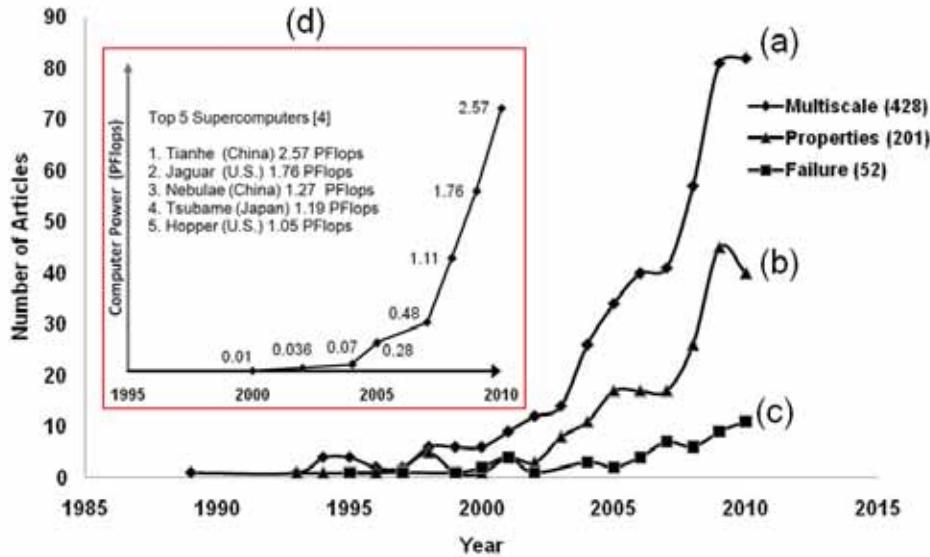


Figure 2. Journal articles from 1989 -2010 on composite materials for (a) MM (b) MM of properties and (c) MM of failure[4]. The development of computer power is shown in (d) [5]. Total number of articles is shown in parentheses.

The rise in MM activity is also evident by the numerous survey articles and books available on the subject, as listed in Table 1. Most of these articles deal with MM strategies, approaches and MM treatments of specific material systems. The current effort is not meant to be an exhaustive or an all-encompassing review on a specific topic in MM— for particular areas, the resources in Table 1 provide an excellent starting point. This present paper seeks to provide a very broad overview on MM by categorizing a number of selected papers by a variety of MM characteristics such as scales, applications (deformation, evolution of structure, failure), MM strategies (serial or coupled) and linking information to bridge scales. By so doing, a somewhat quantitative assessment is made that gives a general impression of MM activity over the last decade.

At the beginning of this effort, it quickly became evident that the field of MM is so vast that some constraints must be introduced. Most of the selected articles are from 2000 to 2010 and focus is maintained on the behavior modeling of structural materials. Although the bulk of papers concern composite materials, some interesting papers on monolithic materials are also included, as shown in Table 2. The inclusion of a wide variety of material systems gives insight into the numerous MM strategies and terminologies that are being used currently.

Table 1. List of survey articles and books on multiscale modeling.

SUBJECT	REFERENCE	MATERIAL
Mean field approximation theories	[6] Baeurle	Polymers
Statistical micro damage mechanics; Spatial and temporal	[7] Bai, <i>et al.</i>	Polycrystals
Damage and failure	[8] Bazant	Heterogeneous
Failure processes in composites	[9] Beaumont	Polymer composites
Scaling laws – cohesive crack modeling	[10] Carpinteri, <i>et al.</i>	Heterogeneous
Micromechanics homogenization techniques	[11] Charalambakis	Layered composites
The Heterogeneous Multiscale Method	[12] E, <i>et al.</i>	Solids
Atomistic / Continuum Coupling Methods	[13] Curtin, Miller	
Nanomechanics & Micromechanics	[14] Ghoniem, <i>et al.</i>	Polycrystals
Computational multiscale tools	[15] Gravemeier, <i>et al.</i>	
Asymptotic Homogenization	[16] Kalamkarov, <i>et al.</i>	Composites
Mean field approaches	[17] Kanoute, <i>et al.</i>	Composites
Momentum transport approaches	[18] Kapellos, <i>et al.</i>	Biological materials
Atomistic approaches	[19] Karakasidis, Charitidis	Nanomaterials
Computational strategies; spatial and temporal	[20] Ladeveze	Composites
Mesomechanics finite element methods	[21] Mishnaevsky, Schumacher	Alloys
Atomistic approaches – dislocations and defects	[22] Moriarty, <i>et al.</i> ,	Bcc metals
Mechanics of Carbon Nanotubes	[23] Qian	CNT
The Atomic Limit of FE Modeling in MEMS	[3] Rudd	MEMS
Atomistics-continuum strategies	[24] Wernik, Meguid	Nanocomposites
Computational strategies and nanomechanics	[25] Zeng, <i>et al.</i>	Polymer NanoComp
Computational multiscale modeling of fluids and solids : theory and applications	[26] Steinhauser	Book
Multiscale modeling and simulation of composite materials and structures	[27] Kwon, <i>et al.</i>	Book
Atomistic methods	[28] Dove	Book chapter

CLASSIFICATIONS

A total of 84 research articles were reviewed and categorized by a number of characteristics applicable to MM. Table 3 gives the general results of the survey. Brief descriptions of each classification category used in this review are listed in Table 4 and given below.

Scales

First, the papers are separated by the number of physical scales that are examined / traversed in a multiscale fashion. Typically, the lowest scale is referred to as micro, intermediate scales as meso and the largest/highest scale as macro. For example, in a fiber reinforced composite material, the micro scale involves the constituents (fiber, matrix, inter-phase), with a “zoom-out” to a mesomodel which is often the representative volume element (RVE) which is used to fabricate intermediate mesomodels (lamina, weave) and finally the macro model which is the composite structure (test specimen, structural component). Scales are separated by the size of structural

features and/or by the failure assumptions that are inherent to the particular scale being considered. The input to each scale is defined by the phenomena that are treated discretely and the output is the homogenized effect of these discrete features; which can then be used as either the boundary conditions or effective properties for the next higher scale. Of the papers reviewed, 65% encompassed 2 scales, 31% treated 3 scales and 4% modeled 4 scales.

Table 2. MM research of Composite & Monolithic Materials

Composite	Polymer matrix composites	[29-41, 112-114]
	Metal Matrix	[42-47, 108, 113-114]
	Woven composites	[48-53, 112-114, 116]
	Nanophased composites	[19, 24, 25, 54-71]
	Particulate composites	[72-77]
	Biological materials	[18, 78]
	Other (fiber reinforced, heterogeneous, concrete, rocks)	[10, 11, 79-84]
Monolithic	Crystalline	[77, 85-91]
	Polycrystalline	[7, 14, 21, 22, 92-102]
	Polymers	[6, 103-107]

Modeling Strategy (Hierarchical, Synergistic, Concurrent)

Modeling methods from finer to coarser scales consist of quantum mechanics, molecular dynamics, micromechanics and finally continuum mechanics. Capturing the interaction between the scales of interest is of key concern to multiscale modeling methods and is entirely dependent on the coupling scheme used, broadly defined herein as Hierarchical, Concurrent or Synergistic. Effort is made to classify articles based on their coupling scheme. Hierarchical or sequential methods are typically strategies that systematically pass information in a bottom-up (or top-down) approach from a finer (coarser) scale to the next coarser (finer) scale as either boundary conditions or effective properties. A key distinction in this classification between hierarchical and synergistic is that this coupling is strictly one-way, either bottom-up (homogenization) or top-down (localization) but not both as often the case in synergistic approaches. The hierarchical approach is typically used for problems that have weak interdependence on length and time scales, whereas with the concurrent approach, all scales (both temporal and spatial) are treated simultaneously due to strong scale interdependence. Synergistic approaches typically attempt to blend these other two approaches for optimal performance. For example, in the case of micromechanics based structural analysis [108], spatially, at each integration point, calculations are hierarchical, yet temporally, all integration points are dealt with concurrently. Another MM strategy is the atomistic-based continuum technique, in which atomic configurations and interactions are described in a continuum framework. Few papers fall in this category; therefore, these will also be listed in the synergistic category. Of the papers considered, roughly 62% of the studies utilized the sequential approach, 20% the synergistic and 17% used the concurrent approach.

Application (Deformation, Life Issues)

Another category of interest involves the primary objectives of the research. These are categorized as linear deformation analysis (usually material properties), nonlinear deformation (hyperelasticity, plasticity, creep, viscoplasticity) or life issues (defects, damage, structure evolution, failure). As seen from Figure 2b and 2c, there are four times as many journal articles dealing with material properties than breakdown properties (i.e., damage/failure issues). To gain

an impression of MM strategies for both issues, an almost equal number of papers for deformation and damage are reviewed and of those, over 70% investigated nonlinear systems.

Experimental Studies

The role of experimentation (physical or virtual) for providing accurate input data and data for model validation is also noted. Due to the increase in computational power and subsequently due to the development of more sophisticated modeling techniques, numerical experiments far outweigh physical experiments; this being one of the primary goals/motivations of multiscale modeling. As expected, continuum modeling (primarily finite element analysis) is the predominant tool in MM. Since particular attention was directed at atomistic modeling, 44% of the articles reviewed had an atomistic modeling component in their MM strategy.

*Table 3. General results of literature survey
(based on 84 research articles)*

2 scales	65%
3 scales	31%
4 scales	4%
Concurrent	17%
Synergistic	20%
Hierarchical	62%
Deformation	50%
Defects, structure evolution, failure	50%
Physical experiments	27%
Numerical/Virtual experiments	56%
Continuum modeling	55%
Atomistic modeling	6%
Atomistic/Continuum modeling	38%

DISCUSSION

Table 5 shows the selected articles separated first by scales and then correlated to the primary type of MM strategy (hierarchical, synergistic or concurrent). A further sub-classification under each approach places the article according to its application of deformation (linear or nonlinear) or any type of life assessment issue such as continuum or discrete damage, progressive damage, crack propagation, buckling or failure or a combination of these.

The goal for most papers categorized as linear deformation is determination of mechanical properties (moduli) and overall constitutive response; applications involving nonlinear deformation involve inelastic behavior [81], dynamic behavior [109], plasticity [94, 96, 101], large deformation [105], etc. Of the papers considered for this study, a notable portion address life assessment issues using a sequential strategy. This includes progressive failure analysis [49], continuum damage [39, 51], tensile strength [29, 40, 46] and several fracture analyses. Several studies employ a cohesive zone model (CZM) which describes the constitutive relationship of interfaces (fiber/matrix interface or grain boundaries) and allows bridging between the microscale and the macroscale. For example, a bilinear CZM is used to predict the damage due to debonding in particulate composites in [74-76]. An excellent example of multiscale modeling is found in the use of atomically informed cohesive laws. Using molecular dynamics simulations, fracture mechanisms are identified and used to formulate CZMs which are subsequently used in finite

element models to predict crack growth [73, 97, 99]. These methods pass information, usually in the form of displacement or force fields, from the lower scale to the coarser scale.

Table 4. Classifications

Scales	Relative to the problem and material system investigated. Scale division is obtained by separation of structural features by size or by failure of assumptions at the implicit level.
Concurrent modeling	Integrated modeling in which scales are interwoven and coupled in a parallel fashion for simultaneous computation.
Synergistic modeling	Effective blending or integration of field variable information at various scales, typically with a two-way information flow. Note these methods typically handle field quantities spatially sequentially and temporally concurrently or spatially concurrently and temporally sequentially.
Hierarchical modeling	One-way serial or sequential modeling in which information is passed in a bottom-up (or top-down) approach from smaller (larger) scales to coarse (fine) grained models.
Deformation	Linear (material properties, linear constitutive/ kinematic relationships, small strain, etc.) and nonlinear (plasticity, viscoelasticity, viscoplasticity, etc.)
Defects/Damage/Failure	Defects, continuum damage, progressive damage, crack propagation - fracture, ultimate strength, progressive failure, buckling
Continuum	Analytical (Rule of Mixtures, Mori-Tanaka, micromechanics, micropolar elasticity, etc.) and numerical (finite element analysis, dislocation dynamics, level set method, etc.)
Atomistic	Quantum approaches (self-consistent, density functional theory), molecular structural mechanics, quantum molecular dynamics, etc. and classical (classic molecular dynamics, Monte Carlo simulations, etc.)

Many studies have turned to atomistic modeling to describe phenomena at the microstructural level. Typically, the input to atomistic approaches involves atomic configurations. Taking a lead from [26], various methods along with their approximate range of applicability, as well as their output are depicted in Figure 3; the output and applications of the various atomistic interface tools (for empirical or quantum methods) are shown in Table 6.

Although atomistic strategies are used for a number of materials (single wall carbon nanotubes [67], polymer nanocomposites [54], crystalline and polycrystalline materials and polymers [86, 88, 104]) and for a variety of applications, the range of application is relatively small. At the other end of the spectrum (continuum approaches), it becomes difficult to establish accurate property-structure relationships because the structure is treated as a continuum rather than as discrete phases/particles. This has led to a rapid growth in a true multiscale methodology which combines atomistic approaches for the salient discrete features and couples the analysis with continuum methods to achieve the most accurate impression of material behavior. This includes the quasi-continuum method [89], the handshaking method [85] which incorporates tight-binding (TB) quantum mechanics approximation, molecular dynamics (MD), finite element (FE), and the heterogeneous multiscale method [12] based on the concept that both the atomistic and the continuum models are formulated in the form of conservation laws of mass, momentum and energy; these methods are primarily concurrent in nature. Table 7 shows the division of papers with respect to the modeling domain of purely atomistic, purely continuum and a combination of both approaches. As can be seen, the importance of including phenomena at the atomistic level is recognized and is increasingly being incorporated in numerous studies. Again, information shared and exchanged between the scales takes the form of forces, displacements and properties.

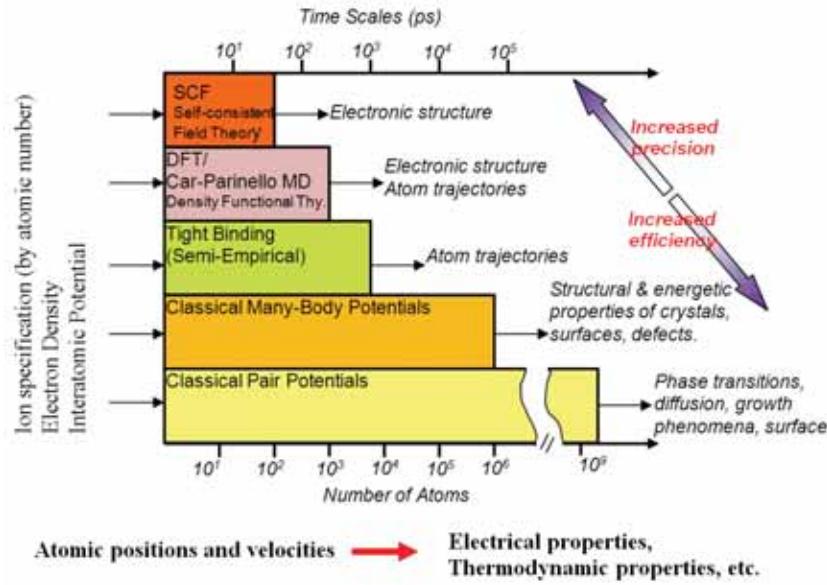


Figure 3. Inputs and outputs of atomistic approaches and their approximate range of applicability[26].

An assessment of MM strategies was performed in which crack propagation in a functionally graded composite was modeled using multiscale models (hierarchical and concurrent) and compared to a purely microscale model [110]. The study concluded that the concurrent strategy, rather than the hierarchical 1) produced results closer to the microscale model, 2) reduced computational time and 3) was able to accurately map the crack path.

Table 5. Classification Based on Computational Strategies: Sequential, Synergistic and Concurrent Modeling

HIERARCHICAL			SYNERGISTIC			CONCURRENT		
Scales	Deformation		Damage Evolution, Failure	Deformation		Damage Evolution, Failure	Deformation	
	Linear	Non-Linear		Linear	Non-Linear		Linear	Non-Linear
2	[30, 37, 95, 107]	[44, 50, 53, 54, 56, 61, 63, 71, 72, 77, 78, 83, 84, 86, 93, 94, 96, 98, 102, 105, 106]	[31, 44, 66, 73-76, 79, 80, 84, 90, 96, 97, 99, 110]	[81, 88, 101, 103, 109]	[32, 45, 55, 58, 64, 67, 89, 91, 100, 110]	[59, 65]	[81, 88, 101, 103, 109]	[32, 45, 55, 58, 64, 67, 89, 91, 100, 110]
3	[52, 57, 62, 68, 69, 104]	[36, 38, 87]	[29, 39, 40, 46, 49, 51, 111]	[112, 113]	[43, 92, 113, 114]	[33-35, 41-43, 85, 95, 115]	[43, 92]	[33-35, 41-43, 85, 95, 115]
4	[70]	[48]	[82]	[113]		[113, 116]		

Multiscale Modeling Strategies

A primary factor in materials design is the development, characterization and validation of predictive models on a hierarchy of length scales so as to establish a multiscale modeling framework (albeit sequential, synergistic, and/or concurrent), as schematically shown in Figure 1 and discussed above. The spatial methods include approaches at the atomistic level (quantum mechanics), microllevel (micromechanics, molecular dynamics) and macrolevel (continuum mechanics) which are linked by either direct or sequential coupling. Each approach has its limitations and advantages, as listed in Table 8.

Table 6. Atomistic Interface Tools [26, 28].

METHOD	INPUT	OUTPUT	APPLICATION
Lattice energy modeling	Atomic configurations / Crystal energy in terms of atomic displacements	Crystal structure and energy	Physical properties (elastic and dielectric constants, etc.), defect energies, surface studies (adsorption)
Lattice dynamics		Dynamical matrix	Thermodynamic properties, phase diagrams
Molecular dynamics		Atomic trajectories (evolution of position and velocities)	Equation of state for range of temperatures and pressure, phase transitions, properties
Monte Carlo simulations		Evolution of ensemble	Averaged thermodynamic quantities (energy, heat capacity), properties

Table 7. Modeling and Experimental Studies

	MODELING	EXPERIMENT	
		Physical	Virtual
Atomistic	[54, 67, 86, 88, 104]	<i>Micro</i> [31, 36, 44, 49, 57, 62, 70, 92, 93, 99]	[55, 56, 59, 61, 65-67, 70, 85, 87-90, 100, 104-106, 109]
		<i>Macro</i> [31-35, 44, 46-50, 57, 62, 63, 70, 72, 82, 84]	[32, 33, 36-38, 40, 41, 43, 45, 48, 51-53, 55, 64, 72, 74, 76, 80, 81, 83-85, 87, 90, 93, 100, 102, 103, 110, 111, 115]
Continuum	[29-35, 37-53, 57, 62, 70, 72, 74-76, 78-84, 92, 93, 96, 101, 102, 110, 111, 115]		
Both	[3, 36, 55, 56, 58, 59, 61, 63-66, 68, 69, 71, 73, 77, 85, 87, 89-91, 94, 95, 97-100, 103, 105-107, 109]		

Table 8. Advantages and disadvantages of atomistic, micromechanical and macromechanical approaches.

ADVANTAGES		
Atomistic	Micromechanical	Macromechanical
<ul style="list-style-type: none"> • Ab initio methods require only a specification of the ions present. • First principles approach generates fundamental information obtained with minimal empiricism. • Enables the design of new materials because material composition can be predetermined electronically. • Acts as a computational microscope. Provides information not accessible by other methods. 	<ul style="list-style-type: none"> • Enables capturing the physics of deformation and damage at more fundamental scale than macro-level. • Captures varying in-situ non-proportional, multiaxial stress and strain states (iso/nonisothermal) • Utilizes simpler isotropic constituent constitutive models and failure criteria than macro-level • Microstructural effects explicitly prescribed • Enables what-if scenarios for design of materials. 	<ul style="list-style-type: none"> • Most computationally efficient • Experimental testing incorporates all in-situ effects (interface, damage, residual stresses, etc.) • Tends to work well for fiber-dominated and linear, isothermal regime. • Aligned with standard ply level design procedures. • Highest technology readiness level.
DISADVANTAGES		
<ul style="list-style-type: none"> • Reliable inter-atomic potentials usually are not available for multi-element materials • Many physical processes happen on length- and time-scales inaccessible by these methods (diffusion in solids, many chemical reactions, etc.) • Computationally expensive • Experimentally expensive • Lowest technology readiness level 	<ul style="list-style-type: none"> • Increased computational expense vs. macromechanical • Need for constituent constitutive response (fiber/matrix) as well as higher level (e.g., composite) testing • Possible need to recalibrate for in-situ effects • Interfacial behavior a constant unknown • Mid technology readiness level 	<ul style="list-style-type: none"> • Requires anisotropic constitutive theory • Requires additional complexities to handle Tension/compression, tertiary creep – damage • Multiaxiality/ hydrostatic interaction more difficult to handle • System specific • Phenomenologically based: accounts for physics of all nonlinearity on the wrong scale • Mathematical form of internal state variable (ISV) evolutionary law – based on monolithic materials • Adversely impacted with non-isothermal loading

Experimental Methods

Studies that include experimentation (physical or virtual) at the micro level and the continuum level are also listed in Table 7. Numerical experiments dominate physical experiments at both the atomistic and continuum levels. Yet physical experimental techniques (and associated necessary equipment) are essential for both structure characterization and model validation. Table 9 lists the various micro and macro-level physical experiments found in the reviewed articles. Standardized tensile, flexure (three or four-point bend), high and low level impact, relaxation, creep and fatigue tests are well established and widely used to determine material properties and overall structural response for a wide range of conditions. Also, nondestructive test methods such as ultrasonic testing, acoustic emission, etc. are widely used for inspection and testing of composite structures

as well. At the micro level, optical-based techniques are primarily employed. Techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM) and focused ion beam experiments are used to observe microstructural details. Measurement techniques to characterize the microstructure include atomic force microscopy (AFM), Raman spectroscopy, X-Ray diffraction (XRD), neutron diffraction and differential scanning calorimetry (DSC). It is noted that much of the progress and advances in nanotechnology in the last decade can be attributed to the advances made in the measuring and manipulating capability at the nanoscale with further development work continuing at the atomic level [117]. Aside from electron microscopy, scanning tunneling microscopes such as the atomic force microscope have allowed the imaging and manipulation of individual atoms. For nanoscale manipulation, scanning probe microscopes, optical tweezers and nanomanipulators (devices used in SEMs and TEMs) are being utilized.

Table 9. Physical Macro-level and Micro-level Experimental Tests.

Macro-level		Micro-level	
Tensile	[31, 34, 44, 50, 57, 62, 82, 93]	Scanning electron microscopy (SEM)	[31, 44]
Biaxial	[50]	Transmission electron microscopy (TEM)	[62, 70, 92]
Flexure	[31, 32, 57, 62, 70]	Electron diffraction (ED)	[92, 93]
Impact	[33]	X-Ray diffraction (XRD)	[70]
Cyclic-tensile	[72]	Neutron diffraction	
Compression creep: uniaxial, triaxial	[84]	Atomic force microscope (AFM)	[57]
Dynamic mechanical analysis	[62]	Differential scanning calorimetry (DSC)	[62]
		Focused ion beam	[49]

Issues/ Challenges

The fundamental difficulty in multiscale modeling is the coupled length and time scales, which is due to the hierarchy and evolution of microstructures. And even though a significant amount of effort has been dedicated to multiscale modeling of materials in recent years, thus far, seamless coupling between the scales has still not been achieved due to the difficulty in incorporating system evolution and computational complexity. Although multiple mathematical methods exist at each level of hierarchy, many tend to over-simplify the problem and depend on parameters that are unavailable. Often, very simplistic unit cells of regular construction are used to model the real, wildly varying, structure of materials. Therefore, more realistic representations of the actual microstructure, through the use of image and signal data or atomic structure, should be incorporated. Links between the solutions of transport and elasticity problems for composite materials would be very helpful as cross-property relations become very useful if one of them can be more easily calculated or measured experimentally. In atomistic modeling, further work is needed to develop more accurate potential energy functions for specific types of atomic interactions [7, 16, 20, 118].

To facilitate the development of a complete multiscale framework, it is the authors' firm belief that identification of one or more model materials (or model class of materials) would be worth consideration [119]. The model material concept would 1) enable experimentation and modeling resources among diverse groups to be focused, 2) facilitate creation of a national database of experimental results at every scale for these model material systems, and 3) enable direct comparison of both experimental techniques and modeling approaches to identify the most

promising directions of research. This would accelerate the development of a viable multiscale modeling framework (that can span all length scales) would be useful to the ICME community.

CONCLUSIONS

A sample of multiscale modeling (MM) papers for a wide variety of materials and applications were reviewed to obtain a broad view of current efforts. The key limitations, both general and focused on particular areas, are expressed in many of the survey papers in Table 1 and left to the reader. However, a few conclusions from this broad overview are expressed. One of the main advantages of computational strategies is the ability to perform “what if” scenarios without the prohibitive expense of implementing a full laboratory experiment. A number of papers [32, 40, 44, 66, 68, 70, 71, 74, 76, 82, 97, 120] conducted parametric studies to determine the effect of particular lower scale parameters on the response of the structure. This is actually the final goal of Integrated Computational Materials Engineering (ICME) – the development of robust, fully validated models that can be used to design and/or analyze a structure with minimal or no physical experiments. A primary limitation is the lack of a robust and thorough validation methodology which verifies each level of a multiscale modeling strategy. For example, in the MM of a fiber reinforced composite laminate, it is possible and customary to measure constituent (fiber, matrix) properties which are used as the input to the micro model; at the macro level (lamina, laminate, structure), physical experiments are often performed to verify and determine the limitations of the multiscale model. However, no physical experiments exist for the validation of the intermediate level (representative volume element) which is the fundamental representation of the composite microstructure. Also, although experimental techniques at the structural level are well established and many benchmark solutions are readily available for simulation approaches, standardized techniques at the atomic level are lacking. Atomistic approaches typically use established force fields or potentials to describe the interactions between atoms valid for a broad class of materials. Parameters for these force fields are adjusted to obtain a required atomic structure. Most studies use a force field for which the parameters are determined at a specific state – the same force field may not apply once the atomic configuration changes.

In conclusion, the field of multiscale modeling is vast – it involves various disciplines which makes communication between scientists and engineers (both analytical and experimental researchers) vital. Further the multi-disciplinary nature of multiscale modeling requires clear understanding of 1) the transitioning requirements between scales, 2) the understanding of the input/output requirements of each scale, 3) the experimental requirements at each scale to enable the exploration, characterization, and validation of models, and 4) the trade-off between fidelity and efficiency to enable practical engineering solutions. In addition the main obstacles encountered while conducting this general overview (that considered a variety of materials, research applications, MM strategies from the quantum level to the continuum level) were the:

- a. Lack of a common paradigm (i.e., a clear understanding of the input, output and importance of proper transitioning between scales),
- b. Lack of a common language (i.e., the multidisciplinary nature of ICME requires significant investment in learning the nomenclature of other disciplines),
- c. Lack of a common framework (i.e., the multiplicity of computational approaches being investigated: sequential/ synergistic/ concurrent/ hybrid),
- d. Lack of a complete and sufficient material response database at various levels of scale.

Consequently, documentation of results should contain explicit statements of 1) the number of scales being considered, 2) the application, 3) the MM coupling strategy, 4) the linking information and all experimental techniques utilized for characterization and validation of the applied MM technique. This will enable the reader to understand the context of the work and

allow identification of trends and new techniques and ideas, thereby facilitating the area of multiscale modeling and ICME.

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ICME: SUCCESS STORIES AND CULTURAL BARRIERS

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INTRODUCTION

Several national academy studies of materials and manufacturing^[1-4] have emphasized the unique opportunity of computational materials engineering. While the breadth of the 2008 ICME study^[1] creates an impression of a field in its infancy, a 2004 study^[2] uniquely charged with identifying best industrial practices for accelerating transition of materials and process technology identified practices which are now mature and ready for broader dissemination. We here update the state of best practices and consider the principal cultural barriers to ICME proliferation.

COMPUTATIONAL DESIGN SUCCESSES: FLYING CYBER STEEL

The first example of a commercial alloy created by computational design is the Ferrium C61 (AMS6517) high durability gear steel now performing well in off-road racing applications^[5]. The first such designer alloy to reach flight qualification is the Ferrium® S53 (AMS 5922) corrosion-resistant landing gear steel allowing a drop-in replacement for current non-stainless landing gear steels, eliminating the need for cadmium plating.^[6] S53 is a secondary hardening steel strengthened by efficient M₂C carbide precipitates and contains sufficient Cr content to provide passivation against general corrosion as shown in the flow-block diagram in Fig. 1. The sequential processing steps experienced by the alloy are depicted on the left-most column of the flow-block diagram and are constrained to existing processes for steels employed in current structural aircraft applications to maximize manufacturability. The subcomponents of the alloy system are connected by process-structure and structure-property relationships, representing the mechanistic modeling tools necessary to employ quantitative computational design.

The application of the system flow-block diagram in conjunction with the computational models begins with identification of key design tradeoffs. Key to achieving the stated design goals is the development of an efficient strengthening dispersion. M₂C carbide is an efficient strengthener in steels due to its high modulus misfit with BCC Fe and its ability to precipitate coherently at the nano scale. Models were utilized, as demonstrated in Fig. 2, to predict the overall precipitation driving force and the normalized coarsening rate constant of the M₂C carbide as a function of the Mo and V content in the S53 alloy. The approach maximizes the resulting strength through the precipitation driving force, while assuring that strength can be achieved with reasonable tempering parameters.

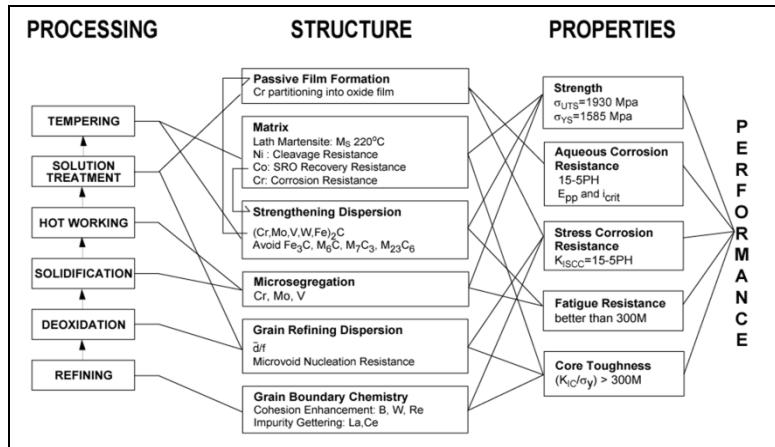


Fig. 1. The flow-block diagram for ultrahigh-strength corrosion-resistant steel indicates the desired property objectives, the microstructural subsystems, and sequential processing steps needed for design. Links between system blocks indicate quantitative models needed to effect the design via science based computation.

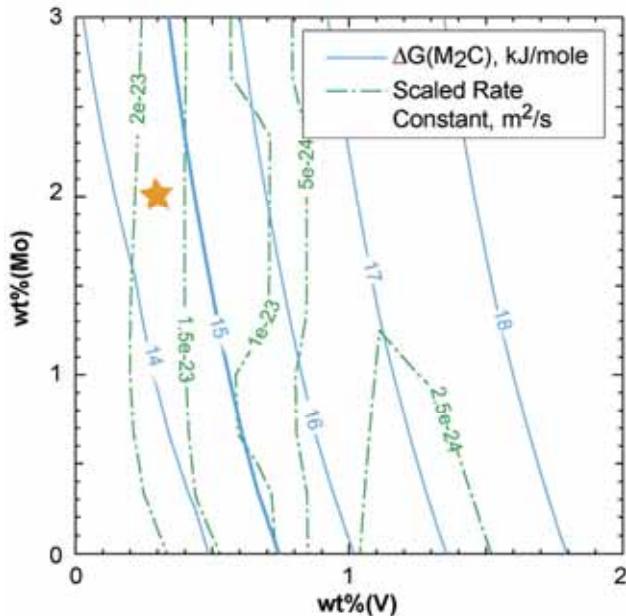


Fig. 2. Maximizing M_2C driving force while maintaining a normalized coarsening rate for adequate tempering kinetics provides a secondary hardening alloy with highly efficient strengthening. The S53 alloy achieves greater than 1930 MPa tensile strength with only 0.2 wt% carbon.

This design also maintains adequate martensite kinetics to ensure a lath martensitic alloy while achieving high strength as another key design tradeoff. Quantitative martensite kinetic models^[7] are used to predict the martensite start temperature along with the M_2C precipitation driving force in Fig. 3 as a function of Co and Ni content.

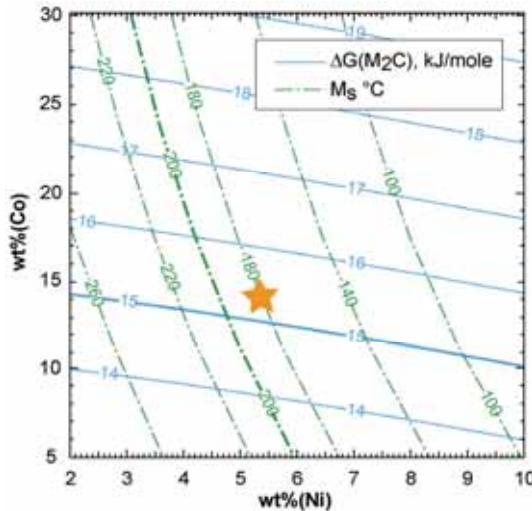


Fig. 3. Maintaining a sufficiently high M_s temperature while maximizing carbide driving force allows efficient strengthening in a fully martensitic alloy. Contours of M_2C precipitation driving force overlaid with the alloy M_s temperature determine optimal Co and Ni content.

Additional constraints on ductile fracture, grain boundary chemistry and grain pinning dispersions are used to complete the design optimization and uniquely identify the alloy composition that represents the best compromise of the diverse design goals and constraints. Grain boundary chemistry considerations are applied based on first principles calculations of impurity and alloying effects on the interfacial cohesion of BCC low angle grain boundaries.^[9] The grain pinning dispersion design was based on calculation of the TiC/Fe interfacial adhesion that demonstrated excellent resistance to microvoid formation.^[10]

Solidification simulations employing 1-D multicomponent diffusion calculations in DICTRA for candidate design compositions ensured production scale processability.^[11] Figure 4 demonstrates segregation profiles across secondary dendrite arms predicted for production scale ingots using VAR. These predictions were validated from actual production ingots. Figure 5 shows DICTRA predictions of homogenization Mo in the as-cast ingot of the S53 alloy. The simulation guides processing recommendations and indicates that sufficient homogenization can be achieved in production scenarios. Figure 6 demonstrates the validation of tensile properties in production ingots of up to 24,000 lb. size.

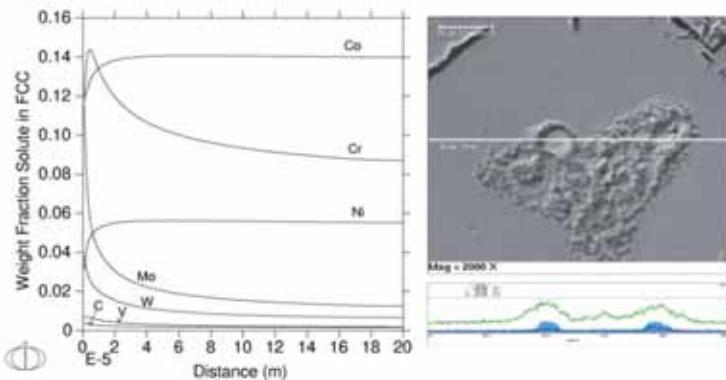


Fig. 4. One-dimensional multicomponent diffusion simulations of the solidification of S53 alloy indicate the extent of segregation that can be expected in final ingot. This segregation is validated by SEM observations of ingot material.

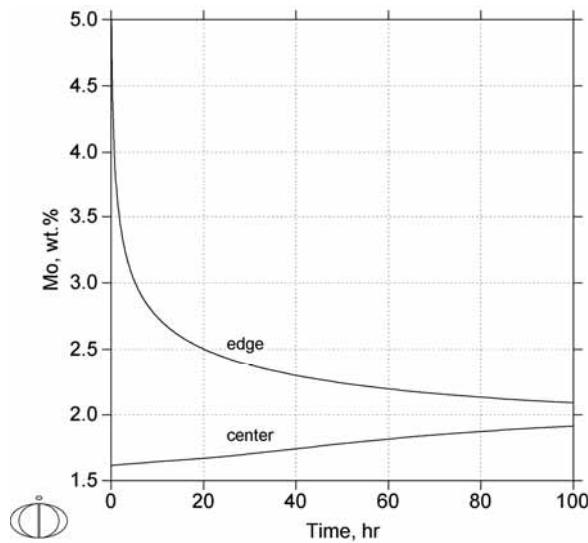


Fig. 5. The homogenization of Mo segregation in the S53 alloy as a function of time at 1350C. The two curves represent the composition of Mo at the dendrite center and edge, and, the initial profiles are provided by the solidification simulations from Fig. 4.

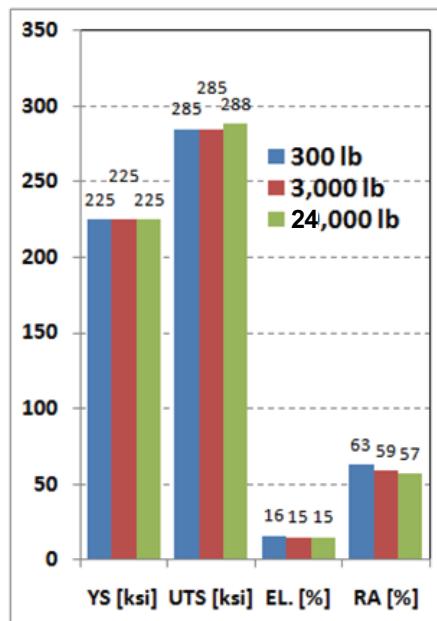


Fig. 6. Validation of scale-up results after the computational optimization of homogenization parameters. The chart represents typical tensile properties for wrought product produced at three production scales, including laboratory 300 lb ingots, intermediate 3000 lb ingots and full production 24,000 lb ingots. The similar tensile properties across all products indicate the ingots are homogeneous across all production size scales.

EXTENDING COMPUTATION DESIGN TO QUALIFICATION AND IMPLEMENTATION

Accelerated Insertion of materials (AIM) methods^[2] were applied to the prediction of the ultimate tensile strength, a primary design objective of the S53 alloy. Prediction of property design minimums, which normally require 10 production heats of alloy and 300 individual observations, were completed using only three heats and 30 individual observations. A large simulated dataset with over 300 simulations was produced using expected process variation and computational mechanistic models of alloy strength. The simulated property distribution was scaled to fit 20 experimental observations from two production heats by a linear transformation function determined by the best fit. This analysis indicated the 1% minimum ultimate tensile strength was predicted to be below the 1930 MPa design goal by at least 10 MPa. This early indication allowed additional process optimization to be completed, increasing the ultimate tensile strength by 10 MPa. The AIM analysis was repeated after a new temper was optimized, using 30 data produced from 3 heats of the alloy, and is shown by the solid curve of Figure 7. The new property minimum estimate shows a prediction of 1930 MPa (280 ksi) meeting property objectives. The resulting full experimental data set of 10 heats and over 600 individual observations are represented by the square points of Figure 7. The AIM prediction is within 7MPa (1ksi) of the 1% minimum tensile strength statistically defined by the 10 heats of data. In this AIM example, if data development had proceeded and the property deficit discovered when the full dataset was complete, over a year of development and in excess of \$500,000 US would have to be repeated to meet the property goals.

The first flight of a Ferrium S53 landing gear occurred on December 17, 2010.

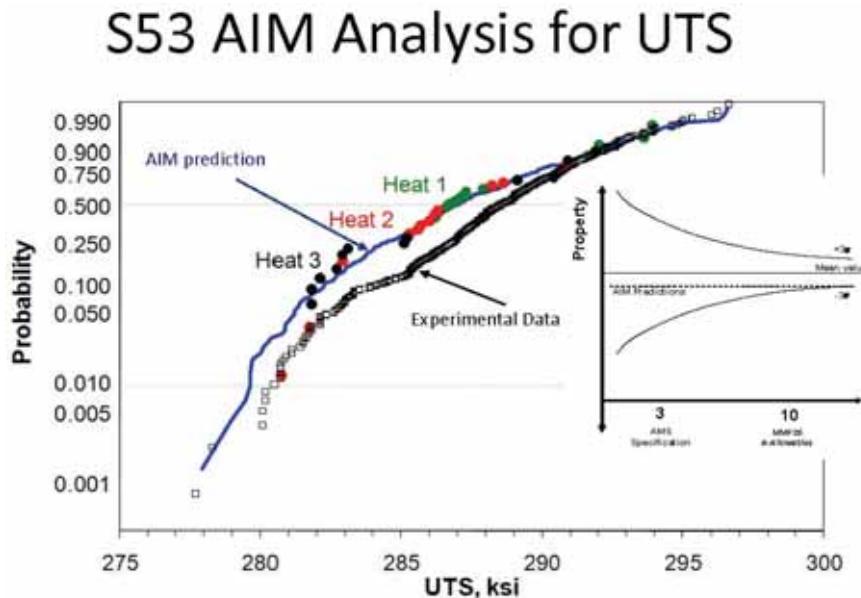


Fig. 7. An AIM analysis of the ultimate tensile strength of S53 using simulation results and 30 data from 3 individual heats agrees well with the completed dataset from 10 heats and over 600 observations in determining the 1% minimum design allowable.

ICME CULTURAL BARRIERS

Primary cultural barriers to the accelerated development and proliferation of ICME technology stem from the broader issue of the opposite nature of science and engineering. It has been much discussed that science seeks the discovery of new knowledge of nature as it is, while engineering applies existing knowledge to bring new technology into existence. The unique position of materials at the interface of science and engineering intensifies the inherent conflict between these opposite philosophies.

With the glorification of basic science by the atom bomb, and the catalytic effect of Sputnik Hysteria, it became temporarily fashionable for post-war American industry to invest directly in basic research. This created historic environments like Bell Labs (with achievements from this period still receiving Nobel Prizes) where science and engineering coexisted in an atmosphere of mutual respect and collaboration, enabling an unprecedented level of science-based technology creation. Concurrent with the development of MBA programs, major industry concluded that such basic research could not be justified in terms of short-term competitiveness, and largely dropped out of science. This in turn created a need for federally funded academic research to take full responsibility for basic science, with the unfortunate consequence that engineering at our research universities has been almost entirely replaced by engineering science. We are left with a system where universities do science and companies do engineering; probably the most egregious example of the much-discredited “over-the-wall” system. While limited technological competence at universities and limited scientific depth in industry offer an opportunity for unlimited finger pointing, the special case of university spinoff companies has provided the best exception to the prevalent systemic dysfunction, and it is no wonder that these have served as the principal source of the ICME methods, tools and databases that are now available for broad dissemination.

While a few elite engineering schools have attracted private funding to conduct actual engineering on campus, there is a pressing need for federal funding agencies to take responsibility for restoration of engineering across our research university system. DoD agencies have provided the best example so far, but far more impact could be achieved by the formation of a National Engineering Foundation as an equal and opposite partner to NSF, with a mission of direct technology creation through design as the complement of discovery. Such an enterprise would powerfully demonstrate societal respect for engineering as the equal of science, would provide a fertile intellectual environment far more capable of achieving the goals of Bayhe-Dole legislation in a technological return on our vast public investment in science, and would create an educational environment for engineering equaling that in place for science.

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CRITICAL PATH ISSUES IN ICME

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ABSTRACT

The initiative in Integrated Computational Materials Engineering offers great potential to add value to products and reduce time to market by combining emerging capabilities for materials modeling and simulation with systems engineering approaches to design and manufacturing. Significant barriers in the critical path of developing ICME are discussed in terms of industry, government and academia.

Keywords: materials design, integrated computational materials engineering

1. INTRODUCTION

Integrating computational materials science and mechanics with manufacturing and design of products is a major opportunity made possible by the confluence of advances in modeling and simulation tools, high performance computing, and quantitative materials characterization. This integration represents a significant leap beyond materials selection in design, as traditionally taught and practiced in engineering [1]. The recent emphasis on *Integrated Computational Materials Engineering* (ICME) [2] demands integration of computational modeling and simulation with product development, and has much common ground with the notion of tailoring materials to achieve targeted properties or responses, commonly referred to as *Materials Design*. ICME includes various aspects of materials processing, manufacturing, fabrication, and performance/property projections and involves materials science and mechanics, computing, experimental methods and validation methodologies, and multidisciplinary design optimization, among other disciplines and sub-disciplines.

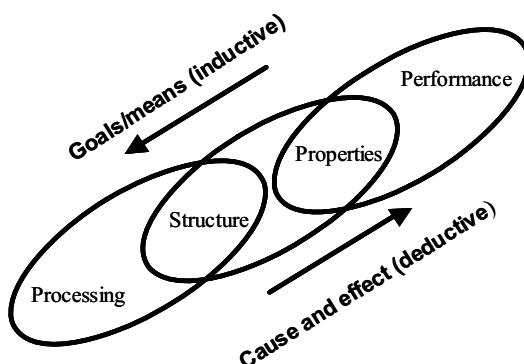


Figure 1. Olson's linear concept of
'Materials by Design' [3].

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As a foundational, enabling element of ICME, materials design will receive the primary focus of the present article. The concept of materials design is clearly conveyed by Olson's schematic [3] of the linear, overlapping relations between material processing, structure, property, and performance, shown in Fig. 1. The important point is that design is a top-down, inductive pursuit, in contrast to the inherently bottom-up, forward nature of modeling and simulation methods. This duality presents a challenge to decision-based design, which necessarily must extract information and guidance from experiments, models and simulations conducted at judiciously selected scales of material hierarchy associated with the dominant design degrees of freedom, as shown in Fig. 2.

The term "materials design" means different things to different people. It is effectively a multi-discipline, incorporating various disparate aspects:

- materials selection
- computational materials science
- materials informatics, data mining and combinatorics
- multiscale modeling
- expert intuition and application of experiential learning
- distributed collaboration
- inherent coupling to product development
- decision support for designers that considers uncertainty and sensitivity
- multidisciplinary design optimization

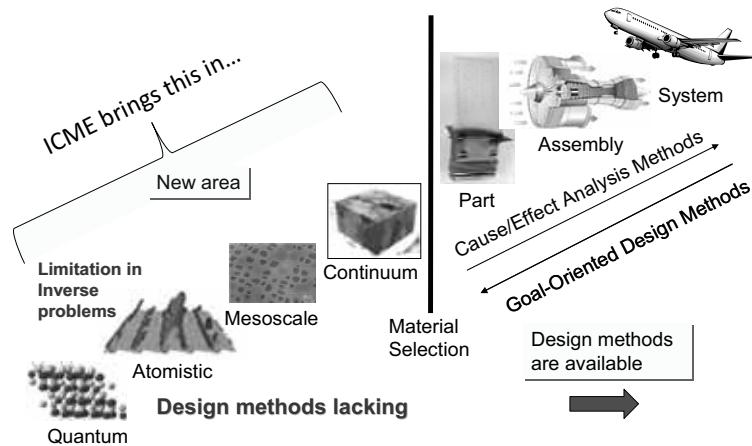


Figure 2. Augmentation of the usual hierarchy of engineering systems design with multiple scales of material structure (left of vertical bar), undergirding the notion of materials design which is foundational to ICME.

With such a broad range of endeavor, it is clear that no single academic discipline or corporate division can address the full scope of either materials design or ICME. Integration of the elements of ICME is a major challenge for any organization, requiring an overarching vision and the ability to evaluate potential payoffs. The notion of materials design has been articulated for several decades [4]. The emergence and maturation of first generation tools for virtual manufacturing and computational materials science, effectively comprising the broad technology infrastructure for ICME, motivated a 1998 NSF-sponsored workshop [5] entitled "New Directions in Materials Design Science and Engineering (MDS&E)", co-hosted by Georgia Tech and Morehouse College. This workshop concluded that a change of culture is necessary in U.S. universities and industries to cultivate and develop the concepts of simulation-based design of materials to support integrated design of material and products. It also forecasted that the 21st

century global economy would usher in a revolution of the materials supply/development industry and realization of true virtual manufacturing capabilities (not just geometric modeling but also realistic material behavior). It recommended establishing a national roadmap addressing (i) databases for enabling materials design, (ii) developing principles of systems design and the prospects for hierarchical materials systems, and (iii) identifying opportunities and deficiencies in science-based modeling, simulation and characterization “tools” to support concurrent design of materials and products. In the intervening years, the envisioned proliferation of small companies specializing in materials design has not yet occurred, nor have materials science and engineering (MSE) academic departments broadly embraced this vision in their curricula. However, several significant federal initiatives have continued to foster development of the foundations of ICME, including the DARPA *Accelerated Insertion of Materials* (AIM) program from 2000-2005 [4, 6].

Crystallization of the ICME initiative in recent years offers solid evidence that industry sees the value added by integration of modeling and simulation to reduce time to market and enhance its competitive position by tailoring materials for products and accelerating insertion of new and improved materials into products. By employing materials design in product development, ICME offers compelling potential to incorporate multifunctional material systems that save weight and space, require less energy, improve aesthetics, enhance sustainability, and improve performance. This article provides a brief perspective on barriers to realization of ICME in industry, government and academia. The interested reader is referred to more detailed recent overviews of materials design by the present author and collaborators [7-10], including a recent ICME-relevant textbook [11].

2. BARRIERS TO ICME

At its core, the concept of materials design outlined in Figs. 1 and 2 is a systems engineering activity. The tailoring of materials is intentional and iterative, having much common ground with engineering design [11]. This differs from the conception of ‘Edisonian’ materials discovery pursued by searching permutations of accessible material structures by either computational or experimental means. The paradigm of materials discovery is more common in the sciences, as well as computing and information systems, for example the NSF Cyber-Enabled Discovery and Innovation (CDI) initiative [12]. Traditionally, the engineering domain has been more oriented more towards materials selection [1], and therefore has relied less on computational modeling and simulation than is required by materials discovery. More systematic approaches to mining databases and combinatorial experiments with informatics [13] can enhance the materials selection process or the rate of discovery of new materials, as well as knowledge discovery. Perhaps the most important step towards realizing the vision of ICME is the integration of systems engineering with computational mechanics and materials science, as well as virtual manufacturing; these communities do not have much professional interplay. The multidisciplinary design optimization community within engineering is often considered “soft” by the “hard” sciences and overlapping engineering disciplines such as MSE. This manifests a history of distinct evolution, each with its own perspectives and challenges to integration. Moreover, certain cultural and organizational barriers in industry, government and academia need to be addressed, as outlined next.

2.1 ICME Barriers in Industry

- Distinct materials development, product design, and marketing/product support teams.
- “Over the wall” interfaces between divisional “bins”.
- Legacy design systems with historical antecedents for inputs and outputs—“our designers need simple algorithms, simple property sets, etc.”

- Unrealistic short term objectives - overselling maturity or progress in ICME, either within an organization or at the national or international scales, may create a credibility gap. ICME will take a long time to fully realize.
- Incentives are essential for keeping up with the recent relevant literature - continuing education and updating of the workforce is essential to realizing ICME.
- The ICME approach must be clearly understood, articulated and incentivized with specificity to each industry involved.
- The central role of probabilistic design and uncertainty must supersede deterministic methods and guidelines, and should appeal to details of physical phenomena and related models.

2.2 ICME Barriers in Government Funding Agencies

- Requests for proposals (RFPs) are typically developed for materials with *point* property specifications rather than *ranges* of properties or responses. Moreover, the taxonomy for evolving material responses (progressive damage, degradation, etc.) is lacking. This encourages adherence to traditional materials selection and incremental refinement.
- Lack of employment of systems tools or strategies in developing RFPs – program managers often operate based on limited experience or intuition. Moreover, property specifications for new and/or improved materials systems are usually based on replacing a material within a given product in a given application, rather than concurrent *redesign* of the product and material. This also promotes instrumentalism and status quo methods.
- Funding programs are typically binned according to material class or application (bio, solar, electronic, etc.), which complicates the review process for something as multidisciplinary as ICME or materials design. Perhaps NSF DMR and other agencies should consider programs in multidisciplinary materials design and optimization, for example, that would address the ICME vision.

A brief foray though on-line websites of various funding agencies in November 2010 revealed very few clearly articulated programs or RFPs with regard to materials design. On the other hand, the notion of multiscale modeling (often concurrent) is more commonly expressed as a focus or objective. Multiscale modeling, however, is a means to an end. Multiscale modeling is an element of materials design; as discussed by McDowell and colleagues [7-9], but the two are not equivalent. Concurrent multiscale modeling is often unnecessary in materials design applications as it may introduce levels of idealization and approximation in the scale transition that compound uncertainty. Moreover, its necessity also depends on the degree of coupling between mechanisms operating at different time and length scales. It is important to realize that some design requirements do not target cooperative response at higher scales, but often involve tailoring the material response at specific microscales or mesoscales (e.g., phase or grain boundary corrosion resistance). With regard to ICME, the input of industry and professional societies is of great importance in clarifying research needs and agendas. It is important for ICME to be anchored in engineering, also involving the materials sciences (including physics and chemistry), computational sciences, and information sciences.

2.3 ICME Barriers in Academia

- Lack of reinforcement of computational methods in materials science and engineering course offerings downstream from instruction in basic computational methods.
- Isolation of multidisciplinary optimization and engineering systems design approaches from the materials research and education community (disciplines of mechanical engineering (ME), civil engineering, and aerospace engineering are much more integrative in this regard, for example).

- Uncertainty, robust design, and design for manufacturing concepts are not routinely taught as part of computational mechanics and/or the materials sciences.
- A focus on bottom-up schemes for materials discovery and development has been perhaps reinforced to some extent by the emphasis on nanomaterials and nanotechnology.
- Capstone design courses in materials often aren't really ICME-related, nor are cross-cutting ICME-related elective undergraduate and introductory graduate level courses commonly offered.
- As an integrative research area in universities, ICME is apparently not yet widely recognized as there is little if any mention of it in advertisements for faculty positions.

In many respects, while industrial needs compel investment in ICME, the “rate limiting step” to fully enable this emerging field is the education of materials and systems engineers who understand and embrace the elements of its vision. From several of the points above, within the academic context the curriculum is a key indicator of the priorities and attention devoted to enabling ICME. Clearly, there are some areas of disconnect in this regard that perhaps owe to historical trends in research training and emphasis. There may be more subtle and substantial trends as well that affect this issue, including the increasing confluence of the engineering sciences and physical sciences in condensed matter physics, chemistry, materials science and mechanics of materials in the past 15 years, driven by the national nanotechnology initiative, among others. It is now common for faculty with training in the sciences to be hired into engineering units, and vice versa to some extent. To effectively pursue ICME, this enhanced richness and blending of cultures and approaches must be balanced by investment in a similar blending of cultures and disciplines *within* engineering, including engineering systems design, manufacturing, logistics, etc. One practical way to achieve this integration is to include materials design as one of the divisions or academic areas of pursuit within MSE departments, or even as a distinct multidisciplinary unit, along with supporting coursework.

There are also several particular points relevant to MSE curricula:

- Principles of computing and numerical methods should constitute a required undergraduate course.
- Software for managing heterogeneous model execution and database management, as well as software for materials modeling and simulation, should be integrated into computational materials science courses offered at the undergraduate level.
- The methods, tools, and benefits of these codes should be systematically reinforced by faculty/GTAs in other follow-on courses, which may require a concerted investment to support these later courses.
- Materials design courses should not be offered in a self-contained manner within MSE academic units, but should convey the multidisciplinary flavor of ICME.
- Capstone design courses at the advanced undergraduate level should integrate materials processing and characterization, experiments, principles and numerical methods for modeling, systems engineering, and cross-disciplinary teams of students and faculty from various academic units.

At Georgia Tech, cross-fertilization between MSE and ME occurs in various ways, including joint faculty appointments, a senior-elective course in materials selection/design, and modeling and simulation courses taken by students in both departments. Both departments require an undergraduate course in numerical methods for engineers. Moreover, two multidisciplinary centers within the College of Engineering facilitate ICME-related research and education collaborations of faculty and students in these units, the Mechanical Properties Research

Laboratory [14] and the NSF-sponsored Center for Computational Materials Design [15], a joint Penn State-Georgia Tech I/UCRC.

But the net to be cast for ICME is even broader than this. Pursuing the vision of ICME involves the confluence of several key developing fields:

- Computational materials science, micromechanics, and ubiquitous computing.
- Advances in high resolution materials characterization and *in situ* measurements.
- Computing and information sciences (information theory, databases, digital interfaces, data visualization for decision support, web protocols).
- Decision theory and systems design (game theory, utility theory, multi-objective optimization).
- Engineering design.

From a broad educational perspective, it is clear that the integration of these fields is mainly to be accomplished in the interdisciplinary graduate curricula. It is important to emphasize disciplinary depth and competence in the undergraduate curriculum, offering students enhanced exposure to computational methods, systems thinking, and design integration. ICME is a multi-discipline, not a single discipline, that draws from various branches of engineering and the computing and information sciences.

3. CLOSURE

The vision of Integrated Computational Materials Engineering is compelling in many respects, not only for the value-added in reducing time to market for new products with advanced, tailored materials, but also for enhanced efficiency and performance. It involves much more than just enhancing the role of modeling and simulation in design and manufacturing processes. This article has attempted to outline some of the basic issues and obstacles facing development of ICME from perspectives of industry, government and academia. A pro-active approach is required to reform historical modes of operation in these sectors to facilitate multidisciplinary collaboration and to clearly articulate the vision and scope of ICME.

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THE FOUR FOUNDATIONAL GROUPS REQUIRED FOR A SUCCESSFUL ICME APPROACH*

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ABSTRACT

This article briefly outlines some of the roles of four foundational groups in fostering rapid growth and implementation of Integrated Computational Materials Engineering (ICME). These roles include development of ICME-related computational, experimental, and cyberinfrastructure tools, and training of the future ICME workforce, in order for ICME to realize its great potential. The four foundational groups considered here include: (1) corporations, (2) government organizations, (3) universities, and (4) professional societies. Finally, a discussion is provided of how materials societies can play an important role in convening the four foundational groups, and providing the venues and mechanisms for members from these groups to integrate and work together to enable ICME to flourish.

INTRODUCTION

In a 2008 study on Integrated Computational Materials Engineering (ICME) organized by the National Research Council (of the National Academies)¹, ICME was described as “the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.” That study went on to provide a wealth of information on the overall vision for ICME as a discipline, case studies and lessons learned, technological barriers, and a look toward the way forward in overcoming cultural and organizational challenges to ICME [1]. One recurring theme throughout that report was the need for people from various materials-related disciplines and organization types to work together not only to provide the foundation for ICME, but also to integrate the proper ICME tools and personnel into broader, multidisciplinary, Integrated Product Development Teams (IPDTs). These IPDTs represent a mechanism whereby new materials and manufacturing processes are designed, developed, and brought to market.

The purpose of this paper is to elaborate on four foundational groups that are not only required to provide the needed computational and experimental tools for enabling successful ICME approaches, but which also must provide for the integration of such ICME tools and personnel into the Integrated Product Development Teams. The four foundational groups outlined here include: (1) corporations, (2) government organizations, (3) universities, and (4) professional societies – as depicted schematically in Fig. 1. This article is written from the author’s direct experience in three of the foundational groups (government, materials societies, and academia), and intimate interactions with the fourth (corporations) through various projects and development

* This article was previously published in the April, 2011 issue of JOM (a publication of The Minerals, Metals & Materials Society), and is being directly excerpted here (with permission from JOM and Springer), as some of its contents were included in a presentation by the author, George Spanos, at the MS&T 2010 ICME symposium from which this proceedings book is based.

teams upon which he participated. Additionally, many of the themes and ideas developed here are directly related to the discussions and recommendations of the 2008 National Academies Study on ICME [1], but with a specific focus here on these four foundational groups. Particular emphasis is placed on summarizing and elaborating on the key roles of each of these groups, and considering how they must be integrated and leveraged with one another, in order to advance and enable ICME in the coming years. Specific consideration is finally given to the role of one of the foundational groups, professional societies, in convening the other three groups, and helping to integrate and provide synergy amongst them.

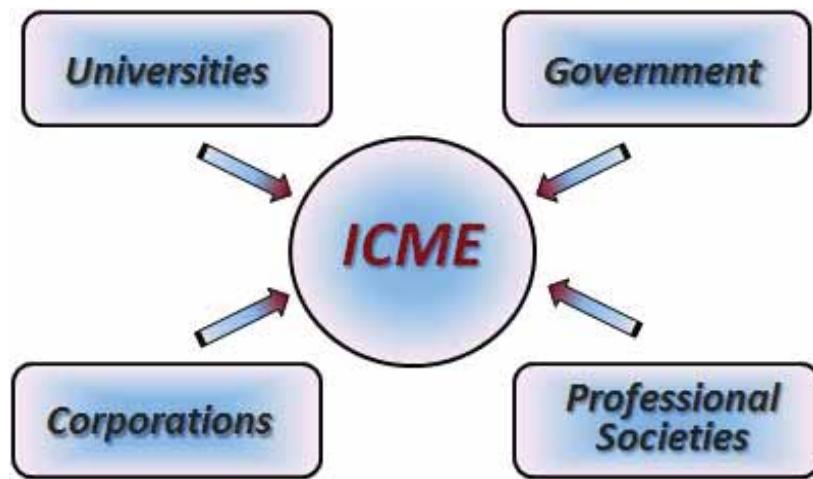


Figure 1: Schematic illustration of the four foundation groups required for a successful ICME infrastructure and approach.

ROLES AND INTERACTIONS OF EACH OF THE FOUNDATIONAL GROUPS

Corporations

One of the most important roles of industry in ICME is implementation of ICME tools and personnel into the product and process design cycle. This is done by integration of these tools and professionals into the broader IPDTs, which are typically assembled by corporations focused on development of a new product or manufacturing process. As discussed in the 2008 study [1], there are a number of cultural and historical barriers that have to be overcome in order for this to be done effectively, on a large scale. An equally important role of corporations is investment of significant resources upstream to support ICME, with the vision of a substantial final return on investment (ROI) (as high as 10:1 for a given product and/or manufacturing process¹), and the promise of a significantly reduced cycle time for product/process design, development, and implementation.

Companies will also be required to partner with academia and national laboratories to develop the computational, experimental, and cyberinfrastructure tools needed for ICME, as discussed further below. Another key role of industry is to work with the other foundational groups in defining the optimum engineering problems for which to apply an ICME approach, to provide for the most efficient use of resources and the largest ROI.

Government Organizations

This foundational group can generally be broken down into two, intimately related organizational types: (1) funding agencies, and (2) national laboratories. A major role of funding agencies is to become champions of ICME [1], and thus to come alongside industry to provide the leveraged funding support needed to develop and implement ICME tools and personnel. These agencies will also play a key role in defining the product and manufacturing needs of various US government sectors to which ICME approaches should be applied; these government sectors include for instance the department of defense, the department of energy, and the commerce department. National laboratories can also work with the funding agencies to provide such input on product/process needs, but even more importantly need to continue to partner with academia and industry to develop and implement advanced ICME tools and cyberinfrastructure. In the present context, ICME “cyberinfrastructure” includes collaborative Web sites, repositories of various types of materials and properties related data, computational modeling tools, and collaboration software.

Just one example of this type of effort in which national laboratories partnered with funding agencies, academia, and corporations was the D 3-D Digital Structures program, which was funded by the Office of Naval Research (ONR) and the Defense Advanced Research Projects Agency (DARPA) (and came to a close in July of 2010). A number of groundbreaking computational, experimental, and materials database tools centered about 3D materials and processing analyses were developed in that program, and can now be integrated into ICME efforts. As emphasized both in that program and in the 2008 ICME study [1], experimental tools and data are critical to any ICME approach (and often compose 50% or more of such an effort), in order to provide for critically needed testing, verification, and enhancement of the computational models, and to generate realistic input for the initial conditions of such models [2, 3].

Universities

One role in ICME for which universities are perhaps uniquely suited, is the initial, foundational development of the workforce, or “human capital”, which will serve as the backbone of ICME teams and efforts for the foreseeable future. The University Materials Council (UMC), which is composed of department heads from materials departments around the US, should play a critical role here [1]. In this regard, the UMC had a meeting in June of 2010 to address educational issues and needs related to ICME, and to the somewhat broader area of computational materials science and engineering (CMSE).

Three interrelated components can be employed by universities to develop the proper educational elements and workforce for ICME, as depicted schematically in Fig. 2. First, academia must develop the proper curriculum, at both the undergraduate and graduate levels, to equip young professionals with the proper training and tools to enter the ICME workforce and begin serving in this capacity on Integrated Product Development Teams (IPDTs). Secondly, Masters and Ph.D. theses centered about ICME or ICME-related topics provide a strong training ground for

ICME professionals. Finally, ICME-related research at universities (which includes the theses just mentioned) provides training not only for the students involved, but also enables ICME expertise to be developed by the faculty, engineers, and technical staff working on these projects.

Related to these university projects, another role of academia in ICME is essentially the same as one shared by the national laboratories and industry - the development and implementation of the computational, experimental, and cyberinfrastructure tools needed for ICME. As mentioned earlier, significant and rapid progress here will not be accomplished independently of the other three foundational groups, but must be done in a partnership in which all the groups work together in a synergist way to accomplish the ultimate goal of utilizing ICME to dramatically reduce design and development cycle times, and associated costs, of new products and manufacturing processes. These university efforts could be funded as part of larger ICME projects/teams, but could also be leveraged with the smaller research and development projects supported at the individual principle investigator level.

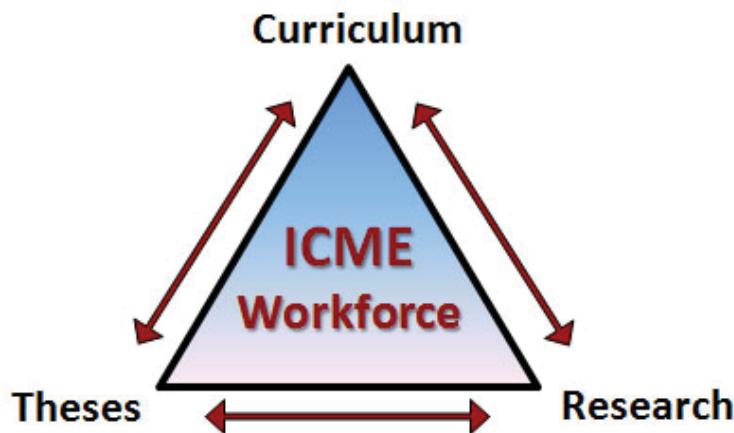


Figure 2: Three (interrelated) components at universities that contribute to the development of the educational needs and workforce required for ICME.

Professional Societies

Professional societies, particularly those associated with materials science and engineering, play an especially important role in convening members of the other three foundational groups in a synergistic way in which their efforts and interactions are integrated and optimized to provide the largest benefit. Materials societies can accomplish this in a number of ways, and although most of the examples provided here are taken from efforts of The Minerals, Metals and Materials Society (TMS), with whom the present author is affiliated and most familiar, other societies such as (but not limited to) ASM-international and the Materials Research Society (MRS) also have members and efforts associated with computational materials science and engineering, and in fact work with TMS members and/or staff on some of these efforts.

First, technical committees within professional societies are an excellent way to bring members from the four foundational groups together to work in concert on projects that will provide the foundational infrastructure needed for effective ICME programs. Additionally, they create a venue for these members from the different groups to get to know one another, work together for common goals, and possibly even begin to form ICME teams. An excellent example of such a structure is the TMS ICME committee, which is composed of more than 50 members, with significant representation from industry, government, and academia, and professional society liaisons. This committee also contains three active subcommittees, centered about: (1) education, (2) ICME cyberinfrastructure, and (3) technical programming (i.e., symposia and conferences). The educational efforts are obviously closely linked with universities and the UMC, while the cyberinfrastructure subcommittee is helping to determine critical components, needs, and synergies of ICME cyberinfrastructure.

Technical programming is one of the ways that professional societies can convene a much larger cross section of the ICME community, i.e. to greatly expand the sphere of influence beyond the members of the technical committees themselves. For example, the TMS ICME committee organized a multi-session ICME symposium at the recent TMS annual meeting in San Diego, and was involved with another ICME symposium at the 2010 MS&T meeting (a multi-society meeting), which was organized by the ASM Materials Properties Database Committee. Additionally, as mentioned in another article in this JOM issue, the *First World Congress on ICME* is a TMS specialty conference, organized in conjunction with the TMS ICME committee, that will bring together more than 200 scientists and engineers working in ICME or ICME-related areas (from 11 countries around the world) on July 10 – 14, 2011, in Seven Springs, PA. This conference will provide for an intimate setting conducive to rich discussions, interactions, and planning amongst the ICME community (see www.tms.org/Meetings/Specialty/ICME2011). These are all examples which provide excellent venues for the ICME community within the four foundational groups to connect, interact, and work together to not only leverage one another's efforts in providing for critical ICME tools and infrastructure, but also to determine the critical directions and pathways of future efforts in ICME.

An equally important mechanism whereby materials societies can convene the ICME community (the four foundational groups) is through publications such as this special group of JOM articles, other special journal issues, conference proceedings, and books. Finally, electronic on-line bulletin boards and platforms, such as the ICME digital resource center at the MaterialsTechnology@TMS Website, will certainly be valuable tools for convening the four foundational groups as well.

CONCLUSIONS

Integrated Computational Materials Engineering (ICME) is an exciting and rapidly growing discipline with great potential for dramatically reducing product and process design, development, and implementation times and costs, thus providing for large returns on investment. But ICME is in its early stages of development, and in order for this great potential to be realized, it will require a firm commitment from four “foundational groups”, or organization types, to develop and implement ICME. These four foundational groups include: (1) corporations, (2) government organizations, (3) universities, and (4) professional societies. More than just providing a commitment to ICME, a concerted effort is needed by members from each of these groups to work together not only to leverage one another's efforts, but to partner in a way to synergistically advance this field at a much more rapid rate than would be achievable otherwise.

More specifically, each of the four foundational groups have various roles (often overlapping) in fostering growth and implementation of ICME, development of ICME-related computational, experimental, and cyberinfrastructure tools, and proper training of the future workforce to provide the human capital required for ICME. Finally, materials societies play an important role in convening the four foundational groups, and providing the venues and mechanisms for members from these four groups to integrate and work together to enable ICME to flourish.

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THE DEVELOPMENT AND IMPLEMENTATION OF INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME) FOR AEROSPACE APPLICATIONS

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ABSTRACT

Considerable effort has been expended over the past three decades developing materials, processing, and behavior models. While many of these models are currently employed in the industry by both engine OEMs and their suppliers, the anticipated major benefits from the use of such models have not been realized. We believe that basic technology approaches for Integrated Computational Materials Engineering (ICME) exist and that an industry-wide plan for the development, integration, and validation of such methods would lead to their broad implementation with significant benefits to the aerospace industry and its customers. This paper presents a general overview of the current state of ICME related to the aerospace propulsion industry, and identifies key challenges and barriers to broad development and implementation.

INTRODUCTION

Many significant advances in jet engine performance and durability have been enabled by advances in the state of the art for structural metallic materials. Notable examples are the introduction of titanium alloys, development of various nickel alloys and superalloys for many critical applications, directionally solidified and single crystal nickel-based alloys for gas path components, and advanced coatings which, when combined with advanced cooling configurations, have greatly increased turbine temperature and efficiency while simultaneously increasing durability and reducing ownership costs. Today, however, the development and validation cycle for a new or derivative metal alloy or coating remains highly empirical, *development and characterization costs are high, and the time required typically exceeds the time available in the product development cycle*. The ramifications are significant: unless a material and manufacturing process are sufficiently developed and mature at the time an engine program commits to detailed design, the program either has to forgo incorporation or carry along a backup material and configuration to mitigate risk until a final decision can be made.

In the broadest vision for what ICME could be, physics based computational models and requisite data bases would facilitate a fully integrated analytical representation of materials from alloy development, through process and microstructure optimization, to final physical and mechanical property prediction, in a manner suitable for integration with the engine development process [1-3]. Such capability could permit rapid material development and characterization for insertion, as well as become an integral part of engine development and optimization analyses. With comprehensive physics-based models, new compositional or microstructural development space

might be explored. Such capability would facilitate much more economical assessment of process and supplier changes, better definition of specification limits, analytical evaluation of “out-of-specification” consequences, and development of derivative or tailored materials. Understanding material property variation and its drivers could reduce characterization and validation test requirements, and facilitate maximum safe utilization of materials through more insightful probabilistic analyses and life prediction.

ASSESSMENT OF CURRENT STATUS

ICME is a nascent, immature discipline and undoubtedly even the concept has varied interpretations within the materials community. While some material scientists view it as a new paradigm describing a better way to build and represent knowledge, almost all cognizant industrial materials engineers hope to exploit the concept to solve problems and replace costly and time consuming experimentation and testing. In 2008, the National Materials Advisory Board’s (NMAB) Committee on Integrated Computational Materials Engineering published the results of a yearlong study to establish a vision and status assessment of ICME [1]. An operational definition of ICME developed by the study is given in the text-box below:

[The ICME] goal is to enable the optimization of the materials, manufacturing processes, and component design long before components are fabricated, by integrating the computational processes involved into a holistic system. ICME can be defined as the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation. ... The emphasis in ICME is on the ‘I’ for integrated and ‘E’ for engineering. Computational materials modeling is a means to this end. [1]

As stated in this definition, the application of ICME is an engineering endeavor involving integrated modeling. In this context, integrated modeling can mean model integration across differing length and time scales for a given phenomena or simply integrated modeling among processing, microstructural evolution and properties. One example of an ICME architecture is shown in Figure 1. The system consists of a suite of models, a database, systems analysis tools, and a graphical user interface all linked and managed via an integration software system.

Modeling

Mechanical engineering has enjoyed a strong mathematical foundation since its inception; so not surprisingly, the development of the finite-element-method (FEM) and modern computers has radically transformed the discipline. Indeed, today the FEM framework is applied to carryout sophisticated continuum heat flow, fluid flow, and structural analysis of complex geometries. Despite its predominant dependence on a single computational framework, it still has taken this discipline over 30 years to build integrated analysis systems whose application has reduced component, rig, and engine testing while reducing the product development time by a factor of three.

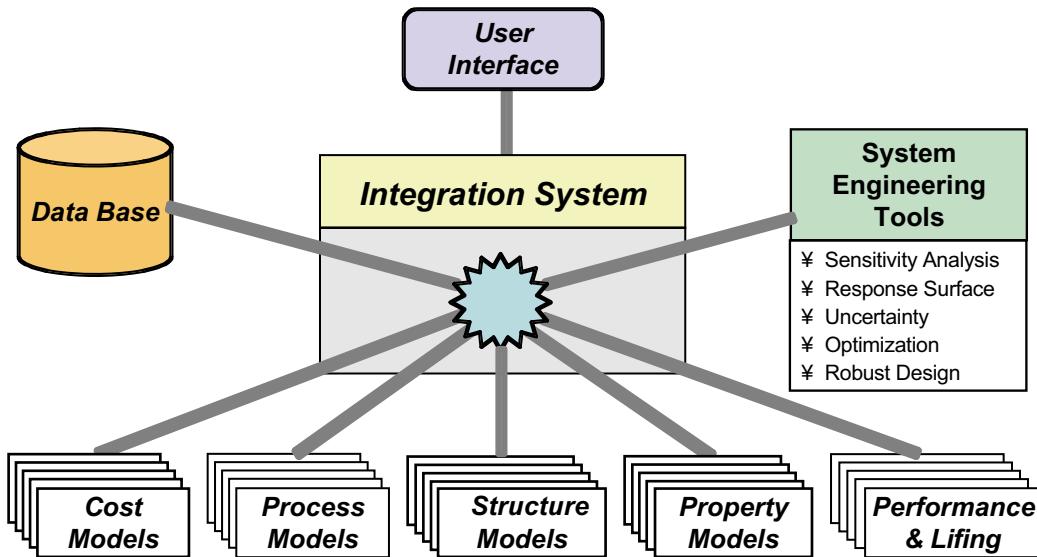


Figure 1: Pictorial representation of the typical elements of an ICME system.

Materials engineering computation has exploited these FEM advances which now serves as the backbone of casting and forging process modeling tools, such as ProCAST™ and DEFORM™, respectively. The mathematical underpinnings of these codes are mature and the FEM implementation within these programs has been validated by comparing results with those from closed-form analytical solutions. Also, well before the ICME acronym had been coined, materials scientists and engineers were physically modeling microstructural evolution and mechanical behavior. Resulting physically based models currently used by materials scientists and engineers are listed in Table 1 [1]. This table illustrates the diversity of materials models, each type employing differing computational techniques, largely owing to differing length scales of the associated materials phenomena. The lack of a unifying computational technique fragments and lengthens development effort, makes validation difficult, reduces incentive for commercial code development, and requires increased specialization among materials modelers. Also, not all models in Table 1 are currently suitable for industrial application because they require excessive expertise and/or they are computationally expensive. Further, while the process models in Table 1 are fundamentally mature some of the ancillary models in these modeling packages, e.g. hot tearing within ProCAST™, are immature. Others such as the thermodynamic codes, Pandat™ and ThermoCalc™, employ validated computational schemes but predictions contain error associated with errors in the thermodynamic database.

Table 1: Physically Based Materials Models

Mode or Method, Required Input, Expected Output, and Typical Software Used in Materials Science and Engineering [1]			
Class of Computational Materials Model/Method	Inputs	Outputs	Software Examples
Electronic structure methods (density functional theory, quantum chemistry)	Atomic number, mass, valence electrons, crystal structure and lattice spacing, Wyckoff positions, atomic arrangement	Electronic properties, elastic constants, free energy vs. structure and other parameters, activation energies, reaction pathways, defect energies and interactions	VASP, Wien2K, CASTEP, GAMES, Gaussian, a=chem., SIESTA, DACAPO
Atomistic simulations (molecular dynamics, Monte Carlo)	Interaction scheme, potentials, methodologies, benchmarks	Thermodynamics, reaction pathways, structures, point defect and dislocation mobility, grain boundary energy and mobility, precipitate dimensions	CERIU2, LAMMPS, PARADYN, DL-POLY
Dislocation dynamics	Crystal structure and lattice spacing, elastic constants, boundary conditions, mobility laws	Stress-strain behavior, hardening behavior, effect of size scale	PARANOID, ParaDis, Dis-dynamics, Micro-Megas
Thermodynamic methods (CALPHAD)	Free-energy data from electronic structure, calorimetry data, free-energy functions fit to materials databases	Phase predominance diagrams, phase fractions, multicomponent phase diagram, free energies	Pandat, ThermoCalc, Fact Sage
Microstructural evolution methods (phase-field, front-tracking methods, Potts models)	Free-energy and kinetic databases (atom mobilities), interface and grain boundary energies, (anisotropic) interface mobilities, elastic constants	Solidification and dendritic structure, microstructure during processing, deployment, and evolution in service	OpenPF, MICRESS, DICTRA, 3DGG, Rex3D
Micromechanical and mesoscale property models (solid mechanics and FEA)	Microstructural characteristics, properties of phases and constituents	Properties of materials—for example, modulus, strength, toughness, strain tolerance, thermal/electrical conductivity, permeability; possibly creep and fatigue behavior	OOF, Voronoi Cell, JMatPro, FRANC-3D, ZenCrack, DARWIN
Microstructural imaging software	Images from optical microscopy, electron microscopes, X-rays, etc.	Image quantification and digital representations	Mimics, IDL, 3D Doctor, Amira
Mesoscale structure models (processing models)	Processing thermal and strain history	Microstructural characteristics (for example, grain size, texture, precipitate dimensions)	PrecipiCalc, JMat Pro
Part-level FEA, finite difference, and other continuum models	Part geometry, manufacturing processing parameters, component loads, materials properties	Distribution of temperatures, stresses and deformation, electrical currents, magnetic and optical behavior, etc.	ProCast, MagmaSoft, CAPCAST, DEFORM, LS-Dyna, Abaqus
Code and systems integration	Format of input and output of modules and the logical structure of integration, initial input	Parameters for optimized design, sensitivity to variations in inputs or individual modules	ISIGHT/FIPER, QMD, Phoenix
Statistical tools (neural nets, principal component analysis)	Composition, process conditions, properties	Correlations between inputs and outputs; mechanistic insights	SPLUS, MiniTab, SYSTAT, FIPER, PatternMaster, MATLAB, SAS/STAT

Although most materials researchers have a strong preference for physically based models, materials engineers often embrace data-driven modeling when there is a compelling need and alternatives don't exist. These engineers who adopt the so-called "80% solution" are merely acknowledging Prof. George Box's well known quote that "Essentially, all models are wrong, but some are useful" [4]. These models are useful when they serve a needed purpose and are formulated based on high quality data, employ relevant modeling forms and variables, are statistically significant, and finally model accuracy, precision, and region of applicability are rigorously determined.

Finally, cost modeling is usually under-appreciated as an important element within the suite of material models [3] and many times it is totally ignored. Too often engineers either assume that material improvements will outweigh any added costs or they totally ignore cost implications thereby potentially violating a key constraint that may prevent implementation. The ability to quantitatively assess the cost impact of material and process changes during ICME analysis allows more accurate and realistic tradeoffs during material design and facilitates optimization by including manufacturing cost within the objective function.

Data

There are three types of data required to develop, upgrade, and execute analyses within an ICME system. These types include: (1) data required for execution of physically based codes (e.g., thermodynamic and mobility databases), (2) data for calibrating constitutive models that feed physically based models or serve as surrogates within the ICME model library, and (3) data needed to validate constituent models and overall system performance. General comments regarding the maturity state and issues for these types of data are described below:

- Thermodynamic and mobility databases are reasonably mature. However, occasionally thermodynamic calculations appear erroneous for certain chemical elements in some alloys.
- There is no community wide database containing physical properties, thermophysical properties, or properties needed for microstructural models (e.g., Anti-Phase Boundary energies, surface energies, precipitate misfit) for most of the alloys relevant to aerospace applications. While some of these properties are available via calculation with programs such as JMatPro™, the uncertainty of resulting values is unknown.
- Publicly available data describing elevated temperature properties relevant to processing models (e.g., emissivity, molten metal viscosity) is limited and of unknown accuracy.
- Some process input data (e.g., surface heat transfer coefficients and forging friction coefficients) cannot be directly measured but must be inferred or calculated using inverse methods that may not be fully validated.
- Validation data for some models is difficult to acquire and subject to variable accuracy. While this issue is most severe with some microstructural models (e.g., measurement of fine precipitate size distributions) it also applies to some mechanical properties (e.g., measurement of elevated temperature dwell fatigue under certain environmental conditions).

While some of these data limitations are relevant to the entire materials community, the limits are greater for the most important aerospace alloys, which are often proprietary and also may be export or International Traffic in Arms Regulations (ITAR) controlled, limiting associated research within academia. Moreover, most research sponsors have limited interest in funding data development research despite its importance to modeling and ICME.

Systems Analysis

Commercial systems analysis software is available from several suppliers; and although this capability continues to evolve it is mature and robust for application to ICME. This software, one example being the Dassault Systemes iSight™ product, provides a robust, user-friendly suite of tools for product improvement. Features often include Monte Carlo methods to simulate variation and uncertainty as well as multiple optimization routines employing both classical optimization routines as well as those based on genetic algorithms and simulated annealing.

System Integration

Much like systems analysis software, integration software is mature and in use by all aerospace OEMs within their product design organizations. These systems allow the user to link a software module with the integration platform and then later channel information between selected programs to establish an interoperable, easily reconfigurable computational network. What this means is that once a suite of models and databases have been linked within the integration system, the user can select a subset of these and logically interconnect them, usually graphically, into a specific network configuration. The output of one program then becomes the input to the next adjacent program in the network and so on until the final output prediction is achieved. Because each “use case” (type of problem) may require a unique set of models and data configured into a unique network, user-friendly reconfigurability becomes a potent integration system feature and such “use cases” can be stored for later use. In addition, integration systems sometimes include systems engineering utilities and interfaces for common mechanical engineering software, e.g., Catia™, Ansys™, MatLab™, Excel™, and ASCII files. For programs that don’t have pre-built interfaces, the user must create the interface which typically requires expertise with a scripting language such as TCL to establish the program interface. Unfortunately, many ICME models will require such interfacing scripts, but the script only needs to be written once and can be shared.

Despite the power and importance of system integration software to build the ultimate ICME system, it is important to address how much emphasis should be given the selection and deployment of this capability in the early stages of ICME exploration within industry. It is likely more prudent to focus development energy and resources on building and demonstrating ICME functionality and benefit for the following reasons:

- The licensing and training costs of such software can be significant;
- For those organizations that already have production software integration systems, management and IT departments will likely resist insertion of ICME modules until they are technically validated and benefit is demonstrated;
- Early application of integration software may divert manpower from more important ICME development needs; and
- Though system integration software is powerful and mature; this technology continues to advance. Future systems will likely be even better.

For those projects and organizations that choose to defer investing in system integration software, many, if not all, near-term integrated ICME applications can be integrated the old-fashion-way by piping information between software programs either manually or via scripting. Taking this approach assures that the associated ICME functionality is indeed useful and also provides integration experience that will inform the future selection of an integration software system.

Community-wide Standards

Since ICME is a nascent technology there are really no known community-wide ICME standards that promote common databases, materials representations, requirements for model verification and validation, interface standards for ICME relevant software, or even mechanisms for achieving such standards. While the materials community adheres to common ASTM standards for common modes of materials chemistry, microstructure, and property measurement and testing, members of the aerospace industry often further refine specific specification measurement techniques to reduce measurement error and improve applicability and data quality.

Early Demonstrations and Lessons Learned

The NMAB ICME report [1] contains a description of early research that developed ICME systems with integrated models, data, and systems analysis tools to demonstrate the potential benefit opportunities. Beyond providing seed ICME systems within the developing companies, these efforts have been important for assessing the maturity of ICME tools, identifying key issues and challenges, and identifying pathways for ICME maturation and implementation. While this whitepaper will give a brief synopsis of two development programs, the interested reader is encouraged to refer to the NMAB ICME report for further details about these two programs and lessons learned.

In 2001 DARPA launched the Acceleration Insertion of Materials (AIM) program to apply modeling and critical data to reduce the development time for advanced aerospace materials. This goal was motivated by the expanding development cycle time gap between empirical materials development and the computational design used for product development. GE Aircraft Engines (GE) and Pratt & Whitney (P&W) collaborated to establish ICME systems supporting development of powder metallurgy turbine disk technology. These efforts used commercial software (DEFORM, ThermoCalc, Pandat, Ansys, iSight) and supported the development of PrecipiCalc and university mechanical property codes relevant to nickel-base superalloys. Both GE and P&W used iSight to integrate these models and relevant databases and then applied the system to analyze typical test problems. P&W successfully demonstrated the ability to reduce forging weight by 21% while increasing disk burst speed by 19%; whereas GE showed how their integrated system could accelerate disk alloy development by 50%.

In the same time period, Ford Motor Company established a virtual aluminum casting (VAC) methodology to reduce the cost and time needed to develop cast automobile components. The VAC modeling system included commercial software (MagmaSoft, Pandat, Dictra, and ThermCalc) and developed a number of microstructural and property models based on the findings of in-house and funded university research. In one demonstration, Ford researchers simulated casting and heat treatment of an engine block and verified VAC predictions via comparison to measured microstructure and properties. While Ford estimates that VAC development involved 25 people and \$15 million dollars, the estimated VAC return on investment was well over 7:1.

Based on the analysis conducted by the NMAB ICME committee [1], these two programs and others reviewed by the committee provide the lessons learned listed below. These lessons are self-explanatory, though further details and justification are provided in the committee report.

Lessons Learned [1]

- *ICME is an emerging discipline, still in its infancy.*
- *There is clearly a positive return on investment in ICME.*
- *Achieving the full potential of ICME requires sustained investment.*
- *ICME requires a cultural shift.*
- *Successful model integration involves distilling information at each scale.*
- *Experiments are key to the success of ICME.*
- *Databases are the key to capturing, curating, and archiving the critical information required for development of ICME.*
- *ICME activities are enabled by open-access data and integration-friendly software.*
- *In applying ICME, a less-than-perfect solution may still have high impact.*
- *Development of ICME requires cross-functional teams focused on common goals or “foundational engineering problems.”*

KEY CHALLENGES AND IMPLEMENTATION BARRIERS

Model Inadequacies

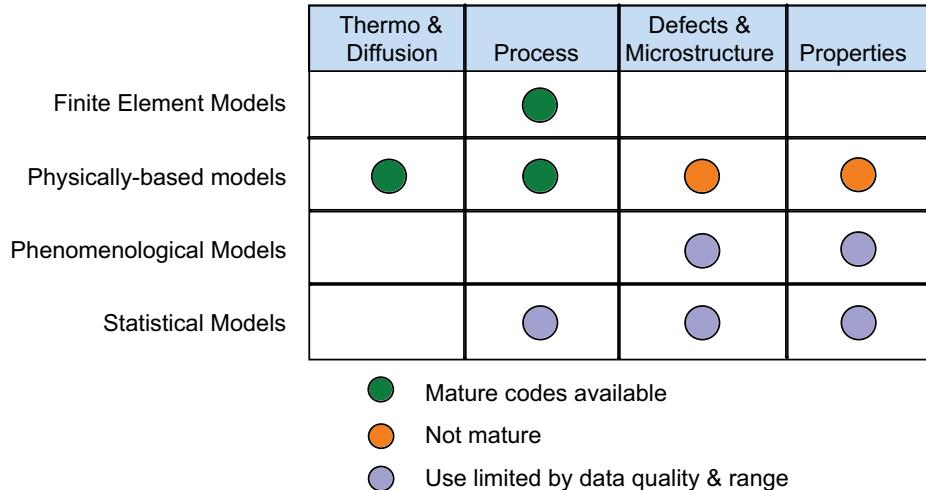
Without doubt, the lack of a complete suite of fully mature validated materials models represents the greatest challenge in constructing a comprehensive ICME system. This shortcoming constricts the number and type of problems solvable using ICME, reduces the realizable near-term payoff, and increases the risk that the fidelity of ICME predictions fall short of application needs. There are some processing and materials models that generally are considered mature, in that they implement proven and reliable algorithms. However, even these models can fall short of providing adequate accuracy owing to inaccurate embedded materials properties, constitutive property model parameters, or boundary condition values. Beyond the repercussions identified above, the lack of mature models have the insidious effect that the repeated failure of models in practical engineering applications taints the potential value of models and builds skepticism among engineers who could otherwise become ICME advocates.

Classifying the maturity of materials and processing models is subjective at best because the accuracy and precision levels of these models are not generally available and the range of applicability is usually not specified in detail. Recognizing this caveat, Table 2 provides a condensed view of maturity for material classes based on both the perspectives and direct experience of the authors. Overall this table indicates that engineers attempting to formulate a near-term ICME system will face challenges that may temporarily require use of provisional data-driven models.

Model Validation Methods and Standards

Commercial suppliers of finite-element-method (FEM) software invoke systematic methods to verify the embedded code and validate the implementation of physics within their FEM products. Validation usually entails comparison of FEM predictions against classical solutions and testing to compare results against those obtained from established software. These software suppliers often encourage and support user groups who provide feedback regarding application issues and enable continuous software improvement and better application practices.

Table 2: Overview of model availability and maturity by type



Unfortunately, the nascent materials modeling realm does not have either agreed upon validation methods or standards whose application convey the magnitude of modeling errors and the range of model applicability. Materials modelers lack benchmark problems whose exact solution is known or alternative widely accepted high fidelity models against which predictions can be compared. Instead, model developers usually must rely on data to test newly developed materials models. However, given the diversity of materials and processes, a model developed and validated against data from one subset of materials may not work for other materials. Model developers sometimes do provide guidance for the range of model applicability but often usually this is limited to specifying the applicable alloy class or referencing the underlying material science research upon which the model was built. Prudent model users often remain uncertain and must test the model for their particular material and process.

Developing validation methods and standards is a difficult endeavor for both cultural and technical reasons. Except for continuum mechanics FEM formulations within processing software programs, most models describing defect formation, microstructural evolution, and property development were and continue to be developed by university researchers. These researchers too often develop models to build and demonstrate understanding of operative mechanisms and have less interest in building widely applicable models for industrial application. Also, materials engineering faculty generally do not include rigorous coursework involving error determination and model validation within their curricula. Finally, increasingly university materials departments are defocusing education and research in structural materials; this change causes less appreciation for industrial modeling needs for these materials and lessened awareness of the level of model fidelity required to supplant traditional empirical, data-driven methods upon which industry has depended historically.

From a technical perspective, model validation is difficult because materials processing, microstructural evolution, and property development entails a rich mix of length and time scales with an equally complex set of interacting phenomena and mechanisms. There are presently no physically based models that incorporate all such phenomena and mechanisms. Instead, currently applicable models introduce simplification, homogenization, and only those mechanisms deemed dominant. Other usable models are only loosely based or inspired by mechanisms including those generally described as phenomenological or constitutive.

Because most currently applicable models do not include all relevant physics, they depend on not only physical properties that can be measured by independent measurement but also calibration (tuning) parameters that depend on the specific material and process under consideration. These calibration parameters must be deduced by comparing model prediction against corresponding experimental results; and of course the range of applicability of the parameters determined in this way depend sensitively on the specific material and process used for the experiment. Therefore, model error varies from one application to the next and depends on the suitability of the model assumptions and constitutive forms, the quality of experimental data and how well calibration parameters are determined, and the skill of the analyst who applies the model. Beyond these difficulties, engineers who adapt these models rarely generate independent validation data sets to confirm model adequacy, calculate accuracy, and identify potential error sources. Even when a validation data set is produced and applied, the range of model applicability is limited by the range on input model parameters contained within the data set. Materials models are often non-linear and therefore the extrapolative power of these models often decreases rapidly the more they depends on calibration data.

Propagation of Variation and Error among Linked Models

When multiple models are linked to form a modeling system, errors from each model propagate through the entire chain and it is impossible to determine the level of error in the system output without additional analysis. Even when the accuracy and precision of each model in the modeling system are seemingly reasonable, the assembly of models can produce unacceptably inaccurate and imprecise modeling results when errors compound and some models have “high gain”. When the accuracy and precision of each model is unknown, reliance on the integrated modeling system introduces significant risk.

Materials and processes are also subject to variation in input variables such as chemistry, process temperature, cooling rates etc. Although each set of input parameters will produce a single deterministic output, it is often important to understand how variation of input (e.g., process) variables affects the variation in the model output (e.g., properties). Much like the propagation of errors input variable variation propagates through a series of linked models in a way that depends on the effective gain of each model.

Monte Carlo analysis is a widely used method to track the propagation of error and variation through a system of integrated models. Application of this technique requires knowledge of the statistical distribution of model input variables, uncertain internal model parameters, and possibly other errors associated with the model formulation or the solver. The method then repeatedly selects random values and parameters from each probability distribution and executes the system of models. After a large number of such iterations, the statistical analysis of output values provides an estimate for output variation associated with error and/or input variation. When the execution time for the modeling system is sufficiently fast, the analyst can use a large number of Monte Carlo iterations thereby assuring an accurate analysis in a reasonable time. However, when the analysis includes extensive computation, such as involving FEM analysis, design engineers have demonstrated Monte Carlo analysis can be accelerated by using response surfaces and approximate fast probabilistic integration methods.

Model Integration Challenges

Models within an ICME system can be integrated in a number of ways depending on the level (tightness) of integration among models and the type of communication interface(s) available for each model. Common interfacing methods include the use of application programming interfaces (API), scripts that port information between modeling programs, user defined subroutines linked

to a master modeling program, and internal linkage of multiple materials models within a single program. Additionally, integration software provides preconfigured interfaces for some engineering software and utilities and procedures to facilitate integration of other software. While most materials programs (commercial or user-developed) can be linked with each other, integration often requires effort and computer expertise to translate and transfer data variables. Such efforts are further complicated by the lack of a community-wide materials modeling standard for data exchange and the absence of a uniform materials representation for either models or databases.

Commercial software suppliers will continue to add subsidiary models and features within their products to better serve their customers' needs and compete effectively with their competitors. This is helpful technically, particularly when the physics of the problem demands tightly coupled solutions or when subsidiary models are fully accurate and validated. It also allows the industrial customer to license fewer commercial codes and limits training costs. However, when subsidiary models are inaccurate or unknowingly inapplicable, a user, committed to unified codes, is powerless to fully understand the deficiency and improve the embedded code to satisfy their particular needs.

Integration Software

Some aerospace companies already use sophisticated integration systems to facilitate and automate their design engineering functions. However, premature attempts to build a full scale integration system before ICME functionality is verified and architectural needs are confirmed, run the risk of diverting critical attention away from more pressing fundamental ICME needs (models, data generation, validation etc.) and ending up with a non-optimal ICME integration system.

Collaborative ICME Development, Intellectual Property and Export Control

ICME encompasses a broad spectrum of technologies supporting a wide variety of materials and processes. The scope is sufficiently wide that ICME development must necessarily engage the wider materials community with collaboration among companies and with academia and the government. And although construction of an ICME system involves commercial software and some models that are pre-competitive or in the public domain, collaborative development of various ICME elements will very likely encounter intellectual property, export control, and International Traffic in Arms Regulations (ITAR) challenges.

Aerospace OEMs and suppliers all protect data and processing information, which is deemed to provide competitive advantage, via patents or proprietary information control. For example, a supplier may safeguard processing methods and parameters, whereas an aerospace OEM may protect material design data and lifing methods. However, these controls can easily frustrate development of an ICME system, which depends on knowledge, data, and models that cross the boundaries between OEMs and suppliers. OEMs and suppliers must collaborate to configure information exchange in a way that precludes inverse determination of process methods or parameters while passing sufficient information to allow downstream ICME analysis. The proprietary nature of aerospace materials data also makes it difficult to assemble community wide databases because so much key mechanical property data is proprietary. However, the community can focus on building databases for common non-proprietary alloys and modeling input property data.

Interaction between ICME developers and software developers may also pose proprietary information challenges. Today many important commercial software providers are headquartered

offshore (e.g., ProCAST™, iSight™, Abaqus™, and JMatPro™) and tailoring and validating embedded modules for some export or ITAR controlled aerospace materials and processes may be challenging when transfer of controlled data is necessary. Additionally, some software developers, domestic or foreign, have adopted business models wherein the developer retains ownership and control of future software enhancements. Though this business model is profitable for the software developer, it may impose undue long-term cost and/or hinder future enhancement for the ICME customer.

Export control and ITAR laws and regulations represent a major hurdle when interacting with domestic and foreign universities or when working with foreign companies. Most U.S. universities have sizeable numbers of international graduate students but don't have the controls and mechanisms in place to assure that non-US persons do not gain access to export or ITAR controlled information. For this reason, it is often difficult, and sometimes impossible, to engage some universities in government subcontract research having ITAR restrictions. Avoiding this challenge requires careful configuration of ICME research projects so that they avoid export and ITAR controlled technologies, possibly by confining work to theoretical issues or experiments involving similar, uncontrolled surrogate materials and processes.

Assessment and Demonstration of ICME Benefits

In the past, it has often been difficult to make a simple, conventional "business case" type of assessment for materials and process development. This has sometimes been due to the strategic nature of an enhanced material or process capability. For example, when increased operating temperature capability is enabling to a proposed product, a strategic decision to invest in enabling materials and process development might very well be made. In such cases, sponsors have invested in materials and process development with technical goals as key objectives, with a schedule constrained to meet the proposed application requirement. The "business case" is made at the product or system level, and materials and process development (if included) is a strategic element (possibly one of several) for the development program.

For the most comprehensive and inclusive future-state vision of ICME, materials and process development would be greatly accelerated, executed at reduced cost, performed without any empirical iterations, and produce results that are technically and economically superior. ICME would ideally be applicable to a broad range of relevant materials, and be applicable for a wide range of applications. Achieving such a comprehensive vision, even for select materials and applications, would require a sustained, long-term effort, and a concurrent commitment of resources for development, implementation, and validation. Such an investment will not be secured from a single sponsor, nor will it be secured at a single point in time. Rather, individual, incremental elements of an ICME capability will have to be defined, and the benefits projected in a quantified fashion – based on acceleration of schedule, reduced development iterations, reduced testing and validation, overall cost savings, reduction of risk, etc. – or more likely, some combination of these factors.

The important point is that many elements of an overall ICME system may have to be defined and assessed for merit as independent elements, in order to fit the schedule and support capability of appropriate sponsors. Ideally, a standard approach for assessment of proposed project or development efforts would be developed, consistent with an overall plan for ICME development. Such an approach would encourage, preferably require, quantitative assessment of benefits, but would not preclude identification of certain strategic elements of ICME which might not be amenable to such assessment.

Listed below are some general attributes and success criteria that are highly recommended for consideration when evaluating any proposed project or task related to an ICME initiative.

1. The project establishes ICME capability that addresses a recognized problem or material system enhancement, (e.g., reduces manufacturing cost, improves properties, or provides information that enhance application of the material).
2. The project develops ICME capability that upon implementation is projected to add value exceeding its recurring deployment cost.
3. The project includes an approach to quantify implementation benefit.
4. The project uses models that are mature or can be reasonably expected to reach acceptable maturity within the project timeframe and resources.
5. Proposed project ICME developments are clearly defined and feasibly achieved within the project timeframe and resources.
6. The project develops methods, models, tools, and standards accessible to the domestic industrial community.
7. The project develops methods, models, tools, and standards that are widely applicable and transportable.
8. The project provides validation and uncertainty metrics for new methods, models, tools, and standards.
9. Project research has a viable approach for overcoming all relevant implementation barriers.
10. The project results in development of a standard practice or procedure that is formally documented by the performing organization.

Such criteria could be used to develop and refine general topic areas as well as specific programs for consideration, in addition to use for evaluation of proposals.

Acceptance by DOD and Regulatory Agencies

The last area for commentary as a challenge for broad implementation of ICME is the acceptance of such methodology by the USAF, Navy, Army, and by regulatory agencies for commercial applications. The general area of acceptance could also be a challenge within OEMs as well, of course, for essentially the same reasons. Such acceptance has importance and may pose a challenge in at least three areas: (1) where ICME methods might affect the approach and execution of a sponsored development program, (2) where conventional testing and validation might be reduced as a result of ICME methods, and (3) where materials behavior including damage tolerance and life prediction might be affected – especially if predicted in whole or in part - by use of ICME methods.

The degree of challenge represented by each of these areas seems directly related to the level of validation and testing that would be required by the associated current, accepted, validated, and highly empirical practices. The first area cited above would likely be least challenging for these reasons – and might be acceptable with least validation of the associated ICME methods and models, since occurrence would generally be in the earlier stages of the development process and significant testing and validation of any output would typically follow later. The more difficult challenges reside in the second and third areas described above. These areas occur later in the system development process, and have historically been addressed by employing significant test and validation efforts. The procedures required for validation and certification of flight engines, and any materials in critical applications within them, would certainly not be changed without substantial validation of any alternative procedure or criteria.

A GENERAL STRATEGY FOR DEVELOPMENT AND IMPLEMENTATION OF ICME

There are many challenges and barriers to broad development and implementation of ICME, as have been previously described. Conceptually, ICME spans an extremely broad technical area, from alloy composition through complex processing and resultant microstructures, culminating with the many physical, mechanical, and life-related properties that must be determined with statistical precision. And, of course, to realize the full potential of the ICME vision as described, the many models and facets of ICME must be integrated, validated, and compatible – not just within the materials engineering discipline, but ideally with the analytical tools of other engineering disciplines. Considering the many classes of materials, processes, properties of interest, and component applications, it seems this is a very ambitious challenge - almost overwhelming when considered in its entirety. Yet, prior programs under AIM and within various companies have demonstrated substantial benefits from an ICME approach for specific applications. Consequently, any strategy should contain short term, focused elements that provide opportunities to demonstrate success on key topics of interest, while generating a framework for sustainable, progressive development and implementation of ICME in the longer term.

The key challenges and barriers to broad implementation of ICME that were described in the previous section can be consolidated into a few broad categories:

Technical –specifically, model capability, maturity, and available data. The recommended approach to address technical development is to select specific **focused project** areas where perceived benefits of ICME application would provide incentive to participants and sponsors to sustain activities and achieve success. Such selection should result in focused requirement for specific model development for each selected project.

Integration and Standards –the development of protocols, etc. that address how various models are linked and interact, common standards for data bases and integration with other tools - especially standard commercial tools, and where interaction between companies is required. The recommended approach here includes establishment of oversight and working committees with charter to develop standards and select or designate appropriate common tools, software and data standards. It is expected that certain of the recommended project focus areas would necessitate inter-company, inter-organizational, or company-government interaction.

Validation –encompasses demonstrated validation protocols for accuracy, range of validity, and variation assessment, as well as assessment of error propagation especially as related to sequential application of predictive models. The recommended approach here is based on appropriate project selection to ensure that specific validation requirements are manageable.

Acceptance by DOD and Regulatory Agencies – such that selected, validated practices may be integrated with other analytical development, analysis, and validation tools to provide concurrent reduction in empirical test and validation requirements. The recommended approach here is to select appropriate project areas, and develop associated validation bases for ICME application, with the cognizance and preferably the participation of appropriate DOD and Regulatory agencies.

In addition to the above, it is helpful to partition the collective concept of ICME into a few general focus areas:

Material development: alloy and composition, processing methods, microstructure, nominal properties. Note that this application would generally be early in the Technology Readiness

Level (TRL) [5] process, and very early in the Integrated Product Development (IPD) process - hence less emphasis on extensive validation. Possible significant integration between supply chain and OEM companies might be required for success.

Process modeling: thermomechanical processing of specific alloy, resultant microstructure, nominal properties, process yields, residual stresses, defect species and occurrence rate. This application would generally be in the mid-to-late part of the TRL process, but still early in the IPD process – hence moderate emphasis on extensive validation. Also, significant integration between supply chain and OEM companies would be expected here, and cost modeling of material and processes would be a critical element for that interaction.

Material behavior: microstructure, properties, service aging, residual stresses, constitutive behavior and life modeling, including variation assessments, and effects of defects. This application region would be late in the TRL and possibly the IPD processes; consequently validation would become a significant requirement. Probably limited integration here between supply chain and OEM companies would be expected; but significant interaction between OEMs and USAF and/or regulatory agencies would be likely.

Although there is clearly overlap, interdependence, and redundancy amongst these three categories, they are useful to help partition the ICME universe into more manageable categories. This is helpful to determine where in the overall IPD or Technology Development Process specific ICME efforts reside. It is also helpful, possibly even essential, to assess appropriate participants and potential sponsors, required fidelity, validation requirements, and benefits that may be achieved for specific ICME development and implementation efforts.

For the near term, the proposed strategy and activities have some common features: the intent should be to define and address focused project areas – developing and exercising ICME capability over a closely defined (possibly even narrow) range, minimizing the requirement for extensive experimental validation, and applying ICME modeling within a framework of existing data. For utilization of ICME in the area of alloy development, for example, the focus could be on modeling to determine the composition ranges for evaluation, with objective of rapidly and efficiently defining the alloying combinations for evaluation, and minimizing or reducing requirement for iteration. This application would by definition be early in the TRL process. Consequently, extensive validation of the ICME models would not be required in this case, as designed experiments to evaluate candidate alloys would ultimately narrow and confirm final alloy selection with experimental data. The role of ICME here would be to guide and optimize the design of experiments (DOE) to be conducted, and ideally eliminate subsequent costly iterations that have characteristically been required in the past. “Error propagation” for such an ICME application would also be of limited concern here, since the final alloy selection would be based on actual measured properties generated for selected critical tests. Subsequent testing on the selected alloy and/or process would generate data necessary for characterization and validation.

Similarly, for evaluation of derivative materials, significant process changes to an established material, or impact of non-compliances, ICME modeling could be exercised with the goal to predict “differential” behavior, rather than absolute properties. Essentially, the goal and benefit of ICME could be to quantitatively predict change from a well-characterized baseline state of microstructure or properties, for example, rather than to predict absolute properties where extensive validation would be necessary. “Error propagation” from alloy and/or process models, to resultant microstructure and property predictions, would also be addressed by subsequent testing here, in that ICME focus would be on development of derivative material and processing, but final property determinations would still be based upon testing. Validation test requirements for such applications could be reduced or even minimized by conducting “point solution” validation tests, as an example, for selected validation of model predictions, while still providing

significant savings of cost and time compared to more conventional empirical approaches commonly used today.

Validation requirements become a more central issue when ICME is applied to predict final material behavior, of course. This application by nature would occur late in the TRL process, or even late in the IPD process, where extensive data and sound statistical bases for properties are essential. The example strategy here would be to select “derivative material” applications, where extensive baseline data on a related material is already available. The ICME application here could focus on differential behavior again, and assessment of variability compared to a baseline material. Validation requirements might then be reduced through reduction of some replicate testing usually required for determination of statistical ranges, and also by use of “point solution” testing for selected validation of both mean property predictions and the statistical range. Success and confidence in the understanding of a derivative material compared to prior, established material(s) could provide the basis for reduced component or system level validation tests, with potential for substantial cost and time savings. We recognize that these comments on recommended approach and strategy are general in nature. The intent here is to provide some general guidelines that would address what we see as the most significant challenges and barriers to broad ICME development and implementation – guidelines that would be applicable to the proposed focus and project areas, as well as the recommendations for coordination and oversight, and integration of university and small business activities.

CONCLUSIONS

It is believed that substantial cost, schedule, and technical benefits would result from broad development, implementation, and validation of ICME for aerospace applications. It is also believed that such development and implementation is necessary, even essential, to ensure that materials engineering play a significant continuing role in aerospace system design and development. Such capability is especially critical to ensure that the development cycle time for materials and processes be made compatible with the timing and technical requirements for overall system design, optimization, and development.

Challenges and barriers are formidable. ICME tools must span and integrate a wide range of physics, materials science, statistics, and even cost models. There are the substantial challenges of model development, generation of requisite supporting data, accuracy, validation, integration, and finally (but by no means least challenging) – acceptance. Yet previous efforts and studies have demonstrated the value and tremendous potential of ICME. Analogous capability is already in routine use by many other aerospace disciplines – where the challenges of model integration, execution, and validation have been successfully addressed. This capability has facilitated the Multi-Discipline Optimization that is critical to future aerospace system development. One can argue that the challenges for materials science and engineering are more wide ranging, less amenable to accurate representation by physics based models, and thus more formidable. But: these challenges should in no way prevent development- and execution - of a long range plan for ICME. It may require that more empirically-based or phenomenological models be used, that the integration of models with sequential dependencies be carefully assessed or even limited, and that early applications focus on areas where extensive validation may not be necessary. The most immediate requirement for successful initiation of an ICME plan is that we define focus areas with quantifiable benefits – and that we get started.

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STANDARDS-COMPLIANT FORMATS FOR MATERIALS TEST DATA

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ABSTRACT

The advent of integrated computational materials engineering (ICME) comes at a time when data science is emerging as a cross-cutting approach to knowledge discovery that has been facilitated by levels of storage, processing power, and communications that have only recently become widely accessible. Data science is recognized as having the potential to have a paradigm affect on the way science is performed, and data science and ICME share characteristic features. Examples include the use of repositories of open data to undertake research outside the context in which the data were generated, the conservation of computer code alongside associated data, and pattern discovery in aggregated data sets. For ICME to become established, it is broadly recognized that standards are a key component of the required infrastructure. However, the scope of the standards, meaning local protocols compared to normative procedures, is open to debate. While local protocols can be anticipated to be appropriate in particular circumstances, such as in-house models that provide an organization a competitive edge, experience shows that there are cases where normative procedures are appropriate. Materials testing is one such case, wherethere is already a globally accepted collection of documentary procedures. With the advent of ICME, and the need for standard formats for capturing, conserving and exchanging materials test data, these procedural standards can potentially find a new use in the form of specifications for developing standard data formats. In this context, CEN (the European Committee for Standardization) commissioned a 12-month Workshop to determine the technical, economic, and logistical viability of data formats (schemas and ontologies) derived from materials testing standards. As well as establishing the viability of standards-compliant data formats, the Workshop proved successful in engaging a broad cross-section of stakeholders.

INTRODUCTION

The engineering community invests significantly in generating materials test data of high inherent worth. Procedural testing standards identify what needs to be recorded, but in the absence of corresponding formats, the data are rarely conserved, and their value diminishes as the material

pedigree, test conditions and results become disassociated. Although the facilities used to generate and process engineering materials test data have evolved to be predominantly computer-controlled, there has not been an accompanying evolution of standard data formats. Consequently, the processes for generating, processing, and storing information are not well integrated, and instead of a digital infrastructure, the materials community is largely faced with a collection of stand-alone, isolated systems. Although aggregating data from different sources is possible, it is far from straightforward because of differences in data formats. Standards-compliant data formats offer a solution to this issue, allowing the realization of a seamless infrastructure of computer-controlled facilities in anticipation of improved business processes and more effective research.

Motivations for Improved Management of Engineering Materials Data

With the emergence of a semantic Web of data, there is a renewed interest in data management in many scientific disciplines. In the engineering materials sector this interest is manifest in the challenge of integrated computational materials engineering (ICME), which itself is reported as depending on the development of a global infrastructure or protocol for information exchange and interfacing of models [1][2]. Presumably this is because advocates of ICME realize the importance of the streamlined storage and exchange of materials data that such an infrastructure would facilitate. Early work reported in the context of ICME suggests great potential for improved understanding and better designed engineering materials. Examples include the use of repositories of open data to undertake research outside of the context of the project in which the data were generated [3], the conservation of computer code alongside associated data, as in the case of empirical potentials [4], and pattern discovery in aggregated data sets [5].

Requirements for Managing Engineering Materials Data

Procedural standards, meaning documentary standards with detailed instruction on common procedures, are an essential resource underpinning many aspects of society. In the engineering sector, procedural standards for materials testing play a vital role in ensuring that the design of structures, monitoring of safety critical components, and the certification of materials for product release are all based on an agreed and validated method for determining material properties.

With tests typically being undertaken in accordance with paper-based versions of such standards, and paper-based certificates or reports being commonly used for reporting and storing such data, it is contended that the precise nature and well-defined scope of procedural standards makes them amenable to translation into corresponding computer-readable formats. To date however this appears not to have been attempted. This is not to say that initiatives to deliver effective data management solutions have been lacking or that there has been no effort to deliver computer readable representations of materials and materials property data. There are many examples of tailored data management solutions, and a number of successful commercial solutions. These though are typically inaccessible outside the host institution, delivering isolated data silos that are not amenable to aggregation [6]. From the modeling perspective, MatML [7] and ISO 10303 Part 235 [8] are examples of materials models with corresponding data formats. While these have failed to find widespread adoption, this cannot be attributed to a lack of stakeholder interest, as various stakeholders using the documentary standards directly or the data so obtained continue to identify the need for greater interoperability of the data, not least in consistency of testing method, storage of tests results, and usage of those results in a wide engineering context.

It is contended that there are significant benefits that may be accrued from developing documentary testing and calibration standards used for the determination of materials properties into formats that allow direct interoperability with computers and computer-controlled facilities. This would allow such standards to be used to set-up mechanical testing machines and allow the

measured output to be transferred directly to material property databases or data processing tools, or enable the material properties to be directly uploaded to product release certificates.

To understand the full benefits that would accrue from improved interoperability, it is important to consider both the mechanics of use of procedural standards, and the subsequent usage of the data by key stakeholders. One of the most ubiquitous materials tests is the tensile test, the procedure for which is documented in ISO 6892-1:2009 [9]. Often this particular test is applied to qualify a particular product against a material specification. A material test certificate produced in that way can have several uses, as illustrated by a simplified ship-building example in Figure 1. Here it is used not only to provide confidence that the ship plate has been produced to the required specification, but it may also be used to demonstrate the quality processes employed during ship-building. In each of those transactions information (that is, data) is taken from the store of the sender, transmitted and re-stored by the recipient.

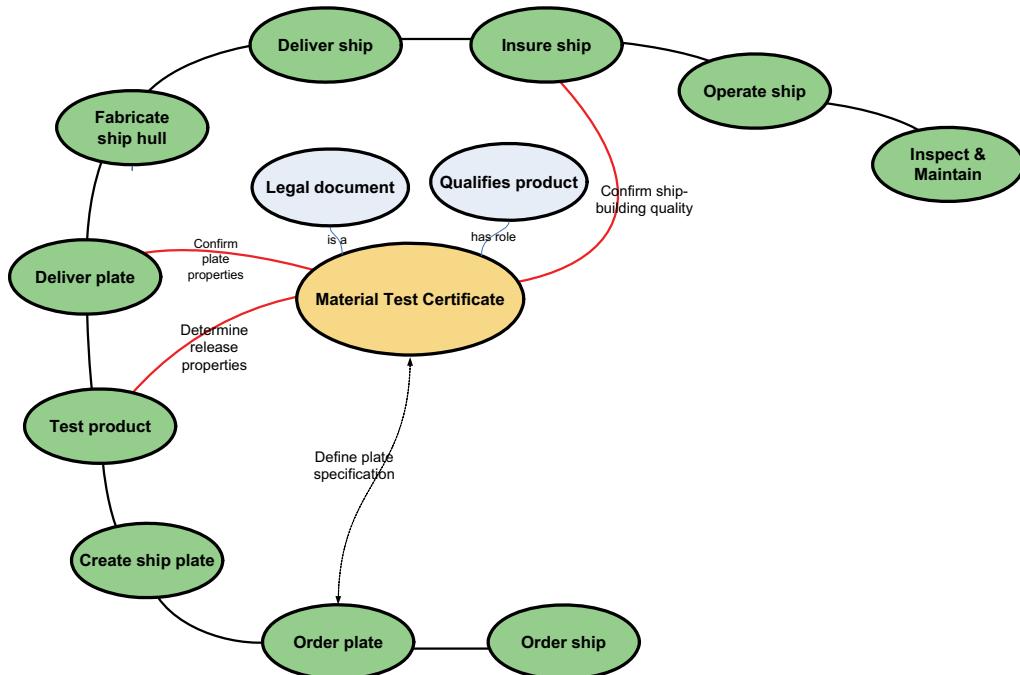


Figure 1. The use of a material test certificate in ship-building and operation.

Data Management Landscape

Studies indicate that while large and widely varied collections of materials data are available, significant issues remain to be addressed [6][10]. The fact that the web-enabled relational databases that typify the facilities available to manage these collections of data are heterogeneous and not amenable to aggregation, has led to their being described as data silos [11][12]. In the materials community, besides this notion of isolated, heterogeneous collections of data with limited aggregate value (meaning their capacity to interoperate and exchange data), studies indicate that other issues to be addressed include provenance and authenticity, database standardization, and extent of metadata [6][13].

Barriers to the Adoption of Effective Data Management Practices

Experiences in the biological sciences, a discipline at the forefront of the revolution in conserving, exchanging, and re-purposing data, indicate that there are very real barriers to embedding data management into mainstream research, not least because information engineers have failed to engage peers in the broader community in the development and delivery of technically sophisticated solutions [14]. Cultural issues and concerns over ownership evidenced in the biological sciences [15] are also echoed in requirements gathering exercises undertaken in the engineering materials sector [16]. Similarly, user acceptance and widespread adoption of formal standards have proved difficult to achieve [17]. In the engineering sector, this reticence to adopt a new culture of data conservation and reuse is further complicated by commercial sensitivities [18].

ICT Standardization

ICT (Information and Communication Technology) standards provide a basis for interoperability across geographically distributed and heterogeneous systems. The internet is built on standards, delivered by organizations such as W3C (World Wide Web Consortium) and OASIS (Organization for the Advancement of Structured Information Standards). Efforts at improved data management in the research sector are also recognized as depending on standards [19]. While conventional standards organizations, such as ISO, CEN, and ASTM, are concerned with standards development in many domains, they are obliged to adopt practices better suited to ICT standardization. This is most evident in the ever increasing dependence of public policy on ICT standards [20], and so the conventional standards organizations are coming under increasing pressure to modify their business models accordingly [21]. While there are indications that these organizations are adapting [22], the implementation of new standardization practices is by necessity a time-consuming process.

Standards are effective in promoting interoperability because they engage stakeholders in a process of defining and achieving consensus on broadly accepted guidelines for a particular process or procedure. The remainder of this paper is concerned with a recently completed year-long CEN Workshop entitled ‘Economics and Logistics of Standards compliant Schemas and ontologies for Interoperability of Engineering Materials Data’ (ELSSI-EMD) that aimed to demonstrate the potential role existing standards for mechanical testing can play in achieving interoperability of test data in the engineering materials sector.

CEN WORKSHOP ELSSI-EMD

The objective of ELSSI-EMD was to deliver formats for tests data that from all perspectives would meet the requirements of the engineering materials community.

CEN Workshop Model

CEN Workshops provide a platform for stakeholders to be involved in standards development activities. A Management Team operates the Workshop, ensuring that formal commitments are met and that its Business Plan and Terms of Reference are observed. A Project Team of paid experts is recruited through an open call, and undertakes work on behalf of registered Workshop participants. The registered participants themselves follow, review, contribute to, and approve the work of the Project Team. In this way, CEN Workshops prioritize stakeholder interests.

The primary deliverable of a CEN Workshop is a CEN Workshop Agreement (CWA) [23]. It is intended to satisfy market demands for a more flexible and timelier alternative to the traditional European Standard (EN). While it possesses the authority derived from the openness of

participation and agreement inherent in the operations of CEN and its national members, a CWA is not intended to support legislative requirements.

Scope and Objectives of ELSSI-EMD

While three primary streams of activity were defined prior to the start of the Workshop, namely development of data formats, business analysis, and standardization practices, the specifics of each activity were defined during the early stages of the Workshop. The immediate objective was to identify a suitable testing standard on which to focus. ISO 6892-1:2009 was selected on the basis that it is the definitive ISO standard for ambient temperature tensile testing and it already incorporates guidelines on data formats in its annex on recommendations concerning the use of computer-controlled tensile testing machines.

Having chosen the particular testing standard, schema implementations and example data sets in XML and ISO 10303 formats, and an RDF and N3 encoded ontology were identified as the focus for the data format development activities. For the business analysis, a transition from paper-based to machine-readable test certificates was selected a suitable case study. For the standardization practices component of the Workshop, it was apparent that HTTP URIs offered the only viable means for publishing the data formats, and that in anticipation of identifying an appropriate host organization, the IPR and revenue generation implications would need to be investigated. Further, for the data formats to find use by the engineering materials community, it was evident that their adoption by TC 164/SC 1/WG 4 (the work group responsible for maintaining the family of ISO 6892 tensile testing standards) would need to be pursued.

RESULTS

ELSSI-EMD involved a broad cross-section of stakeholder in three primary streams of activity—development of data formats, business analysis and standardization practices. Its findings are reported in a CEN Workshop Agreement entitled *A Guide to the Development and Use of Standards-compliant Data Formats for Engineering Materials Test Data* [24].

Stakeholder Engagement

The overall number of participating organizations exceeded 30. Component manufacturers numbered 5 and materials data providers (a category comprising organizations involved the materials supply chain, including materials producers, test machine manufacturers, and software houses producing data management and processing tools) numbered 7. Standards bodies and fora numbered 4, while representatives from the digital curation community (which besides large organizations promoting curation best practices and technologies, included SMEs delivering information engineering services) numbered 6. Academic institutions numbered 5, as did participating materials research institutes.

In terms of country participation, the United States, Japan, China, Australia, the Czech Republic, Sweden, Italy, France, Germany, and the United Kingdom were represented.

Data Formats

ELSSI-EMD delivered a schema and ontology that provided a computer readable version of ISO 6892-1:2009. The development efforts delivered the modeling artifacts (UML diagrams) that will provide a basis for similar efforts for other test types. While the clarity and scope of the underlying standard contributed to the ease of the development process, the dialog with engineering materials experts proved indispensable.

Business Analysis

The business analysis focussed on the impact of a transition from paper-based to electronic test certificates. It examined the test certificate lifecycle from material production to delivery to the OEM, and a survey was undertaken to establish the value chain and gauge reactions to the proposed introduction of electronic test certificates. While the findings were positive, with broad agreement that the general concept is desirable, there is a risk for software houses and organizations with well-developed test certificate generation and delivery processes.

Standardization Practices

The standardization practices effort extended to establishing a mechanism for publishing the standards-compliant data formats and to promoting their adoption by ISO TC 164/SC 1/WG 4. The preferred mechanism for publishing the data formats is as permanently available HTTP URIs, and CEN acting in the capacity of HTTP URI host was the subject of a document submitted by CEN WS LT to the CEN ICT Forum on the subject of namespace policy. Although at the time of writing there has been no decision, the matter is the subject of review. The initial response from ISO TC 164/SC 1/WG 4 was positive but there is a recognition that there are development and maintenance implications. To ease the route to adoption, the ELSSI-EMD CWA includes an Annex A template for incorporation into any mechanical testing standard.

DISCUSSION

While it is reasonable to claim that ELSSI-EMD has proved successful in demonstrating that standards-compliant data formats are viable from all perspectives—technical, business, and standardization—the outcome is not wholly unexpected. The procedural standards for mechanical testing are not dissimilar to written ICT specifications, and have proven to be amenable to translation to computer-interpretable formats. Further, the fact that a transition from paper-based to electronic certification and reporting mechanisms is more efficient is not surprising when the health care sector has already undertaken a similar transition [25].

Stakeholder Engagement

Critical analysis of the state of data management in the engineering materials sector tends to be pessimistic compared to other disciplines. It is not the case though that other disciplines have overcome the inherent resistance to integrating effective data management practices into mainstream research. In fact, evidence suggests that far from encouraging participation, the introduction of sophisticated technologies has alienated the communities they are supposed to serve [14]. Stakeholder engagement is thus a fundamental requirement for any effort to promote effective data management, and this was a governing factor in the choice of a CEN Workshop as the vehicle for undertaking the work reported herein. This, and the decision to frame the work in the context of an existing procedural standard, have proven particularly effective in engaging the engineering materials community in the development of the data formats needed to establish a viable framework for the conservation and exchange of materials test data.

The large collections of well-established procedural standards themselves should also be recognized as a valuable resource in the development of a viable data management framework. The activities of the W3C Health Care and Life Science Interest Group (retrieved 12th July, 2010 from <http://esw.w3.org/HCLS/ClinicalObservationsInteroperability>) indicate that standard procedures (clinical protocols in this case) are a prerequisite to the development of technologies that will address systems interoperability and effective data collection and conservation. Delivering technically robust procedural standards and achieving consensus is a time consuming process. If these activities are considered to be a prerequisite for the development of data formats

for interoperability, then the materials community, having already invested decades of expertise in the development of procedural standards for mechanical testing, is far closer to achieving an effective solution than critical analysis suggests. In its large collection of procedural testing standard, the materials community has an important resource at its disposal and, if the necessary efforts are taken to convert to computer readable formats, there is the opportunity to deliver standards-compliant formats that will address interoperability in a relatively short time. This was an underlying motivation for ELSSI-EMD, and the results of the Workshop indicate that this motivation was well founded.

Data Formats

The process of deriving of the data formats and rule sets proved relatively straightforward due to the clarity and scope of the underlying technical standard. For the schema, the structure of the standard allowed identification of the main classes, and the terms and definitions to annotate the schema. The terms and definitions also proved to be a key resource in the development of the controlled dictionary and ontology. It is important to emphasize, however, that domain experts from the information engineering and engineering materials communities worked together to develop the formats, and the CEN Workshop provided the perfect vehicle for this collaboration.

During the Workshop concerns were raised over the fact that in the ISO 10303 Part 45 [26] and Part 235 [8] specifications, there already exist standard data formats that are able to describe materials and materials properties. It is suggested though that these standard data formats should be considered to be part of a broader solution—one that allows other more widely adopted standards to be used, such as XML and XML Schema. Further, standards-compliant data formats are fundamentally different to standard data formats. Standards-compliance infers that irrespective of the implementation technology used, a data format complies with an existing procedural standard in a given domain, in this case engineering materials testing. This difference is significant insofar as one of the key outcomes of ELSSI-EMD is that framing its work in the context of an existing procedural standard appears to have engaged the engineering materials community in an unprecedented way. There are various possible reasons, including a sense of ownership and control over the development process, and a guarantee of long-term development and maintenance inherent to a standard that is produced by a recognized standards body.

During the course of the Workshop concerns were also expressed in relation to scalability to other test types. This concern derived primarily from the fact that as a path-finding exercise, ELSSI-EMD was necessarily limited in its scope. While it is true that the work focussed on a single test type, it is considered that the procedures for creating standard-compliant data formats are applicable to any test type. In anticipation of data formats being developed for other mechanical testing standards, the ELSSI-EMD CWA is entitled ‘A Guide to the Development and Use of Standards-compliant Data Formats for Engineering Materials Test Data’.

The capacity of the data formats to adapt to different data management requirements is also an issue, and trials with industrial sector data have confirmed that the ISO 6892-1:2009 XSD does not meet all requirements. Examples encountered to date include a lack of support for time and date of test (not mentioned in the standard), Ramberg-Osgood coefficients, and materials metadata, such as material composition and manufacturing route. Since well-designed schemas are amenable to aggregation with other schemas and to extension, this lack of support does not invalidate the ISO 6892-1:2009 XSD. To support the materials metadata, the solution is to aggregate the ISO 6892-1:2009 XSD with a materials schema, such as MatML or JRC:MatDB (retrieved 12th July, 2010 from https://odin.jrc.ec.europa.eu/MatDB_XMLschema/matdb.xsd). For other test and property specific data, the solution is to extend the ISO 6892-1:2009 XSD.

Business Analysis

The business analysis relied on desk-based research and surveying. It suggested that the implementation of a standardized machine readable certification process has the potential to facilitate the realization of a relatively larger number of certificate management infrastructures at a relatively lower unitary cost without significantly altering the balance of interests within the sector. The steps necessary to realize this new paradigm and the transition towards it have to focus on the end result. Namely a more efficient, less time consuming and cost saving way to achieve integration of the internal functions of an organization pertaining to the management of test certificates and the facilitation of data transfer, handling, archiving and updating between the various stakeholders involved in mutual business transactions.

The conclusion that the business analysis accomplished was to highlight the strong general interest of the stakeholders for machine-readable test certificates. The analysis, however, raised questions on the particular interests of stakeholders and how these can influence the standard setting framework. To provide sound guidelines on the transition to standardized machine readable certification process, a larger sample survey is needed in order to probe deeper and report with some degree of statistical significance. Such a survey will have to include a consistent sample of organizations involved along the value chain of test certificates and probe into the particular interests of each group of stakeholders as well as into their different approaches to linking business opportunities to the change in the certification method.

During the course of the Workshop, although there was broad agreement that a transition to machine-readable test certificates is desirable, concerns were voiced by participants representing software houses that new data formats have the potential to impact negatively their business interests if they simply add to, rather than replace, existing formats. Further concerns became evident during the ratification of the CWA when, although a significant majority (>90% of registered participants) approved the CWA, one manufacturer was unable to ratify the work on the grounds that it would not be in their commercial interests. Although a concern, it would be unusual to achieve unanimity, and dissent is a feature of standardization activities.

Standardization Practices

A close examination of the development of mechanical testing standards and ICT standards indicates that the introduction of machine readable data formats that correspond to individual mechanical testing standards is feasible. It is also apparent that individually the standardization practices that would facilitate the introduction of said formats have been implemented separately by different standards bodies and technical committees. These practices include the creation of subcommittees to deliver specialist competency, publishing standards and parts of standards as HTTP URIs, and publishing ICT standards free-of-charge. The difficulty that ELSSI-EMD faced is that these different practices appear not to have been implemented together by any single standards body or technical committee.

At the level of the technical committees responsible for mechanical testing standards, the added value of standard data formats is recognized. This is not surprising considering the present-day reliance on information technology and the internet. There is though a quite justified concern that the development of standards-compliant data formats will place an additional burden on the technical committees concerned, and that the additional responsibilities will have to be delegated to personnel with the needed ICT competencies. For recommendations that ISO TC 164/SC 1/WG 4 adopts the data formats to be successful, trials will be needed to establish the implications and verify the data formats, perhaps in the context of VAMAS TWA 35. There is also a requirement to address the lack of any widely adopted standard representation of

engineering materials. While ELSSI-EMD was concerned solely with representing tensile test data, without the corresponding materials metadata, the test data is meaningless.

Besides the adoption of the data formats by ISO TC 164/SC 1/WG 4, a key concern is that the data formats are published as HTTP URIs. While the standards organizations have yet to embrace the publishing mechanisms on which ICT standards often depend (meaning as persistent identifiers, commonly manifested as HTTP URIs), it is difficult to imagine that such organizations can operate in the ICT standardization domain unless they are amenable to employing such publishing mechanisms. ISO already makes schemas and other ICT standards and parts of standards available from its site at <http://standards.iso.org/iso>. ISO has also addressed the issue of publishing standards in the ICT domain without charge [22].

Motivations for Improved Data Management Practices

Improved data management practices are motivated by different imperatives in the research and business sectors. In the research sector, when applied to large bodies of quality data, computer methods such as data mining and pattern discovery have the potential to drive knowledge discovery, not only through conventional research but also the emergent phenomenon of user-led scientific innovation [27]. Access to raw data is also clearly in the public interest for reasons of transparency (as in the case of the UEA climate data controversy [28]) and regulatory compliance (as in the case of the tree rings FoI ruling [29]). Especially in the case of public inquiry, the engineering sector has a vested interest in ensuring data is properly managed in sectors such as nuclear power and air transport.

In the business sector, ever more stringent auditing and traceability demands in industries such as power generation and aerospace favour the introduction of a robust data management framework. What is significant for engineering materials data is that the same procedures for qualifying and generating data are found in both upstream and downstream activities. Upstream, the refinement of existing test procedures and the introduction of new test procedures, such as the small punch test, offer the potential for more efficient and flexible qualification procedures. Downstream, the automated testing procedures employed in the manufacturing sector have the potential to generate the large volumes of quality data that are fundamental for data-centric research to deliver reliable discoveries.

Given the many potential motivations, there are clearly compelling reasons for the fact that improved data management practices have largely failed to be embedded into mainstream research and business processes. Recent studies suggest researchers are concerned that sharing their data will benefit others at their expense [16]. To counter such concerns, and so promote the generation, conservation, and sharing of quality data, the international DataCite initiative (retrieved 12th July, 2010 from <http://www.tib-hannover.de/fileadmin/datacite/index.html>) provides a mechanism for data citation.

In the business sector, commercial sensitivities make determining the sophistication and extent of data management more difficult. It is clear though that in its dealings with the research sector, the commercial sector is very sensitive to lapses in confidentiality that have the potential to damage competitiveness [18]. Conversely, at the level of the individual organization, the ELSSI-EMD business survey indicates that the business sector anticipates benefiting from improved data management practices. These will be driven both by commercial imperatives, such as improved efficiency, mitigation against data loss, and reduced redundancy (meaning repeated experiments), as well as by more stringent traceability and accounting guidelines.

A Unified Architecture for Engineering Materials Data

During the Workshop it became clear that a unified architecture for engineering materials data is feasible that combines the priorities of engineering materials community with the rigour of the information engineering community. As shown in Figure 2, the Zachman Framework formalizes the observation, and suggests a coordinated and integrated approach is feasible.

	Why	How	What	Who	Where	When
Contextual	Goal List	Process List	ISO 6892-1 Terms and Definitions	Organization Unit & Role List	Geographic Locations List	Events List
Conceptual	Goal Relationship	Process Relationship	Entity Relationship ISO 10303-235 ARM	Organization Unit & Role Relationship Model	Locations Model	Events Model
Logical	Rules Diagram	Process Diagram ISO 10303-235 AAM	ISO 10303-235 AIM Diagram	Role Relationship Diagram	Locations Diagram	Events Diagram
Physical	Rules Specification	Function Specification ISO 6892-1 Process Specification	Data Entity MatDB MatML	Role Specification	Locations Specification	Events Specification
Detailed	Rules Details	Process Details	TENSTAND Data Details	Role Details	Locations Details	Events Details

Figure 2. Representation of materials data standardization activities using the Zachman Framework.

Overlaid on the diagram are the materials standardization activities that ELSSI-EMD encompassed. The fact that these activities occupy adjacent categories in the Zachman Framework provides a good indication that, although undertaken independently, these activities are complementary, and so can be aligned into a common, unified architecture.

CONCLUSIONS

As a path-finding exercise, ELSSI-EMD proved successful in establishing the viability of standards-compliant data formats from technical, economic, and standardization perspectives. This is not entirely unexpected, as the engineering materials community has always shown considerable enthusiasm to develop technologies for data conservation and exchange. Initial concerns that stakeholders had become disillusioned after years of unsuccessful efforts to secure the funding needed to support such activities have been dispelled. Framing the work in the context of an existing standard is considered to be the reason ELSSI-EMD proved so successful in engaging the materials community. However, there is no room for complacency in taking forward the work reported herein, and the real challenge lies in ensuring the work is sustained and diffuses into the wider engineering materials community.

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ONTOLOGY ENGINEERING: COMPUTATIONAL INFORMATICS FOR AN ICME INFRASTRUCTURE

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ABSTRACT

To develop a truly sustainable cyberinfrastructure for Integrated Computational Materials Engineering (ICME) one needs to develop a scientific framework that can convert digital libraries from simply being a source for search and retrieval of information to one of knowledge discovery. While issues such as markup language, user interfaces and data management systems that can be read by computers are important to enable a cyber infrastructure, their use in materials science and engineering continues to be predicated on phenomenological classification schemas of materials behavior. In this paper we introduce the concept of “ontology engineering” which can provide an approach to classifying and organizing data, based on informatics principles. The emphasis of this discussion is how we may use data clustering/ partitioning schemes based on statistical learning to help identify metadata that can help probe databases in a meaningful manner. This computational framework can help to define new and/or alternative ontologies for information queries and convert digital *libraries* into digital *laboratories* that truly promote the ideals of integrated computational materials engineering.

INTRODUCTION: ONTOLOGY ENGINEERING

This paper introduces the concept of “ontology engineering” [1] as a way to guide the management and integration of data in materials science. The term ontology as used in the present discussion refers to a formal representation of knowledge by a set of concepts. We show how we can use the mathematical formalism of informatics to identify key data descriptions (e.g. Metadata) that can serve to guide linguistic based relationships for establishing links between data. Discovering (i.e. engineering) those linkages and similarities in metadata in a mathematical robust manner is one of the critical steps in building an integrated computational materials engineering (ICME) infrastructure. Ontology refers to the linguistic expression of correlations between scientific data. These correlations are not linear and can be best expressed in terms of networks of information. Discovering the connections in this network is often done heuristically and with built in *a priori* assumptions and hence ontologies simply reflect the phenomenological nature of data gathering.

A high level of granularity is necessary to enable efficient data sharing and meaningful data mining to capture descriptions of data across length scales. Application of an ontologically based approach needs to be more than simple keyword-based methods for information retrieval. Not only can semantic queries be formed, but axioms that specify relations among concepts can also be provided, making it possible for a user to derive information that has been specified only implicitly. The challenge of building a successful ICME infrastructure is to manage the complexity of information, and identifying and/or ranking which data is important and which sets of correlations are important. The problem involves a potentially large array of multivariate correlations leading to a high dimensional data set. A first step in this process is reduce the dimensionality of data such that we can begin to make subsequent data mining tools to seek

patterns of behavior and make predictions as well. There are many mathematical approaches to reduce the dimensionality of data; however we will focus our attention on robust linear methods known as principal component analysis.

META DATA SELECTION THROUGH DIMENSIONALITY REDUCTION METHODS

As noted by Searls [2]; understanding the relative roles of the different attributes governing systems behavior is the foundation for developing models. A good and effective ontology for an ICME infrastructure must be able to reflect the integration of disparate data. When data from different sources reflecting the same phenomenon are combined, the signals are often mutually reinforcing, emerging from uncorrelated noise that tends to cancel itself out. The challenge of engineering an ontology is to identify those correlations and to assess how the different data mutually reflect a given materials property. Data can be modeled as a set of entities, which are general classes of objects, such as compounds. Associated with entities are attributes, which comprise features or properties such as crystal structure. Attributes take on particular values, and each entity can then correspond to a table in a database, so that the model specifies a schema for that database. When integrating multiple data domains, attributes can collapse on entities that are recognized as identical or even similar, which increases dimensionality in the sense of '*arity*' or number of attributes. Integration can result in recognizing new relationships among distinct entities, which increases dimensionality in a different sense, that of connectivity. Increasing connectivity can simply result in a proliferation of data, but at the level of classes of entities in underlying data models, additional connections increase the complexity of those models and resulting database designs.

Hence the computational challenge is to find the key "*arity*" or attributes and their respective connections that form the basis of ontology. One basic approach to address this problem is to use Principal Component Analysis (PCA). This is a technique to reduce the information dimensionality that is often needed from the vast arrays of data as obtained from a combinatorial experiments, large databases or simulations, in a way so that there is minimal loss of information [3-13].

It is a geometrical ordination method which is used to compress a set of variables into a smaller number of derived variables or components. It is used to pick out patterns in the relationships between the variables in such a way that most of the original information can be represented by a reduced number of new variables. Algorithmically let us consider the case of a vector x of p number of variables. With $\alpha_1^T = [\alpha_{11}, \alpha_{12}, \dots, \alpha_{1p}]$, the variance of the linear function $z_1 = \alpha_1^T x$ is maximized in PCA. The linear function, $z_2 = \alpha_2^T x$ which is uncorrelated with $z_1 = \alpha_1^T x$, can then be calculated to capture the remaining variance. Therefore the k -th linear function, $z_k = \alpha_k^T x$, is calculated to have maximum variance and to be uncorrelated with $\alpha_1^T x, \alpha_2^T x, \dots, \alpha_{k-1}^T x$. Consider the case where the vector of random variables x has a known covariance matrix S . α_k is an eigenvector of covariance matrix S corresponding to its k -th largest eigenvalue λ_k . If α_k is chosen to have unit length ($\alpha_k^T \alpha_k = 1$), then the variance of z_k is $\text{var}(z_k) = \lambda_k$. To populate the first projection vectors α_1 in $z_1 = \alpha_1^T x$, PCA finds maximum variance, such that

$$\alpha_1 = \arg \max[\text{var}(\alpha_1^T x)] = \arg \max[\alpha_1^T S \alpha_1] \quad (1)$$

With the constraint of unit length of α_k and maximum variance of z_1 , the method of Lagrange multipliers can be applied as

$$\max(L) = [\alpha_1^T S \alpha_1 - \lambda(\alpha_1^T \alpha_1 - 1)] \quad (2)$$

where λ is a Lagrange multiplier. Since differentiation gives the maximum value, equation (2) results in

$$(S - \lambda I_p)\alpha_1 = 0 \quad (3)$$

where I_p is a $(p \times p)$ identity matrix. This is known as the problem of eigenstructure for the covariance matrix. To avoid a trivial null solution, $(S - \lambda I_p)$ should be zero. λ and α_1 should be an eigenvalue of S and the corresponding vector respectively. Therefore, the eigenvalue λ represents the variance because:

$$\text{var}(\alpha_1^T x) = \alpha_1^T S \alpha_1 = \alpha_1^T \lambda \alpha_1 = \lambda \quad (4)$$

Since variance should be maximized in PCA, the eigenvalue λ must be as large as possible. The vector α_1 is the eigenvector corresponding to the largest eigenvalue λ_1 of S . The second principal component maximizes the variance.

$$\alpha_2 = \arg \max [\alpha_2^T S \alpha_2] \quad (5)$$

subject to the constraint, $\text{cov}(\alpha_1^T x, \alpha_2^T x) = 0$. Thus, it should be uncorrelated with $Z_1 = \alpha_1^T x$. Using the method of Lagrange multipliers,

$$\max(L) = [\alpha_2^T S \alpha_2 - \lambda(\alpha_2^T \alpha_2 - 1) - \varphi(\alpha_2^T \alpha_1 - 0)] \quad (6)$$

where λ and φ are Lagrange multipliers. The following relations result in $(S - \lambda I_p)\alpha_2 = 0$. The vector α_k is called the loadings for the k -th principal component (PC). The algorithms for calculation of principal components are mainly based on the factorization of matrices. Singular vector decomposition (SVD) and eigenvalue decomposition are the main techniques for factorization of matrices. For any $(I \times I)$ matrix A and P which are non zero orthonormal matrices, the eigenvalue problem can be expressed as

$$AP = P\Lambda \quad (7)$$

where Λ is an eigenvalue matrix and its components are $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_I\}$. Then matrix A by eigenvalue decomposition is

$$A = P\Lambda P^T = \sum \lambda_i p_i p_i^T \quad (8)$$

Here, the property $P^T = P^{-1}$ was used from the fact that P is orthonormal. If a covariance matrix S of X is a matrix A , the data manipulation involves decomposition of the data matrix X into two matrices V and U , and V is orthonormal,

$$S = X^T X = V U^T U V^T = V \Lambda V^T \quad (9)$$

The columns of U are known as scores (e.g. property values of a material) and those of V are called loadings (e.g. attributes of the types of data being relevant to the functionality of the material). PCA decomposes eigenvalues of a covariance matrix, S , of a given data matrix. The loadings can be understood as the weights for each original variable when calculating the principal components. The matrix U contains the original data in a rotated coordinate system. The mathematical analysis involves finding these new data matrices U and V . The dimensions of U (i.e. its rank) that capture all the information of the entire data set of X (i.e. # of variables) is far less than that of X (ideally 2 or 3). One now compresses the N -dimensional plot of the data matrix X into 2 or 3 dimensional plot of U and V . While the eigenvalues geometrically represent the length of each of the principal axes (i.e. scores), the eigenvectors of the covariance matrix

represent the orientation of principal axes of the ellipsoid (*i.e.* loadings). By using just a few latent variables, the dimensionality of the original multivariate data sets are reduced and visualized by their projections in 2D or 3D with a minimal loss of information (Figure 1) . Clustering and similarity analysis of the latent descriptors, (ie the meta data) associated with the data defining materials characteristics can be used to map out which variables are highly correlated or clearly unique as outliers or variables that have a strong independent component of influence.

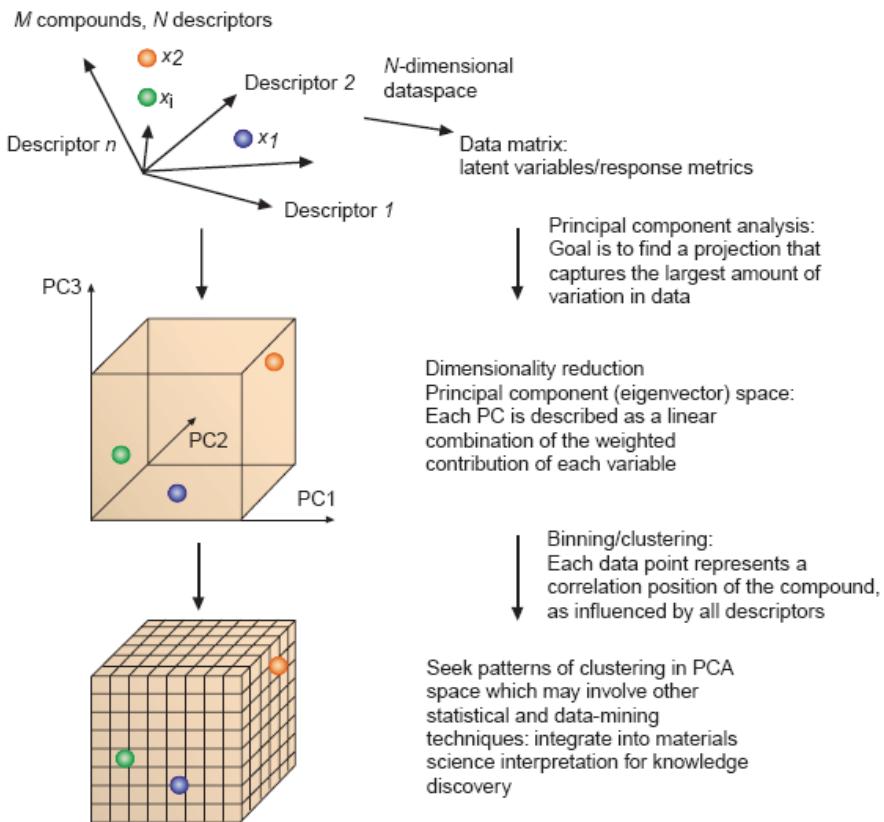


Figure 1 summarizes the procedural logic of PCA. From a set of N correlated descriptors, we can derive a set of N uncorrelated descriptors (the principal components). Each principal component (PC) is a suitable linear combination of all the original descriptors. The first principal component accounts for the maximum variance (eigenvalue) in the original dataset. The second principal component is orthogonal (uncorrelated) to the first and accounts for most of the remaining variance. Thus the m th PC is orthogonal to all others and has the m th largest variance in the set of PCs. (from Bajorath-Ref.3)

Once the N PCs have been calculated using eigenvalue/ eigenvector matrix operations, only PCs with variances above a critical level are retained. The M -dimensional principal component space has retained most of the information from the initial N -dimensional descriptor space, by projecting it into orthogonal axes of high variance. The complex tasks of prediction or classification are made easier in this compressed space. If we assume that information from the data can be gained only if the variation along an axis is a maximum, we have to find the directions of maximum variation in the data. In addition, these new axes should again be orthogonal to each other. In order to find the new axes, the direction of the maximum variation should be found first in order to take it for the first axis. Thereafter we use another axis which is

normal to the first and rotate it around the first axis until the variation along the new axis is a maximum. Then we add a third axis, again orthogonal to the other two and in the direction of the maximum remaining variation, and so on (ideally we can capture all the meaningful relationships in 3 dimensions).

ONTOLOGY ENGINEERING THROUGH META DATA SELECTION

In this section we provide a brief example of the use of data dimensionality reduction methods. Figure 2 shows a PCA plot of a multivariate database of high temperature superconductors [4,6]. The initial data set consisted of 600 compounds (i.e., the rows of our database) with data on eight different attributes or variables associated with each compound (i.e. the columns). The PCA analysis shown below indicates a clear pattern emerges which maps out the granularity of the database.

Every data point in the PCA plot represents a compound with all the attributes embedded. It should be noted that this process of inspection and data association has to be deliberate and careful process of understanding what data was inputted and how to infer interpretations from these patterns. In the context of what PCA can do, all the data points refer to different compounds and their spatial position with respect to each other indicates how they relate to each other when defined simultaneously by all the latent variables or parameters that may be used to characterize or influence their superconducting behavior. These variables form the basis of the ontology system that we need to construct. As it turns out the interpretation of this 3 dimensional projection of information of an eight dimensional data set (i.e. 8 variables or descriptors for each compound). The geometrical visualization of the key variables that define the ontology can help guide the construction of the ontology for superconductors. These can be classified as:

- Compound chemistry
- Structure type
- Superconducting transition temperature (the materials functionality defining the database)
- Materials properties
 - Cohesive energy
 - Ionization energy
 - Valency
 - Pseudopotential radii
 - Electronegativity

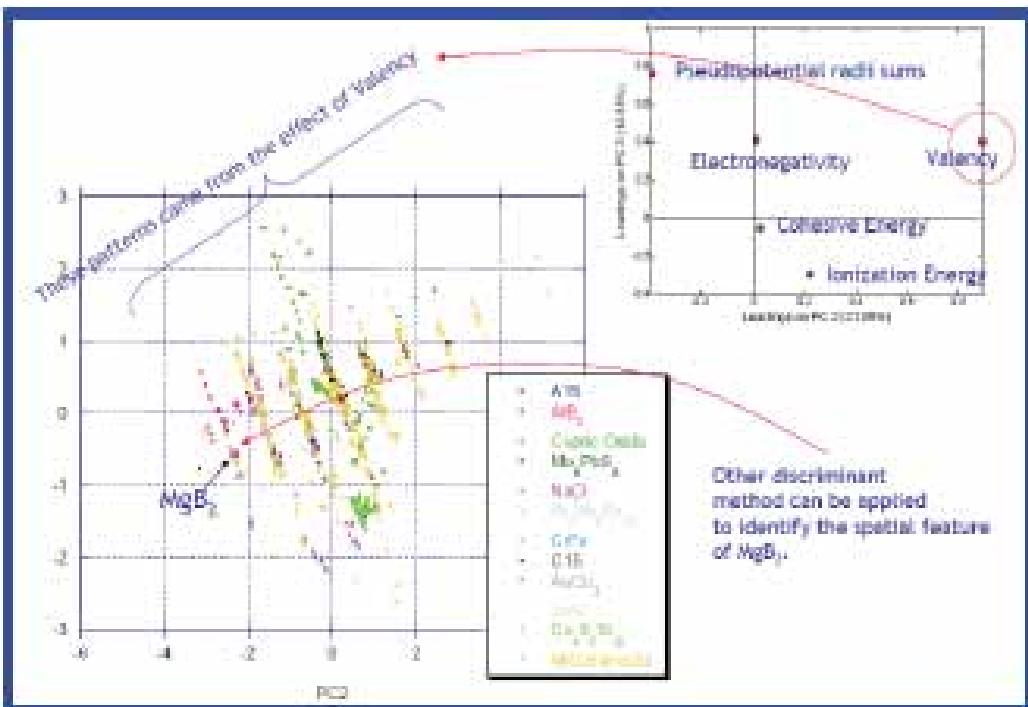


Figure 2: A scores and loading plot (top inset) for a high T_c superconducting dataset. Each point in the scores plot corresponds to a specific compound chemistry and the color code corresponds to a given structure type. In the loading plot, each point is an attribute associated with the compound data set and are labeled appropriately. The power of data dimensionality reduction methods in mapping high dimensional information is exemplified by the fact that both intermetallic and oxide superconductors all fall within unified pattern of behavior suggesting that a common ontology for a superconductor database can in fact be developed using the attributes used for these dimensionality reduction calculations. As an aside, the mapping of MgB_2 (an unexpected discovery at the time) as following the systematics of behavior of the other superconductors is also indicated; something that would not have been easily uncovered in a conventional database.

By inspection and comparison to prior data [14] on these materials and unsupervised learning methods, the linear clusters were found to be associated with systematic valency changes among the compounds studied (Figure 3). These associations discovered by our data dimensionality reduction methods provide the guide of building the ontology framework for representing the information network of our database (Figure 4)

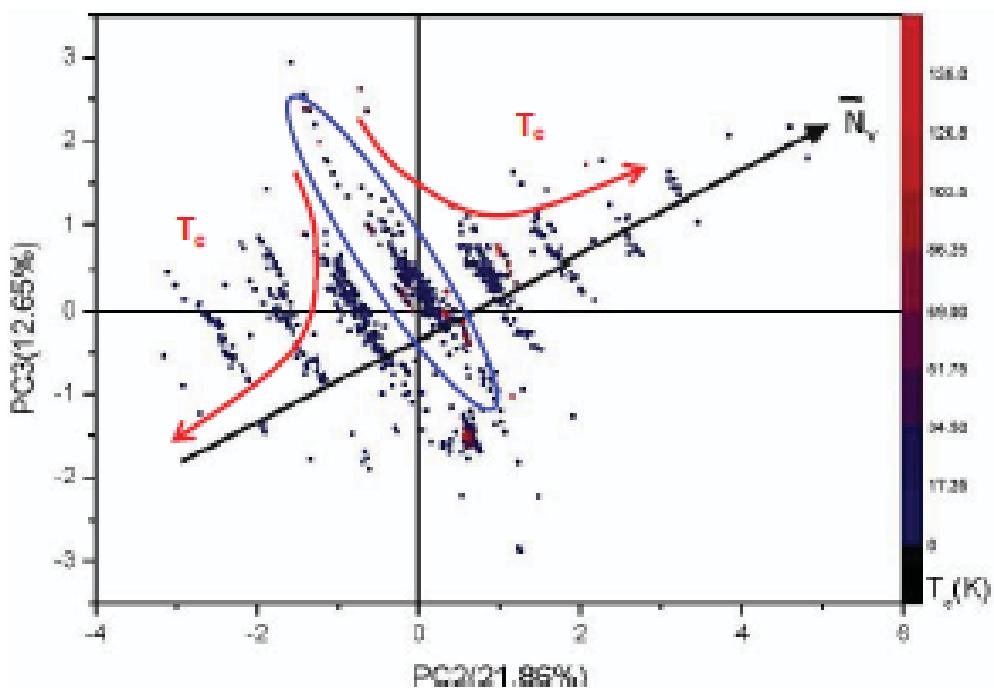


Figure 3. An analysis of the scoring plot for known superconductors showing the direct correlation of one of the key ontological terms (“net valency” N_v) with systematic trends in the superconducting transition temperature. The red arrows indicate the direction of the gradient of decreasing T_c . Hence the compounds with the maximum T_c (cupric oxides) are in the middle cluster (circled). For clarity comparison with Figure 2 to provides the ontological relationship with specific compound chemistries and crystal structures.

A conventional approach to building a materials database will list compounds with their respective attributes and properties. Such a database will have an ontology that simply reflects the phenomenological nature of data gathering. It does not provide any *a priori* insight into how to integrate information. For instance, the loading plot in Figure 2 suggests that the cohesive energy does not play a major role in discriminating among compounds in terms of the linear clustering projection, as it near the origin (0, 0) position of the loading plot. However parameters such as pseudopotential radii are a very dominant factor, while valency and ionization energy play a important but lesser role. The loading plot also indicates the noticeable negative correlation between ionization energy and pseudopotential radii in terms of their influence on average valency clustering of the compounds as they reside in opposite quadrants.

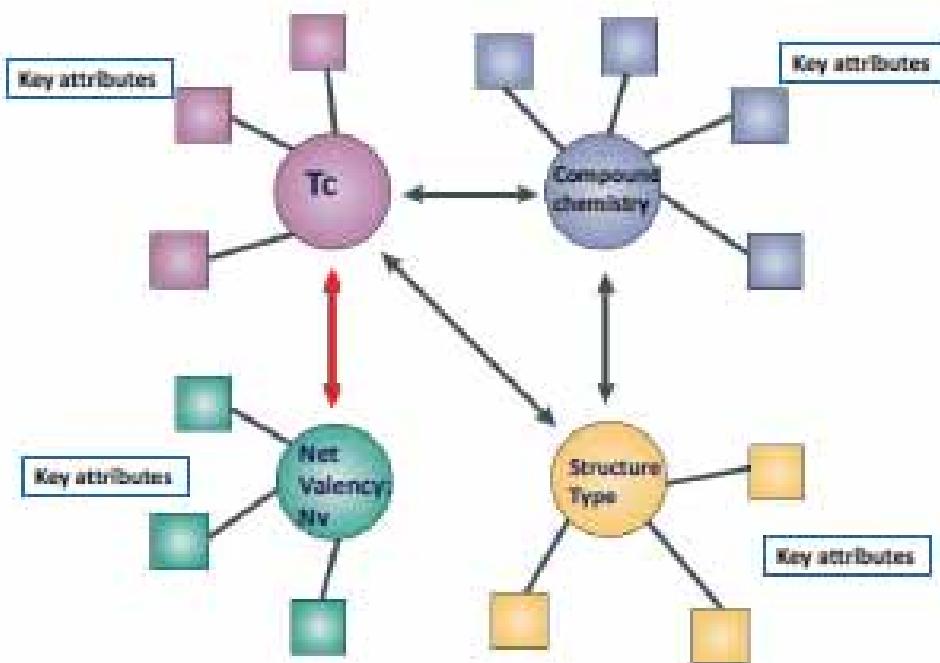


Figure 4: A network representation (figure adapted from Searle-Ref. 2) of an ontology for a superconducting compound database. The nodes (i.e., the key hubs for information classification) are identified as materials chemistry , materials functionality (T_c), structure and “net valency”. The latter was discovered through unsupervised learning methods aided by dimensionality reduction methods. As shown in this diagram, N_v has a direct correlation (highlighted by the red arrow) that can be mapped to T_c , independent of its relationship to compound stoichiometry and structure as shown in Figure 3. The “key attributes” would be the loading parameter variables and their linkages in both strength and number can vary. For instance the principal component equations as derived from the eigenvalue analysis yielded: $PC_2 = 0.89 N_v + 0.01X - 0.39R + 0.03C + 0.22 I$ and $PC_3 = 0.41 N_v + 0.41X + 0.75R - 0.06C - 0.29I$. Note that for PC_3 , the weighting coefficients for valency and electronegativity is the same (0.41). Also the weighting coefficients for cohesive energy is very small (0.03 and -0.06) for both principal components, suggesting that this attribute plays a very small role in defining relative to the other attributes or latent variables.

CONCLUSIONS

The key operating word in ICME is integration. No matter how sophisticated the modeling and experimentation, integration requires the application of other tools into the computational framework. That toolkit is informatics, encompassing a broad range of subject areas including dimensionality reduction, statistical learning, data mining. Informatics techniques provide a robust mathematical framework for integration, when judiciously linked to the physics and chemistry of the materials science problem. We have shown how tools such as data dimensionality reduction methods coupled to clustering and unsupervised learning methods can uncover new taxonomies for information classification and organization. This provides the basis of not just organizing information (i.e. databases) but also how to build databases that can integrate information. Databases then become learning platforms and not simple static

repositories for information queries in a search and retrieve mode. To extract knowledge from databases requires one to engineer how one can effectively search and discover new information... hence ontology engineering.

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MANAGING MULTI-SCALE MATERIAL DATA FOR ACCESS WITHIN ICME ENVIRONMENTS

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ABSTRACT

Integrated Computational Materials Engineering (ICME) is an emerging discipline that has the potential to enable both innovation and efficiency gains in the materials engineering process. In this paper, we begin by considering examples of the potential benefits of ICME, for nickel-based superalloys and composite materials. Using the composite example, we then explore some of the requirements for enabling ICME: the need for an effective, relational materials database; a test data interface; and the requirements for effective interfacing with analysis and modeling tools. Finally, we explore a step beyond simple integration in which computational tools can be made interoperable by embedding within them interactive access to shared materials data. We find that most of the requirements for a system to enable ICME exist today, for example, in the system developed by the Material Data Management Consortium – an international collaboration of leading aerospace, defense, and energy enterprises.

Keywords: Integration, Materials Information Management Software, Traceability.

INTRODUCTION

The behavior of engineering components and structures is dependent on their characteristics at many length scales:

- the composition and atomic structure of the constituent parts;
- the microstructure – grain orientation and size, phases, dislocations, and imperfections, which are strongly affected by the processing history;
- the macro-structure – mixing and structuring of the components in a composite; and,
- the structural scale, where cracks, flaws, and stress concentrations can dominate performance.

The material properties that result from this mix of factors can be highly complex, varying with many parameters such as loading and unloading rate, temperature, time, operating environment, specimen processing, specimen geometry, and loading history.

Computational methods, from curve-fitting test data to advanced micromechanical and continuum models, can provide invaluable information and insight across the range of length scales and operating conditions. Yet these methods are often applied in isolation, without reference to other complementary methods and data.

Integrated Computational Materials Engineering (ICME) should offer major benefits [1]. The phrase suggests a ‘grand unified’ approach, in which predictive methods from the quantum level to the structural scale are united in a ‘black box’, enabling prediction of material performance with little or no empirical input. Such a vision may be unrealistic, but a more practical, yet still immensely valuable, vision of ICME is well within reach. In this, test data from all relevant

length scales, model information, and validation data are integrated and shared across computational and empirical calculations, and are available in the right form at every stage of the engineering process.

TWO EXAMPLES OF THE NEED FOR ICME

Consider the following example: for nickel based superalloys, a series of computational processes could be chained together in order to control the specific properties across a component and to identify the processing parameters needed to create the necessary microstructure, residual stress levels, etc. To achieve this, mechanical properties, chemistry, and background pedigree data might be captured and stored in a database along with micrograph(s) for each ‘lot’ of material. This data could then be accessed by specialized analysis software to calculate the volume fractions of the various phases present, e.g., ‘Widmansttten Alpha’. The results of these analyses could be returned to the central system along with any associated metadata for future examination. In this way, slowly-varying trends in the various lots (such as volume fraction of Widmansttten Alpha) might be plotted against lot tensile strength and linked to the appropriate processes’ parameters values.

With large volumes of this data available from many multiple lots and from many vendors, it might be considered suitable to push the data and meta-data out to a pattern recognition system or to train a neural network to generate models describing properties as a function of microstructural features and processing values. The results of the analysis would themselves be loaded back into the central system so that the next processing analysis package could use this data as input to control the processing parameters and generate the desired microstructure after a forging or heat treatment step.

An interface making this data accessible to more sophisticated modeling systems (e.g., implicit or explicit finite elements) is also of benefit, enabling analyses of, e.g., residual stresses in production components.

Another area of focus for ICME is advanced composite materials, for example, analysis of the distortion of components during molding. The residual stresses which cause these distortions result from temperature variations and thermo-chemical shrinkage of the resin system during cure. These residual stresses lead to changes in the dimensions of a component on removal from the mold, commonly referred to as ‘spring back.’ Distortions due to ‘spring back’ often result in multiple trials during tool manufacture, which extend lead times and incur high cost penalties during production by increasing the tooling costs and scrap rate. To predict the mold shape successfully – so as to account for spring-back – requires multiple modeling runs in which temperature distributions through the mold cavity are calculated as a function of time, allowing for the exothermic chemical reaction of the matrix materials superimposed on the heat input from the tooling. The chemical reaction of the matrix continues until gelation, after which any local strains are locked-in and must be considered in the final calculation of residual stress, and hence any derived residual strain.

To model the whole process we must integrate information and calculations on the chemo-physical behavior of the resin, the physical and mechanical properties of the reinforcement, and the geometry of the component and mold. Having confidence in the model requires its validation. It is therefore essential to compare the outputs of the model to the measured behavior of test components. The role of ICME is to help optimize the entire process by ensuring that the related data is organized in a unified way, and that computed and experimental data can be easily exchanged, applied, and compared.

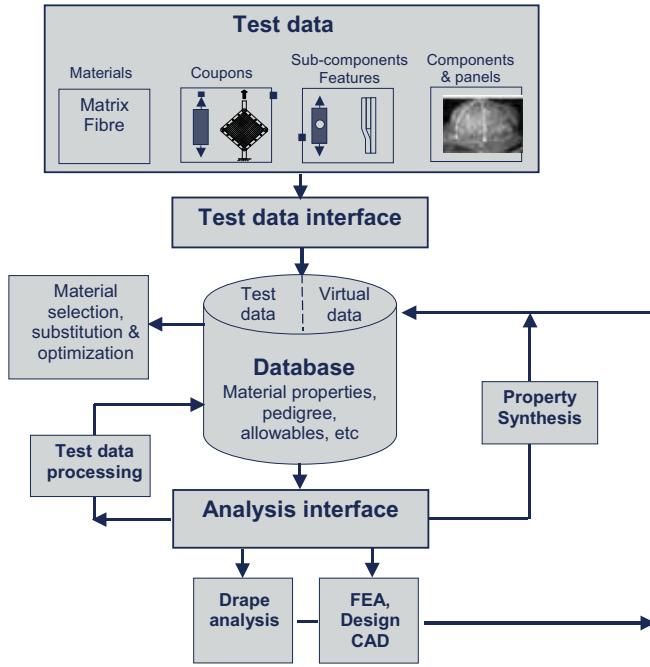


Figure 1: An example ICME architecture for composite materials.

AN ICME ARCHITECTURE

An example ICME architecture for composite materials is shown in Fig. 1. Test data at a variety of length scales – constituent materials, intermediates, coupons, sub-components, and entire panels – is imported through a common *test data interface* and stored in a *structured database*. Data about the constituent components, the processing history (pedigree) data, test data, and all derived information are organized in a way that is transparent for users, while preserving the complex inter-relationships between the data elements. Once the test data are stored, it is possible to give access to them via an *analysis interface* to perform statistical and other analyses to reduce the data to a form usable by designers and analysts – for example calculation of ‘design allowables’. Property synthesis tools can also access the data to predict the properties of ‘virtual materials’ – for example, varying composite lay-up or constituent components. If the predicted properties are stored in the database, then it is straightforward to validate such methods and models by direct comparison with test data. Finally, further *analysis interfaces* to numerical analysis tools, including ‘user material’ constitutive models in FEA systems, draping systems, etc. enable analysis and design of complex structures, based on test data for constituent elements. Again, storage of model predictions in the database makes validation of such models a natural part of the analyst’s workflow.

We will now explore in more detail each of the key elements required to deliver such an architecture – a relational database system that can handle all of the relevant data along with their complex inter-relationships; a test data interface that makes it easy to capture this information into the database; and a two-way interface delivering data to analysis tools and capturing their outputs for further use.

ORGANIZING MATERIALS INFORMATION IN A RELATIONAL DATABASE

Many data formats are necessary to describe material behavior and performance. Layers of complexity can be added to even the simplest property as the range of operating and processing conditions expands. This is best illustrated with an example. The room-temperature strength of a material can be described with a single number. If the operating temperature can vary significantly, the necessary data changes from a single point to a function of temperature. This can become a more complex multidimensional function with inclusion of exposure time, strain-rate, product form, thickness, etc. Every variable adds a new dimension to the data. Figure 2 shows strength data for a 7075 T6 aluminum, taken from the MMPDS database [2], which requires a family of curves for each specific product form and thickness.

There are, of course, other data types that have to be accommodated. These include Boolean data, ‘discrete’ data (e.g. ‘A, B, C, D, E’), text, mixed tables of numbers and text, images, media files, and mathematical functions.

Storing materials information so that it is useful and accessible requires the appropriate data type or attribute to be used for each item in conjunction with an accurate description of the relationships between them. The ‘map’ of these data types is known as a database *schema*. An example of such a schema for the composites database described above is shown in Fig. 3. This schema was designed by the Material Data Management Consortium (MDMC), a group of materials-oriented organizations involved in the aerospace, defense, and energy sectors [3].

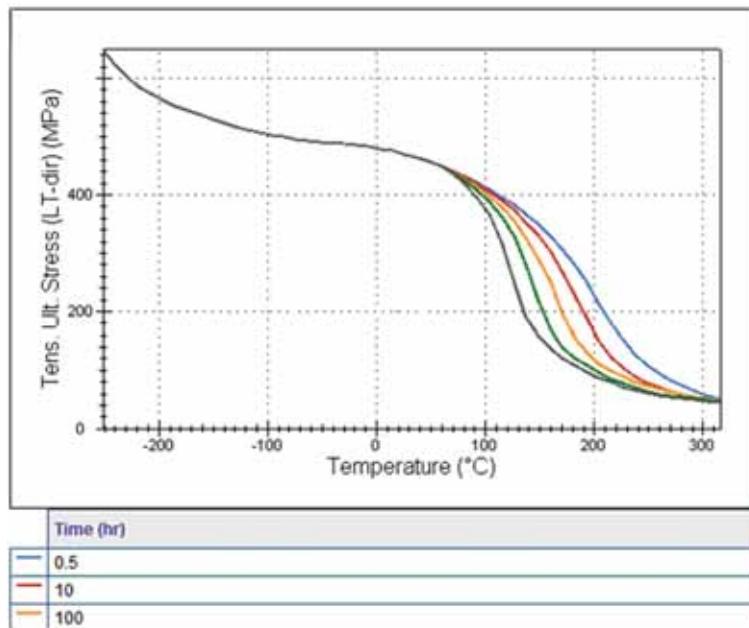


Figure 2: Strength data for 7075, T6, Clad Sheet, Thickness: 0.012 to 0.04 in, AMS-QQ-A-250/13, A basis materials from MMPDS database [2].

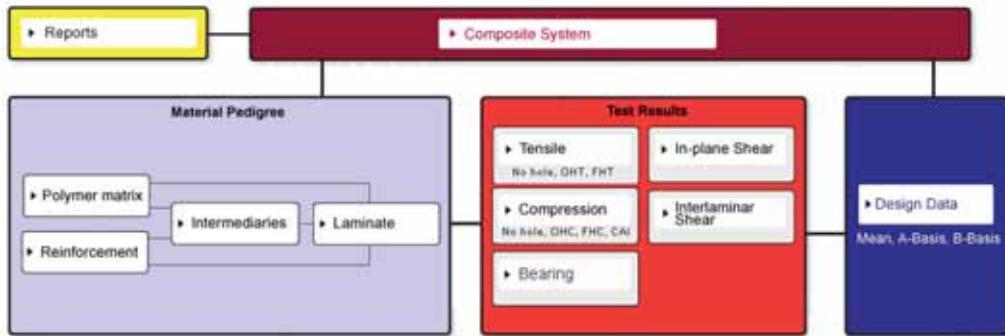


Figure 3: High-level overview of the MDMC schema for storing data for composite materials [3, 4].

The schema comprises five major areas. The “Composites System” area is a general entry point containing generic high-level information about each of the materials systems. The “Reports” area is where pdf files and other resources referenced in the database are stored, supporting the ‘traceability’ of data to its source. The “Material Pedigree” area stores the relationships between materials or components and their constituent parts as well as the processing history. Each *laminate* (or component or sub-component) is typically represented by a record containing ply lay-up data and other processing data along with basic information about it, such as areal weight, thickness resin and fiber volume fractions, etc. This is the pivotal record of the test data system and acts as the focus for the results of tests carried out on coupons cut from the laminate. Laminates may be created from one or multiple intermediaries. A single pre-preg can be processed into a laminate, it could be used to create the skins of a sandwich structure, or it could be combined with one or more different pre-pregs (or other intermediaries) in a hybrid, which itself could be one skin of a structure... It must be possible to represent all of these possibilities for all of the composite types. However, data about a specific pre-preg (gel time, areal weight, nominal ply thickness, etc.) belong on a single record. Links from the pre-preg record connect it to the constituent materials, in this case a fiber and matrix. Data for the sizing or strength of the fibers or gel time and viscosity profiles of the resin are stored at this level.

The “Test Results” area contains the output of a variety of different types of material tests as well as coupon conditioning data. This is because coupons from the same laminate might be subjected to different condition environments. One complexity accounted for in this schema is the storage of results where multiple tests are performed sequentially on a single coupon, such as compression after impact. It is usual to analyze the test data statistically and store the results in the “Design Data” area.

What lessons do we draw from exploring this schema? We see that a typical materials database contains many specialist data types and must ‘hard wire’ in a lot of materials domain knowledge, particularly about the connections between these types. We also see, however, that the structure must be flexible. For example, it must be possible to add support for a new type of test, and to represent all of the possible combinations of system components. This is generally true when designing ICME systems: data structures must be designed with a careful application of materials domain knowledge, supported by information technologies that allow them to be adapted and refined.

TEST DATA INTERFACE

A successful database structure will allow the processing history of every constituent of a test piece to be collated, whatever its origin. With reference to Fig. 1, we will need to import this data, ideally automatically. There are hundreds of possible test types within materials engineering, all generating data of differing types, complexity, and different formats. A few examples from the world of composites are rheological data for the polymer resin systems, strength data for reinforcement fibers, and glass transition data for a green-stage intermediate. Not only do we need to enter these results into the database efficiently and without error, we ideally want to link together related records as we do this – for example, connecting test data records to the relevant process history data. And we want to record information about the test-piece and ensure that this is also linked to the results. These links preserve that vital ‘traceability’ so that we can understand the full context of any piece of test data.

Test data is delivered either in an ASCII file format or in some compiled form of ASCII and digital objects. An ICME system can be set up to read the formats for common test machines by default. But there are far too many for this coverage to be comprehensive. The essential requirement is for configurable importer “templates” that allow the user to map specific items of information from each test data file format onto a format that can be read by the database system. Once the mapping has been done once for a given type of file, it can be re-used for all future files of that type. It is usual for these importers to store a copy of the original data file within the database for complete traceability. It also makes sense to couple importers to ‘smart linking’ capabilities that can automatically generate links between the test results and related data – for example, to scan imported tensile test data for the names of particular reinforcement fiber batches and to link the result to the record containing the process history for that batch.

ANALYSIS INTERFACE

Whether the data in the system is for a composite, a superalloy, or something else, it is of limited use to computational materials engineering unless the appropriate information can be made available to engineers or external analysis systems when they need it and in the format they need it in. This is what really delivers the “I” of ICME.

Modern analytical tools and mathematical models of material behavior are becoming increasingly complex. In order to understand and predict the behavior of materials during processing, to control the final shape or property envelope, or to predict service life, they need access to many variables for each materials form apparent during the modeled event [5]. These variables are often functions of multiple parameters and need not necessarily represent a measurable material property. Modeling tools need to consolidate the necessary information from the volumes of test data using appropriate theory. However, the key feature which characterizes them is that they will want to read data out from the database before entering their modeled parameters back into a separate area of the same system.

Consider a simple example. Figure 4 shows a screenshot from an Excel-based tool for fitting a model to measured fatigue crack growth data. The parameters generated by the model are on the right hand side with the quality of fit shown on the left. An effective ICME system should be configurable so that a tool like this can be ‘hooked in’ to it. For example, an engineer might select a set of records within the database and choose to apply the tool – the necessary input data would be extracted from the database and placed in the appropriate place in the spreadsheet.

The parameters resulting from the model would then be read back into the database and stored along with meta-data identifying the raw data population used and information about the algorithm and assumptions used in the analysis. This information is then available for use in further analyses. This creates a well documented and traceable flow of information *from* the central database to dedicated software and then *back* into the system, complete with all necessary meta-data, at every stage of the engineering process.

The challenge here is that true ICME requires us to integrate *any* possible analysis tool in this way. In theory, this requires programming work every time we want a new analysis tool to communicate with the database. We can, however, greatly simplify this process with a well-designed system. First, an ICME system should offer generic integration with Excel. It should have utilities that allow a user to specify what data should be transferred to/from an Excel analysis tool when the tool is invoked, and where in the Excel spreadsheet to place/find that data. This integration should only need to be set up once for each analysis tool – subsequently it will work in an automated fashion each time the tool is used. Secondly, the system should have an open and well-documented Application Programming Interface (API) – a tool that allows any reasonably-proficient programmer to connect in analysis tools using, for example, C++, C# or web-services technology.

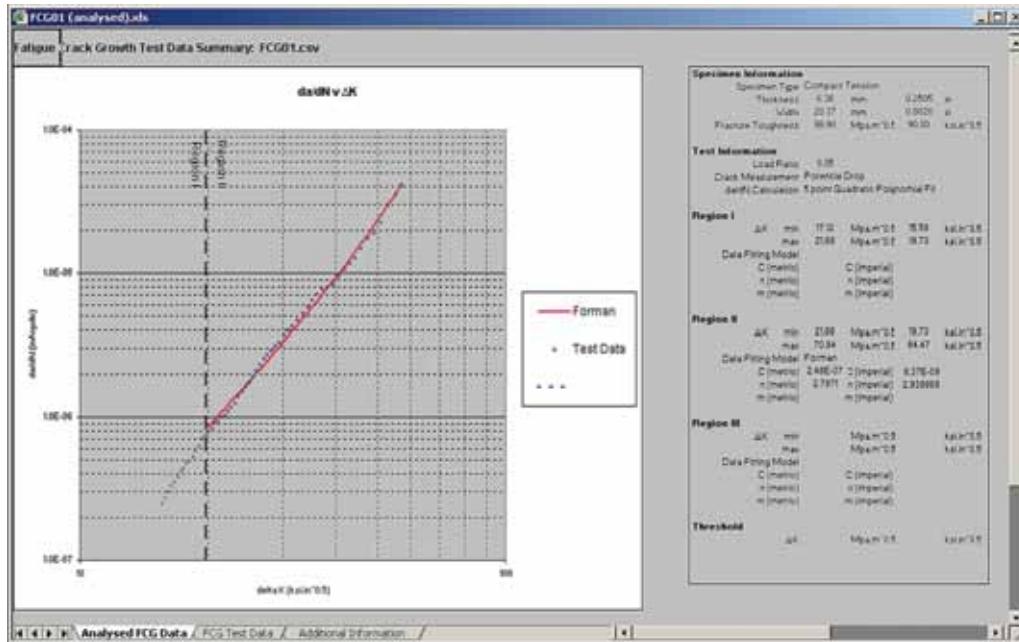


Figure 4: A tool for fitting a model to fatigue crack growth data.

BEYOND SIMPLE INTEGRATION – INTEROPERABILITY

We have covered each of the three key steps for an ICME architecture outlined in Fig. 1. For the test data and analytical interfaces, the core requirement is technologies to exchange data effectively with the database. We can, however, go a step beyond this simple integration, to full interoperability. An example is shown in Fig. 5. Here, materials data in a central materials information system is being accessed directly within the user interface of the Abaqus/CAE analytical system, and can be applied immediately to the model shown. In the same way, fully traceable stored model coefficients could be extracted directly and applied within an FE tool, or

other computational packages. In the GRANTA MI system [4], such interoperability is provided by MI:Materials Gateway. This is a cross-platform rapid integration technology that uses web-services technology and the SOAP protocol to access data and business logic within the GRANTA MI materials information system, and webkit technology to provide a user experience within the client software (e.g., the Abaqus/CAE system, in Fig. 5).

Importantly, flexible tools are needed to transform material models from the data stored in the database into the specific form needed by each modeling package. This can involve a range of activities: from converting the names of attributes, to unit conversions, simple data transformations, and even multi-variable, nonlinear curve fitting. Automating these transformation processes can be challenging, particularly since manual intervention and human judgment are sometimes needed.

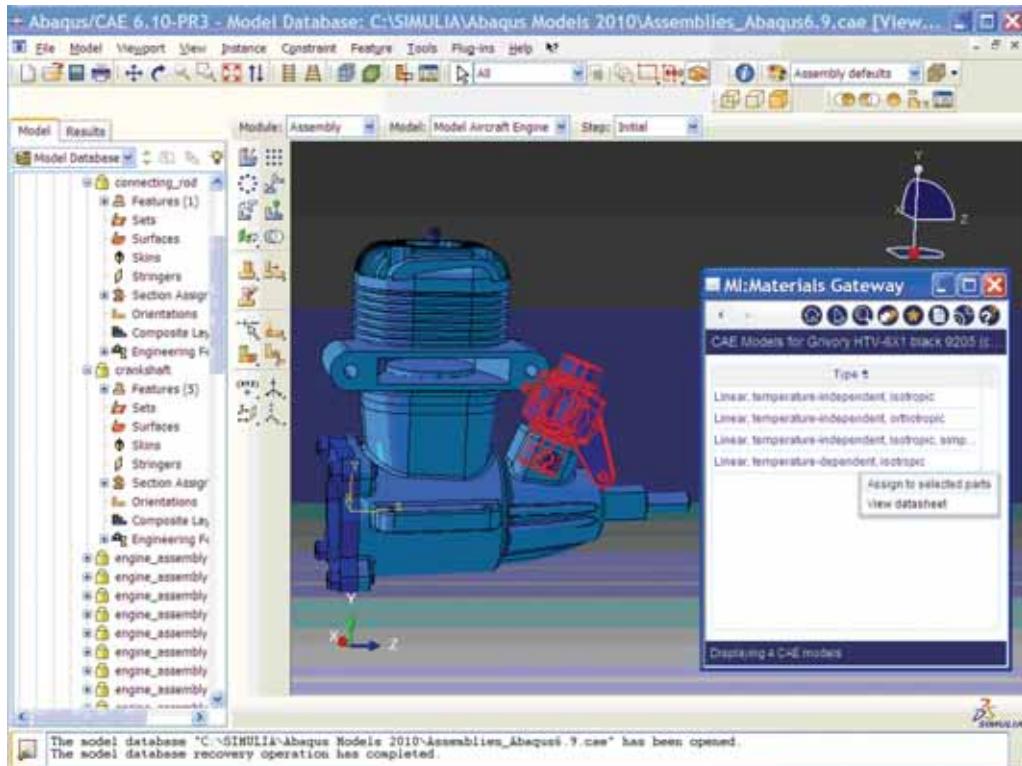


Figure 5: Accessing materials data from within the Abaqus/CAE software, using GRANTA MI:Gateway integration. The front window shows how detailed records can be viewed through a standard web-browser.

CONCLUSIONS

An ICME system does not *replace* analysis tools: its role is an *enabling* one, helping engineering enterprises and collaborative research projects to ‘stitch together’ computational tools with each other and with experimental data. The goal should be to maximize the amount of ‘infrastructural’ materials information software shared between users across disciplines and organizations. This minimizes development and maintenance costs and enables materials engineers to focus on the engineering and the detail of computational methods, not on the IT.

The goal of ICME is a seamless transition between simulations and test data across the full range of length scales. In this paper we have explored the necessary system components for storing and sharing materials information, models, and validation data. The good news is that such technology already exists and, indeed, is in widespread use. For example, the GRANTA MI system mentioned in the previous section was specified by members of the Materials Data Management Consortium, who use it to manage test and design data in the aerospace, defense, and energy sectors.

ICME can be enabled by exploiting the capabilities of such systems to link together more and more computational tools. This allows a coherent flow of data throughout the complex processing chain. Such integration reduces time, risk, and cost in highly sophisticated engineering processes.

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ATOMISTIC SIMULATIONS FOR ENGINEERING: POTENTIALS AND CHALLENGES

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ABSTRACT

Atomistic simulations, both electronic structure calculations and empirical methods such as molecular dynamics, are gaining in popularity and utility to treat a wide range of nanoscale phenomena and materials. The methods have great promise, both on their own and as pieces of an Integrated Computational Materials Engineering (ICME) approach because they can be used to calculate properties (with uncertainties) as input to continuum-level models or as qualitative guides. However, there are a number of issues to be addressed for atomistic simulation to be more widely used in engineering applications. Some are technical, while others are cultural. We will discuss these in the context of the NIST project on atomistic simulations, particularly the issues raised in the annual workshops related to industrial use of atomistic simulations and the NIST Interatomic Potentials Repository (<http://www.ctcms.nist.gov/potentials>) that provides a distribution mechanism for fully referenced interatomic potentials for numerous materials in various formats.

INTRODUCTION

Atomic-scale simulations are increasingly being used to examine nanoscale phenomena, both for stand-alone calculations and as input for higher-level techniques such as finite element analysis (FEA), phase-field modeling, or Calphad approaches [1]. Methods such as electronic structure calculations and molecular simulation (e.g., molecular dynamics) offer the possibility of physical insight into properties that are difficult or impossible to examine experimentally. Atomistic simulations can be used to treat many types of materials including metals, polymers, semiconductors, etc., with applications in the aerospace, automotive, energy and electronics industries. They can be used to examine materials defects, interfaces, surfaces, phase stability, and the effect of system size on properties. They are also part of an Integrated Computational Materials Engineering (ICME) approach [1]. Inexpensive computers and large computational facilities, such as the National Science Foundation Teragrid [2], are providing resources unknown a few decades ago, and this is allowing the treatment of larger systems with more accuracy.

However, electronic structure calculations, while more accurate than classical atomistics (for example, molecular dynamics and Monte Carlo without explicit quantum-mechanical calculations), are still limited to small system sizes on the order of hundreds of atoms. Classical atomistics usually use interatomic potentials or forcefields to control the interactions between atoms, and they can be used to treat billions of atoms in complex configurations, but at the cost of approximations that reduce the calculation accuracy. Cluster expansion methods [3-7] provide one way to apply quantum-mechanical calculations to larger systems by approximating the energy of a system as the cumulative contributions of all of the pairs, triplets, etc., of atoms. While all of these methods are useful in different contexts, in this work the primary focus will be on atomistic simulations using interatomic potentials.

In this paper we briefly describe ICME and outline how atomic-scale simulations fit into the ICME approach. We will then discuss how workshops, including the annual NIST Workshops on “Atomistic Simulations for Industrial Needs” [8] have helped to identify and address challenges associated with the wider use of atomistics in engineering. Some of these challenges are related to the availability and accuracy of materials-specific interatomic potentials [9]. It is important to note that the accuracy of simulations is significant in a scientific, as well as engineering, context -- predictions of invalid mechanisms and transitions can stem from an inaccurate simulation. This discussion will be followed by sections related to data and materials informatics, interatomic potentials, cyberinfrastructure, and the need for robust methods to connect length and time scales. Finally, we will address some of the cultural barriers that are hindering the wider use of atomistics and ICME. All of these topics will be discussed in the context of the NIST Interatomic Potentials Project [8] and other efforts.

ICME AND ATOMISTICS

Besides being integral to scientific inquiry and much of modern life, computation has revolutionized product design through the use of sophisticated computer-aided design and engineering approaches. However, advances in product design have become increasingly constrained by the slow development of new materials. This is in part due to the complexity of many materials with wide ranges of compositions and microstructures, each with different associated properties. Since the development time for materials is often measured in multiple years to decades, materials are generally viewed as static for the purposes of design, meaning that designers select from a database of existing materials with known properties (for example, the database and software products from Granta Material Intelligence [10]). While this approach may work if a material exists and has been characterized, it still relies on materials development that is divorced from product design.

ICME, and the related Materials by Design approach to develop new materials with desired properties, is an approach that is designed to improve how materials development and incorporation in engineering applications occurs with the goal of improving product development times, lowering cost, and increasing reliability [1, 11, 12]. An example of an ICME approach would be the following. A set of required properties would be identified for a particular application. Based on these requirements, an engineer would then choose a set of materials (including composition) plus processing, fabrication, and heat treatment conditions that would result in a microstructure that would most likely yield the required properties. Ideally, these materials would not be limited to a specific type (for example, metals or ceramics) if other materials could meet the objectives. Given the initial conditions, the microstructure would be modeled with resultant properties and performance determinations made. Finally, the cost would be evaluated for that set of conditions. Using that information, an iterative process would be used to optimize the material, composition, and processing conditions. Then a sample of the resulting material would be made and tested experimentally to evaluate the conditions and validate the models. In addition to that single optimized solution, the approach would also encourage a robust design by allowing exploration of how much the processing conditions or composition could vary without significant loss of performance.

This combination of computation and experiment substantially reduces the time and cost of product development over traditional trial and error methods. The approach has been successfully applied in projects such as the Ford Motor Company Virtual Aluminum Casting project [13] and the DARPA Accelerated Insertion of Materials (AIM) program [14], but ICME as a field is still immature and needs sustained efforts and organizational support to mature. To apply this approach more broadly, there must be accurate, scientifically-based predictive models at all

required length and time scales and accurate materials data to use as a part of the model development and validation processes. Additionally, it must be understood how accurate those models are and the uncertainties associated with them. The 2008 National Research Council (NRC) report highlighting ICME discusses many of the benefits and challenges for this approach [1].

Within the ICME approach, perhaps the area of greatest unmet promise is atomistic simulation. Atomistics primarily fit into ICME and multiscale modeling methods by providing data to use as input or validation for higher-level models, either through weak coupling (calculating a property and its uncertainty to feed into another model) or strong coupling where the atomic-scale simulations feed directly into other simulations (for example, passing deformations calculated from local atomic displacements to an FEA simulation and new atomic coordinates back to the MD in response to the FEA calculation). They can also be used to validate continuum-level predictions. However, as with the ICME approach in general (as outlined in the NRC report), there are issues that need to be addressed before atomistics can be more widely used. This is particularly true in an engineering context where safety (derived from accuracy and uncertainties), tight timelines, cost, and required performance objectives are all critical.

In particular, the NRC report notes that the following is necessary in relation to atomistics: “Extensions of atomistic simulations to longer times through the use, for example, of accelerated dynamics methods and to broader classes of materials systems through the development and validation of force fields for application to heterogeneous/mixed materials, especially at the interfaces between material types (for example, metal-ceramic)” [1].

As with the rest of the ICME approach, it is important not to set expectations too high. Otherwise organizations might adopt ambitious programs, only to scale them back substantially or abandon them when it becomes clear that the goal will not be met immediately or without substantial investment. The NRC highlighted ICME as a key engineering approach, but that must happen by laying a groundwork and then building upon it.

WORKSHOPS

The Interatomic Potentials Project was created at NIST to facilitate the use of atomistic simulations through workshops, data-, and standards-related activities. This is a collaborative project that seeks to bring together various researchers interested in atomistic simulations and the issues associated with them. We work with users and developers of interatomic potentials and related software, both in academia and industry, as well as with experts on different modeling methods, data analysis, and standards. One of the primary means to do that is the annual NIST-hosted “Workshops on Atomistic Simulations for Industrial Needs.”

These workshops are designed to facilitate interactions between industrial and academic researchers, identify barriers to the wider use of atomistic methods in engineering applications, and address these challenges. Participants have come from various companies, national laboratories, and universities, and include industrial researchers, developers of interatomic potentials, experimentalists, and software developers. We discuss the state of elemental and alloy interatomic potentials, including transferability, or how well a potential works for a range of conditions such as temperature, pressure, or composition. We also address validation methods using experiments and/or electronic structure calculations, as well as the use of classical atomistic and first-principles calculations as input for phase-field models, FEA, and Calphad approaches. The workshop topics change with expressed participant interests. In 2010, participants presented interatomic potentials, tools, and applications. Various presentations from the 2008-2010

workshops are available on the project website [8]. The workshop participants, along with those participating in various ICME meetings (for example, the 2009 Gordon Research Conference on ICME [15] and the 2010 TMS Materials Science and Technology Meeting symposium on ICME [16]) and numerous one-on-one discussions, echo many of the points in the broader NRC ICME report within the context of atomistics. Many of the issues faced by the industrial research community are also important in the wider simulation community, and thus addressing industrial concerns benefits other researchers as well.

Participants have specifically highlighted the need for a repository of interatomic potentials of known history; standard methods, tools, and benchmarks; validation tools and reference data (experimental and quantum mechanical); accurate multicomponent models; user-friendly, high-throughput, physics-based methods; and standardized ways to link software platforms. They have noted that a partial solution is often enough to guide development -- the perfect answer is not always necessary and waiting for it can preclude its use.

The participants have also noted that trends across the periodic table and in composition space are useful, even if the predictions are qualitative rather than quantitative. Effects of system size on thermodynamics and kinetics (for example, chemical ordering and phase stability in nanoparticles) are also studied. Interfaces are key, both within materials in the form of internal interfaces (e.g., grain boundaries) and externally (e.g., surfactants), and interfacial free energies (solid-solid and solid-liquid) frequently arise as areas of industrial interest. Additionally, atomistic simulations can provide a way to explore the effects of temperature, composition, stress/pressure, and radiation on properties. Many of these studies need to be done for non-equilibrium conditions at elevated temperatures where processing often occurs, and accelerated aging studies are relevant for life prediction. In short, industrial researchers have expressed a desire for a wide range of materials and simulations.

DATA, MATERIALS INFORMATICS, AND CONNECTIONS

Key requirements for ICME outlined by researchers and the NRC ICME report are data and materials informatics. Materials informatics includes databases of information, and the mining of large datasets to identify patterns that give insight into previously unknown physical relationships [1]. Data is needed as part of the process to fit and validate models at all levels, including atomistics. Reference data, trusted experimental measurements, and physical constants are key. Due in part to experience generating and maintaining Standard Reference Materials (SRM) [17] and Standard Reference Data (SRD) [18] programs, the NRC ICME report outlined a major data role for NIST. This includes archiving and curating databases. Relevant NIST projects also include the NIST Diffusion Data Center [19] and Calphad-based thermodynamic and diffusion databases [20]. Interatomic potentials are of more recent interest -- both the potentials themselves and the property comparisons with reference data used to evaluate them. For atomistic simulations, reference data can be obtained from experiments and high-quality electronic structure calculations. Estimates of uncertainties are also essential.

As part of the effort to provide users with data for decision-making, we also perform property comparisons against experiment and electronic structure calculations where available. Recent work has highlighted the importance of the choice of interatomic potential in the predictions of properties for aluminum melts [21] and nickel stacking fault energies [22]. It is important to note that the purpose of this project is not to declare that any potentials are “The Best” since that may depend on the application being considered.

In addition to accurate and reproducible atomistic simulations, robust methods to link simulation scales are necessary. This link can be through the calculation of properties that are used as input for higher-level models (e.g., interfacial free energies that are calculated with molecular dynamics and used as input for phase-field models) or the explicit coupling of simulations such as first-principles molecular dynamics where forces used in the molecular simulation are determined by electronic structure calculations. In either case, it is necessary to assess accuracy, uncertainties, and the sensitivity of the higher-level models to those uncertainties.

INTERATOMIC POTENTIALS

A major need is for the interatomic potentials (also known as forcefields) that describe the interactions between atoms in an atomic/molecular simulation such as molecular dynamics or Monte Carlo. The potentials need to treat not only single elements, but also multicomponent alloys and interactions between types of materials such as metal-polymer interactions, where the most important materials interactions reflect the application under consideration.

Interatomic potentials can have many different functional forms and be analytical or non-analytical [23]. Examples include the Lennard-Jones [24], embedded-atom method (EAM) [25], modified embedded-atom method (MEAM) [26], and ReaxFF [27]. Some are more directly tied to theory (semi-empirical) while others are fully empirical in nature. They often include/emphasize different physics and chemistry (for example, metallic versus covalent bonding, bond breaking and forming, charge, etc.). Developers of interatomic potentials usually use different data as part of the fitting process, so interatomic potentials can differ widely for what is nominally the same element. Transferability, or how well they work outside the fitting region of phase space, is also an issue. Tradeoffs are generally made between calculation speed (system size) and accuracy. Understanding uncertainties and how they propagate through simulations and analysis is important.

Generally a functional approach is chosen and an initial guess for the parameters is made. The trial function is then used to calculate physical properties that are deemed most relevant. Changes are made, and the process proceeds iteratively until satisfactory agreement is reached between the calculated and target properties. Besides the properties included in the fit, developers also calculate properties that were not used as fitting data to evaluate the predictive capabilities of the potential. This process is often considered as much art as science. Once the developer is satisfied, the potential may be published as a set of equations and parameters, tables of numbers, etc. Often files are used to hold the information and control molecular simulation software.

A major challenge associated with interatomic potentials is their accuracy, particularly in the treatment of multicomponent systems. Deciding which data to use for fitting and validation, along with the relevant uncertainties, is sometimes difficult. For example, widely differing experimental measurements may have been made for a quantity, and it is sometimes unclear which are the most accurate. Heavy reliance on inaccurate data would impact the accuracy of the potential. Even with good experimental data, it is not always clear how to use those measurements for comparison (i.e., is the quantity really the relevant one? Which models and assumptions were used to interpret the measurements?).

More practical challenges for users include finding, evaluating, and comparing interatomic potentials. Sometimes potentials are implemented differently in different pieces of software, and these formats can be incompatible. Additionally, there are issues related to version control -- files may be corrupt, users implemented models incorrectly based on equations in papers, multiple versions of the same potentials exist with different properties, or websites created as part of a

grant are allowed to lapse and become out of date. To solve some of these problems, unique identifiers are necessary, and models need to be calibrated and validated. True reproducibility depends on having the same potentials and software. The NIST Interatomic Potentials Repository (IPR) [8] was created to address many of these issues and is described in the next section.

CYBERINFRASTRUCTURE

Cyberinfrastructure includes the tools, software, linkages, databases, etc., necessary to support scientific computation generally and an ICME approach in particular. Various tools exist for these computations, some of which are widely used. Examples include molecular simulation packages such as the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS, [28]), the ITAP Molecular Dynamics program (IMD, [29]), and Accelrys Materials Studio [30]. There are various approaches to link software platforms (for example, EnSight [31] and MedeA [32]). However, work needs to be done to improve compatibility between pieces of software (e.g., using the same interatomic potential file for various molecular dynamics packages) and transfer across simulation types (for example, electronic structure to molecular dynamics or molecular dynamics to FEA). One approach to this problem is developing common formats and consistent, transparent inter-program communication and information transfer (open-platforms). Analysis of the uncertainties associated with the software, not just the models, is also necessary.

Once interatomic potentials have been fit as previously described, there are issues related to their distribution and comparisons. We work with developers to make available the files that are used with molecular simulation packages. While no particular file formats are required, documentation about formatting and usage are. Most interatomic potentials available on the website are compatible with readily-available molecular simulation packages such as LAMMPS and IMD. The files have been approved by their submitters, but it is still the user's responsibility to ensure that the potentials give expected results.

There are currently more than 100 element and alloy potentials available for download at <http://www.ctcms.nist.gov/potentials>. Since April 2008, usage of the site has increased to more than 3500 content pages served per month to more than 600 distinct IP addresses (as of November 2010). The site is currently the primary distribution source for several interatomic potentials developers. While the available potentials were initially metals and alloys of the embedded-atom and related forms, all types of potentials and materials are welcome.

The website contains an overview of the project, a listing of recent additions, links to the potentials pages, a FAQ, statistics on site usage, and links to other resources of interest. For each interatomic potential, there is a citation, formatting information, a link to the potential file(s) or parameters, and additional notes including corrections and information on who submitted the files.

This work builds on the experience at NIST with the SRM and SRD programs and does not depend on grant cycles to provide support for long-term archival capabilities. The IPR is a tool for developers to distribute interatomic potentials in their chosen formats and for users to be able to identify what they have. It is not meant to judge the quality of the interatomic potentials posted there. The IPR complements other efforts at NIST to "develop and curate precompetitive materials informatics databases" (NRC ICME report recommendation 4).

We also work with developers to make their potentials more accessible by converting file formats for use with different pieces of software. In the case of conversions between file formats, validation results are posted to demonstrate that the converted format is faithful to the original.

More recently, we have become involved with automated testing and standardization efforts through the Knowledgebase of Interatomic Models (KIM) collaboration [33].

CULTURAL ISSUES

Besides technical challenges, there are also cultural barriers, some of which affect the ICME approach in general, while others are specific to atomic-scale simulations in particular. One general issue is the disruption of current practices that have been developed over years by the introduction of something new and unproven. The need to invest in new people and technology makes this type of change even more daunting. Ultimately the success of ICME, including atomistics, rests on the economic benefit to organizations. The approach needs to satisfy the short timelines for product development with robust models, results, and software.

From discussions related to ICME, it has become clear that there is sometimes a perception that researchers using atomic-scale methods are not concerned about the accuracy of the simulations since comparisons are often not made with experiments. However, it is important to recognize that this is not a simple issue. Atomistic simulations are often attractive because the experiments are difficult, expensive, or impossible. Even if experimental measurements are available, it can be difficult to assess their quality and applicability. Thus there may be no relevant or trusted experimental work to use for comparison. Even so, these simulations would benefit from greater collaboration between experimentalists and those performing simulations, as well as more comparison with experiment and high-quality electronic structure calculations.

These challenges are exacerbated by the fact that easy-to-use tools are increasing the number of simulations performed, but black boxes and lack of experience can lead to results that are misleading or wrong due to lack of knowledge of the relevant physics or incorrect application of techniques. This situation reinforces the need for critical analysis of results.

Another challenge to the use of atomistic simulations in ICME is the proprietary nature of much industrial research. Interatomic potentials are taken from the public domain and modified for internal use without being released for others to use and improve further. For potentials developers, there is the additional challenge of understanding which systems are relevant for industrial use when companies will not release that information, except possibly to a few academic or government partners. By the same token, academic researchers need to recognize that proprietary or sensitive information is key for many industrial researchers and respect that limitation. Similarly to the modeling, the results of experiments done by industry are often not released into the public domain and thus can not be used to validate interatomic potentials or show where they need to be improved.

To overcome these cultural barriers, it is necessary for experts in different fields to interact and collaborate. Modelers also need to be knowledgeable in other areas such as software, experimental methods, numerical analysis, other engineering disciplines, etc., or collaborate with those who are. Researchers and managers who are experienced in atomistics and other ICME areas, and can properly set project scopes, will also help.

SUMMARY

Classical atomistic simulations are playing an increasing role in materials research, both academic and industrial. They have been widely used to understand nanoscale phenomena, especially in areas where experiments are difficult or currently impossible. However, the model chosen can have profound implications for the accuracy of a simulation. The use of these

simulations in an engineering context is particularly challenging. This is due in part to concerns over accuracy and uncertainties. Methods need to be proven and reliable to be incorporated into a design process with defined performance goals and cost considerations. These and other issues related to data, cyberinfrastructure, interatomic potentials, and culture have been discussed. The NIST Interatomic Potentials project was created to work with the community to provide referenced models for download, property comparisons to assist researchers, and standardized model formats. Annual workshops are also held to address outstanding issues and facilitate communication between industrial and academic researchers. This represents a step forward, but much more needs to be done to make this a mature engineering tool and component of ICME.

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MULTISCALE MODELING OF ALUMINUM OXYNITRIDE

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ABSTRACT

The computational modeling linkage from the atomistic to the continuum scales of homogeneous and discrete deformation mechanisms (twinning, cleavage, micro-cracking, stacking faults, et cetera), nano- and microstructure and defects, to dynamic failure processes in brittle materials should provide pathways to designing improved mechanical performance through controlled processing. This paper will review results from an internal multiscale computational program in first-principles design of armor ceramics, with a focus on an optically transparent armor ceramic, polycrystalline ($\sim 200 \mu\text{m}$ grain size) aluminum oxynitride (AlON) spinel, that uses a multiscale modeling approach, and will overview the special computational challenges that are required for linking the vast spatiotemporal scales from the quantum to the continuum. The grand challenge for such multiscale model development, also known as integrated computational materials engineering (ICME), is to be able to design materials atom by atom and to predict ballistic performance. Gaps and barriers using the ICME approach are addressed in this paper through illustration of an ongoing Army program to model the multiscale constitutive and failure response of AlON.

Keywords: ICME, multiscale modeling, validation, materials in extreme dynamic environments, quantum mechanics, molecular dynamic, continuum mechanics.

INTRODUCTION

The computational bridge between the atomistic and continuum length scales is addressed in a hierarchical fashion (Fig. 1) through development of: 1) a first principles unit cell model to predict the anisotropic elastic properties of AlON, 2) a classical molecular dynamics model through periodic replication of the unit cell model for the study of single crystal slip and twinning dynamics, 3) a single crystal anisotropic plasticity model to account for the kinematics of crystal slip and twinning mechanisms in AlON, 4) a mesoscopic polycrystalline computational finite element model that incorporates single crystal deformation kinematics, and explicitly includes microcracks that are represented on the grain boundaries using cohesive interface laws that allow investigation of crack nucleation, growth, and coalescence, and 5) a continuum computational finite element model with the particular challenge of development of algorithms for transitioning microcrack coalescence behavior at the mesoscale to the continuum.

Critical in the development of the hierarchical multiscale model outlined above is the experimental validation of the individual scales. Quantum and molecular dynamics predictions of the three independent anisotropic elastic constants of AlON, C_{11} , C_{12} , C_{44} , should be consistent with each other, and with experimentally determined values on few tens of micron size oriented single crystals of AlON, using for example, Brillouin spectroscopy or focused-ion-beam (FIB)/SEM compression and tension tests. The chief challenge for modeling brittle armor materials is to correctly account for the growth kinetics of microcracks, inelastic deformation mechanisms, and the influence of defects in a multiscale computational environment. The

propagation of microcracks at smaller scales will be “coarse-grained,” to higher scales where global fracture failure and fragmentation is observed. Such coarse graining algorithms can be validated through continuum-scale experiments that measure dynamic crack propagation speeds, mixed-mode failure, and crack bifurcation phenomena using the in-house coherent gradient sensing (CGS) and/or high speed imaging techniques. The development of consistent coarse-graining algorithms for fracture and other localization phenomena, which are associated with failure and loss of material stability, is a relatively unexplored but critical aspect of this research.

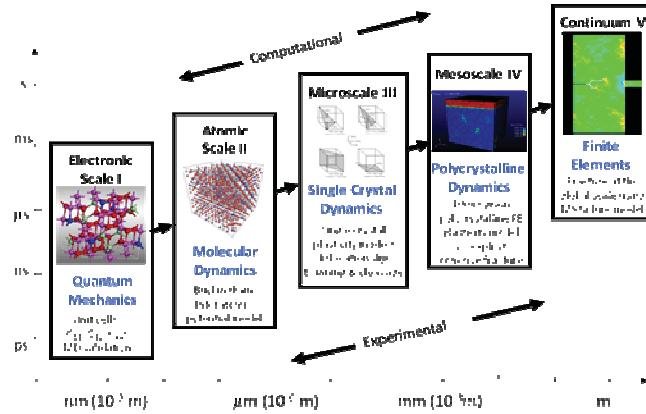


Fig. 1. A multiscale constitutive and failure model for AlON that illustrates the spatiotemporal dependence of the scales [1].

EXPERIMENTAL OBSERVATIONS

Dynamic Fracture and Inelastic Deformation

The complex fracture patterns that are observed in polycrystalline AlON from an Edge-on-Impact (EOI) by a spherical steel impactor travelling at ~ 430 m/s reveal the multiscale nature of fracture in AlON (Fig. 2).

A scanning electron micrograph (SEM) image of fracture surfaces of post mortem samples of AlON from an EOI experiment (Fig. 3(a)) illustrate the complex nano- and micro-cleavage patterns from these dynamic tests. Chen and McCauley are also carrying out systematic indentation studies on single crystal AlON grains to determine the deformation mechanisms in an intrinsically confined test. A high resolution transmission electron microscopy (HRTEM) image of a cross section through an indentation into AlON is illustrated in Fig. 3(b).

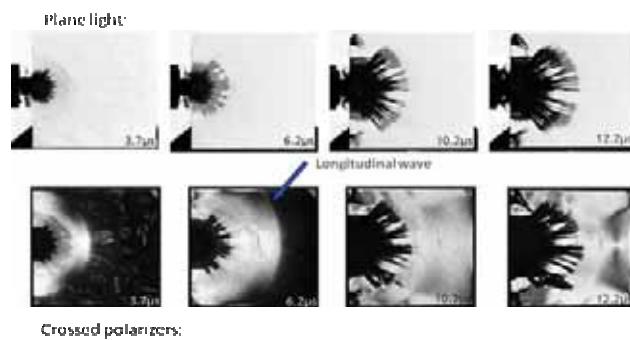


Fig. 2. Shadowgraphs corresponding to photographs at various times after impact from a spherical projectile [2].

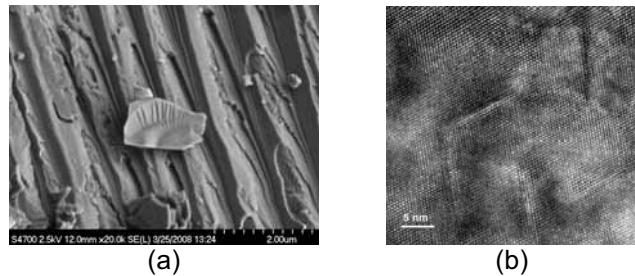


Fig. 3. a) SEM of microcleavage fracture from an EOI test, b) HRTEM showing a high density of dissociated $<110>$ dislocations along $\{111\}$ planes have been identified.

In addition to dynamic compressive strength measurements carried out in a Kolsky bar arrangement, impact transitional velocity measurements are also being determined. Figure 4 shows a flash X-ray radiograph of AlON being penetrated during this test. The transitional velocity was measured as 1207 m/s. Of course, a major challenge is to predict these experimental observations using the multiscale modeling and simulation approach.



Fig. 4. X-ray radiograph of penetration into AlON above transitional velocity [3].

FIB/SEM Experiments

We have developed a custom test apparatus for in-situ scanning electron microscope (SEM) mechanical testing. Our system utilizes a 5-axis piezoelectric positioning system that enables precise placement and alignment of the micro-specimens, either within the tensile grip or near the compression platen. Loads are applied using a high-resolution linear actuator with a reported resolution of ~ 1 nm and measured with a strain gage based S-beam load cell. The load cells have a capacity of 10 or 100 g with a resolution of ~ 0.01 g. Specimen load/stress and crosshead displacements are measured using a customized data acquisition program, while the specimen strain is calculated from SEM micrographs using an open source digital image correlation script developed by Eberl and coworkers for Matlab®. We use focused ion beam (FIB) machining to fabricate micro-compression and tension samples with minimum dimensions of 1-10 μm . Compression specimens typically have a uniform cross-section with a 2:1 aspect ratio while the tension samples are higher aspect ratio “dog-bone” specimens. In Fig. 5, we show a single-crystal SEM micrograph of a high-aspect-ratio compression specimen with a width of ~ 5 μm and overall length of ~ 20 μm that is axially loaded to failure with measured strengths ranging from 5 to 10 GPa on specimens of unknown crystallographic orientation. Tension and compression tests on oriented single and bi-crystals of AlON are pending.

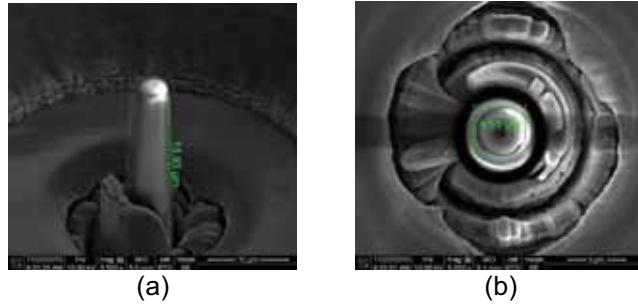


Fig. 5. (a) Single crystal AlON compression specimen, (b) axial view loaded to failure.

Coherent Gradient Sensing of Dynamic Fracture

Despite its long history, capturing relevant data and creating models for the dynamic failure of materials at the macro-scale is a non-trivial task. Material failure in the form of cracks or other localizations is a discrete event, reducing the effectiveness of many traditional material characterization testing techniques that rely on homogenization. Full-field data, particularly when over-driven cracks may bifurcate or a failure-mode transition might occur, is highly informative for observing phenomena as well as developing models for failure events.

The full-field method of coherent gradient sensing (CGS) [4] was implemented at the Army Research Laboratory to study the dynamic fracture of transparent brittle materials. CGS is a full-field imaging technique that produces fringes based on the out-of-plane strain gradient, making it insensitive to noise and capable of discerning the tip of a crack when the crack-opening-displacement is small. Employing an 8-watt 532-nm wavelength laser coupled with a Cordin 222C-16 camera allows framing rates as high as 10-million frames per second (limited by laser power), which is critical in capturing cracks traveling several kilometers per second. Crack bifurcation in poly(methyl-methacrylate) (PMMA) at a nominal crack velocity of 745 m/s [5] is shown in Fig. 6. CGS and the method of caustics have allowed observation of high-speed crack propagation in polymers, glasses, and ceramics, resulting in the computation of the dynamic fracture toughness as a function of crack speed for mixed-mode cracks common in ballistic penetration. Initial work with the transparent ceramic AlON revealed decided thickness effects; ongoing work seeks to determine whether this effect is due to the material itself or the testing methodology.

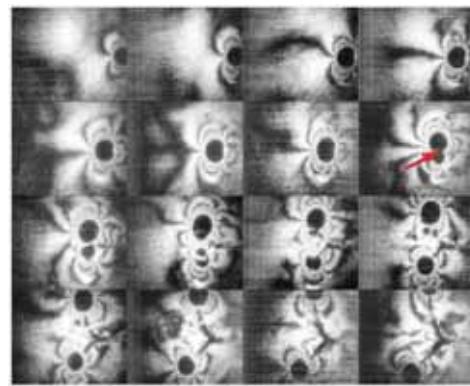


Fig. 6. CGS images of crack bifurcation (initiation indicated by red arrow) in PMMA.

Simulation of dynamic crack propagation at the macro-scale currently relies on the data obtained from the macro-scale laboratory tests discussed above along with the computational technique of the adaptive insertion of cohesive zones. The adaptive insertion of cohesive zones, pioneered by Ortiz and his co-workers [6] allows the connectivity of the finite element mesh to be changed based on a specified failure criterion. Rate-dependent cohesive laws for the fracture of PMMA were developed and implemented into finite element codes featuring adaptive insertion based on the extensive experimentation documented in [5]. Current simulations can accurately predict crack propagation speeds and bifurcation; validation experiments to test the methodology with multiple mixed-mode cracks in a complex geometry have yielded positive, if mesh dependent, results. Ongoing experimental efforts with AlON and the mesoscale work underway at ARL will hopefully provide a similar rate-dependent cohesive law and illuminate the crack propagation mechanisms (intra- versus inter-granular fracture, localized plasticity, et cetera) critical in predicting dynamic failure.

Shock Compression Experiments

Shock compression of AlON has been reported by Cazamias et al. [7] to 15 GPa, by Vaughan et al. [8] to 21 GPa, by Sekine et al. [9] from 61 to 180 GPa, and by Thornhill et al. [10] from 5-89 GPa. These studies included the Hugoniot Elastic Limit (HEL), Hugoniot measurements to 180 GPa and phase transition, shear strength, and spall strength. The densities of AlON used in the investigations of Cazamias et al. [7] and Vaughan et al. [8] varied between 3.51-3.59 Mg/m³. The density of AlON used by Sekine et al. [9] and by Thornhill et al. [10] was 3.67 Mg/m³. Dandekar et al. [11] analyzed the results of these shock compression investigations to determine the shear strength of AlON. The results of these studies may be summarized as follows: (i) The HEL of AlON varies between 10.5 and 12.1 GPa. (ii) The shear strength of AlON at the HEL range from 3.3 to 3.9 GPa. AlON continues to maintain shear strength between 4.4 and 6.0 GPa above the HEL even when the compression of AlON indicates a softening around 16.5 GPa. (iii) Sekine et al. [9] observed a softening in compression around 50 GPa and postulated a phase transition for the reported shock compression of AlON around 130 GPa. (iv) Spall strength of low density AlON was reported to be 0.14 and 1.7 GPa for impact stress of 9.5 and 4.8 GPa [7]. Thornhill et al. [10] failed to detect any spall strength in AlON when shocked to 5.4, and 7.8 GPa, respectively. The compressive durations in two spall measurements each of Cazamias et al. [7], and Thornhill et al. [10] were 0.36 and 0.18 μ s, and 0.35 and 1.16 μ s, respectively.

The puzzling/inconclusive results of the previous spall experiments, lead us to postulate a hypothesis that the magnitude of spall strength of AlON is dependent on both shock induced compressive stress and its duration. A suite of experiments have been designed to test this hypothesis. The selected compression durations for these experiments are 0.18, 0.54, and 1. μ s if needed. Spall behavior of AlON will be determined to 10 GPa with the two selected compression durations. Results of two spall experiments performed at 3.1 and 3.2 GPa are shown in Fig. 7. The compressive profiles show unexpected fluctuations. The reason for the observed fluctuations is not currently understood. Similar fluctuations were also present in previous studies [10].

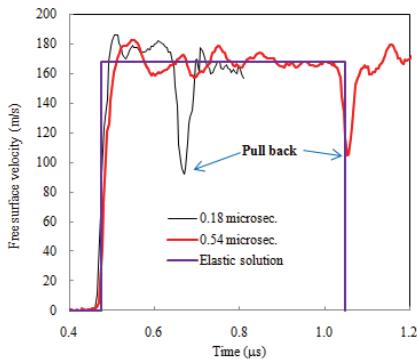


Fig. 7. Free surface velocity profiles in AlON.

The elastic solution provides the magnitude of fluctuations during the compression of AlON. The effect of duration of shock wave compression is clearly seen in these wave profiles. The magnitude of pull back velocity is larger for the smaller duration of compression. The calculated values of spall strength of AlON when shocked to 3.1-3.2 GPa for the compression durations of 0.18 and 0.54 μ s are 1.65 and 1.09 GPa, respectively, i.e., a 33% decrease in the spall strength.

COMPUTATIONAL MODELING

Quantum Mechanics (QM)

The atomic structure and elastic properties of aluminum oxynitride spinel (AlON) at high pressure (up to 40 GPa) have been calculated from first principles. We have assumed an “ideal” stoichiometry of cubic AlON with 35.7 mole % AlN using the constant anion model [12]. Our QM calculations support the model, and the Al vacancy on the octahedral site is \sim 0.5 eV lower in total energy than the vacancy on the tetrahedral site with the same distribution of N atoms. The elastic constants were calculated from independent strains that were applied to a unit cell, parameterizing the total energy as a function of the strain and from a stress-strain relationship. The methods gave quite close values of elastic constants, which indicate convergence of energy of cut-offs and total energy (Table 1). The purpose of the calculations is to determine if the location and/or segregation of N atoms in the unit cell affects the elastic properties of AlON. The calculations have been carried out for two random (Fig. 8(a)) to clustered (Fig. 8(b)) arrangements of nitrogen atoms in the unit cell.

At ambient conditions a clustered distribution of N atoms has \sim 1 eV per 55 atoms higher total energy than for a random distribution and slightly, but systematically lower elastic constants. The pressure dependence of C_{11} , C_{12} and C_{44} for random and cluster distributions of N atoms was calculated in the range of 0-40 GPa by performing six finite distortions of the lattice and deriving the elastic constants from the strain-stress relationship. The calculated values of dC_{11}/dP are in the range of 4.0-6.2 and for $dC_{44}/dP \sim$ 0.8-1.5.

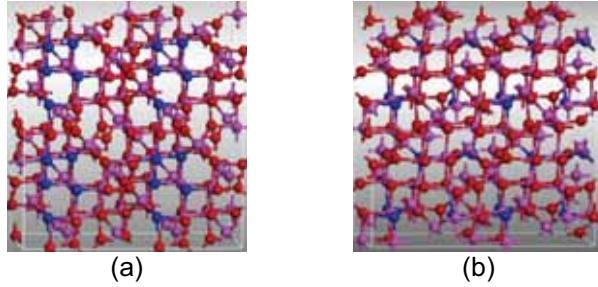


Fig. 8. Cluster (a) and random (b) distribution of nitrogen atoms over oxygen sites.

Molecular Dynamics (MD)

As MD simulations are to be used to explore failure mechanisms for AlON, it is crucial that the interaction potential used in the MD simulations be assessed for suitability in describing this system. It is equally important that the simulation supercell adequately depicts the physical system. The interaction potential model we are using is based on the Buckingham potential

$$V(r_{ij}) = A_{ij} \exp\left(-\frac{r_{ij}}{\rho_{ij}}\right) - \frac{C_{ij}}{r_{ij}^6} + \frac{q_i q_j}{r_{ij}}, \quad (1)$$

where the first term represents an overlap repulsion, the second term is an attractive van der Waals force, and the last term is the electrostatic interaction. Polarization of the oxygen atoms is achieved via the shell model of Dick and Overhauser [13]. Values for the parameters (A , ρ , C , and q) were taken from previous MD studies of AlN and Al₂O₃.

Random Generation of Initial Configuration

In the constant anion model, about one-third of the aluminum atoms are located in tetrahedral coordination, the remaining aluminum atoms are found in octahedral sites, and one site remains vacant. First principles calculations [14] on an idealized unit cell (in which the vacancy and location of the N atoms are assumed) have demonstrated that the most stable structure of AlON has the Al vacancy at the octahedral site, with six O nearest neighbors (VO₆). The positions of the five nitrogen atoms and the one vacancy in a 55-atom unit cell are not actually known nor are they unique. Anisotropic NPT simulations (in which angles between cell vectors were constrained to be orthogonal) of small supercells composed of repeating unit cells in which the locations of the vacancy and N atoms were the same produced crystals that were not cubic.

Size Effect of Cubicity

Ten systems of 1485 atoms were generated, as well as ten systems of 11880 atoms, in which the locations of the vacancies and N atoms are randomly selected. Each system was simulated in the N_oT ensemble, where both the simulation cell lengths (a , b and c) and the angles between cell vectors (α , β and γ) are unconstrained. If an individual system is cubic, such a simulation should result in the averaged simulation cell lengths being equal ($a = b = c$), and the angles orthogonal ($\alpha = \beta = \gamma = 90^\circ$). Fig. 9 shows the average cell dimensions ((a) and (b)) and cell angles ((c) and (d)) for the two system sizes. While no simulation cell ended up being purely cubic, increasing the system size (and corresponding degree of random distribution of Al vacancies and N) clearly improves the cubicity of the system, as the data points get closer to the overall average values, with decreased error.

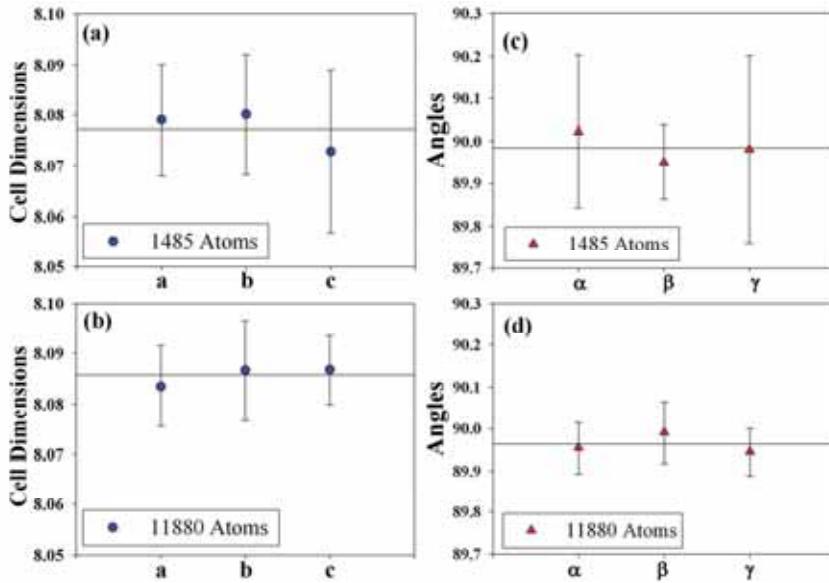


Fig. 9. Effect of system size on the cubicity of the simulation cell in which the locations of vacancies and N atoms are randomly selected within individual unit cells. Average cell dimensions are shown for the (a) small system and (b) large system, and the average cell angles of the (c) small system, and (d) large system, with standard error bars. The reference lines indicate the overall average values for that system size.

The cubic elastic constants, C_{11} , C_{12} and C_{44} , of AlON have been predicted using QM and MD methods, and from these, Voigt averages (upper bounds) for Young's, E_v , shear, G_v , and bulk modulus, K_v , have been determined and compared with experimental values from polycrystals [15] (Table 1). The QM model contains either a random or cluster distribution of N atoms [16] resulting in the range of values shown in Table 1. For MD systems consisting of 1485 atoms, both shell and no-shell configurations also predict a range in elastic constants. Voigt averages for the QM model more closely predict values obtained from polycrystals. As seen in Table 1, the difference between the material properties of AlON calculated from QM and MD are striking. The discrepancy is most likely due to inadequacies in the interaction potential used in the MD simulations, which was not fitted for this material. However, further investigation is necessary to ensure the accuracy of the QM and experimental results, which are currently in good agreement. First, the QM values were obtained from simulations of a single 55-atom unit cell, and only two configurations were used. This is a small sampling of possible unit cell configurations, considering the possible locations of the five N atoms and the single Al vacancy. Furthermore, since the defects result in small trigonal distortions of the cubic unit cell decreasing with growth of number of atoms, the use of larger QM systems may be required. The experimental data was obtained from polycrystalline samples, and single crystal experimental data will shed light on the validity of these values.

Table 1. AlON elastic constants.

	QM	MD	Experiment
C_{11}	296-306	367-394	-
C_{12}	151-158	224-228	-
C_{44}	164-183	242-262	-
E_v	315-341	430-467	307-320
G_v	127-139	173-190	123-128
K_v	199-207	273-283	206-214

Single Crystal Dynamics

A continuum mechanics model for behavior of AlON single crystals has been developed. The next sections summarize model features and results. A more complete description is forthcoming [17].

Material Model

The structure of AlON is presumed spinel, with cubic symmetry. Deformation gradient \mathbf{F} is

$$\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X} = \mathbf{F}^E \mathbf{F}^P, \quad (2)$$

where \mathbf{F}^E accounts for thermoelastic deformation and \mathbf{F}^P accounts for slip and twinning. Specifically,

$$\dot{\mathbf{F}}^P \mathbf{F}^{P-1} = \sum_i \dot{\gamma}^i \mathbf{s}^i \otimes \mathbf{m}^i + \sum_j \dot{f}^j \gamma_T \mathbf{s}^j \otimes \mathbf{m}^j, \quad (3)$$

with $\dot{\gamma}^i$ the slip rate on system i , f^j the volume fraction of a material element that has undergone twinning on system j , \mathbf{s} the slip or twinning direction, and \mathbf{m} the unit normal to the plane of slip or twinning. For spinel, twinning shear $\gamma_T = 2^{-1/2}$. Slip and twin systems [18,19] are shown in Fig. 10.

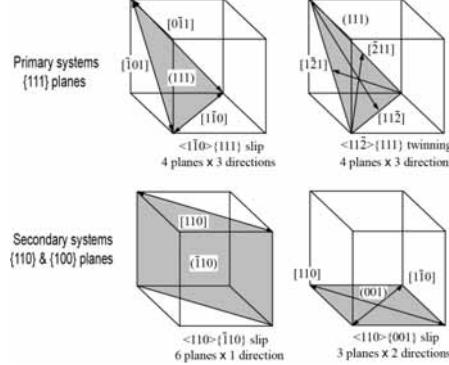


Fig. 10. Slip and twin systems in spinel ceramic crystals.

Nonlinear thermoelasticity of single crystals with defects is addressed. Helmholtz free energy density Ψ is

$$\Psi = \Psi(\mathbf{E}^E, \theta, \rho_{\perp}, \eta_T), \quad (4)$$

with $\mathbf{E}^E = (\mathbf{F}^{ET} \mathbf{F}^E - \mathbf{I})/2$ elastic strain, θ temperature, ρ_{\perp} dislocation density, and η_T twin boundary density. The explicit form of (4) includes anisotropic nonlinear thermoelasticity, dislocation line energy, and stacking fault/twin boundary energy [20]. Kinetic equations dictate slip rates and rates of twin volumes. Resistance to slip or twinning increases with shearing rate and dislocation density. Strength varies with temperature or pressure in proportion to the elastic shear modulus.

Model Calculations

Thermomechanical responses of AlON single crystals and polycrystals subject to homogeneous field \mathbf{F} are studied. Loading pertinent to plate impact is considered: adiabatic uniaxial strain at a high rate ($10^5/\text{s}$). In Fig. 11, predicted axial stress σ (normalized by isentropic bulk modulus $K_0 = 216 \text{ GPa}$) versus V/V_0 closely fits experimental data [11]. Calculations for polycrystals reported in Fig. 11 require incorporation of nonlinear elasticity, self-consistent treatment of voids, and pore collapse with pressure. Void collapse results in the kink in the stress-volume curve for $0.96 > V/V_0 > 0.91$. The model overestimates axial stress in high pressure regime $V/V_0 < 0.88$, suggesting the pressure derivative of the bulk modulus under shock compression is lower than the value used in this model [15] and/or a need for elastic constants of even higher order.

Because resistances to deformation mechanisms shown in Fig. 10 are not known a priori, several possibilities are explored: equal strengths of all systems, exclusive $\langle 110 \rangle \{111\}$ slip, preferred $\langle 110 \rangle \{110\}$ slip, and preferred $\langle 112 \rangle \{111\}$ twinning. Each is sufficient for matching experimental shear strength data [11]. Representative slip and twin resistances τ_c are listed in Table 2, accounting for rate sensitivity at loading rate $\dot{\gamma}_0 = 10^5/\text{s}$ and normalized by tangent shear modulus μ , the latter $\approx 130 \text{ GPa}$ at the HEL. Tabulated values are 1.4%-3.8% of the shear modulus, providing for post-HEL polycrystal shear strength $\approx 3-4 \text{ GPa}$. When extrapolated to the quasi-static limit, shear resistances are comparable to values for other spinel [19] and to Peierls stresses for full dislocations on $\{111\}$ planes. Such extrapolation may underestimate strength in the static limit because rate sensitivity tends to decrease with decreasing rate as drag mechanisms decline.

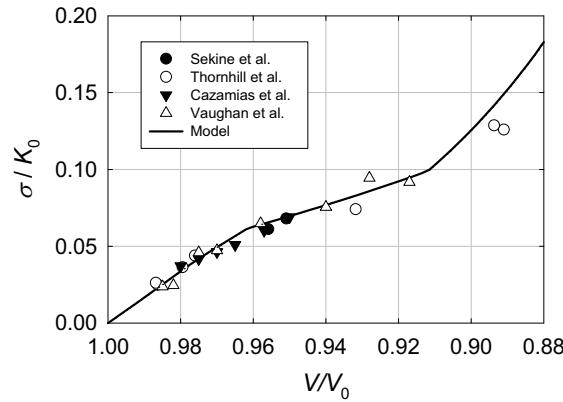


Fig. 11. Normalized axial stress in adiabatic uniaxial strain; data points for plate impact of AlON polycrystals.

Table 2. Dynamic strengths of slip and twin systems.

System	Model	Normalized shear strength τ_c / μ			
		All Equal	Exclusive $\{111\}$ slip	Preferred $\{110\}$ slip	Preferred twinning
$\{111\}$ slip		0.026	0.019	0.029	0.038
$\{110\}$ slip		0.026	∞	0.014	0.038
$\{100\}$ slip		0.026	∞	0.029	0.038
$\{111\}$ twin		0.026	∞	0.029	0.019

Calculations of thermomechanical responses of single crystals oriented for compression along [100] and [110] directions demonstrate that maximum shear stresses can vary by over a factor of two at a compressive strain corresponding to the polycrystalline HEL ($V/V_0 \approx 0.97$) depending on

lattice orientation and choice of slip/twin resistances from Table 2. Furthermore, at $V/V_0 = 0.97$, resolved shear stresses attain maximum values on the order of 25% of the theoretical strength of $\{100\}$ planes, the latter with a value of ≈ 14 GPa. Results demonstrate that AlON single crystals can be highly mechanically anisotropic as a result of slip/twin mechanisms, regardless of the degree of anisotropy of their cubic elastic coefficients. Shock experiments on Mg_2AlO_4 spinel single crystals [21] suggest that slip and twinning on close-packed $\{111\}$ planes may be preferred inelastic shearing mechanisms at high rates and large pressures. Fracture toughness for Mg_2AlO_4 spinel is lowest on $\{100\}$ planes [22], though atomic modeling [23] and experiments [24] suggest that cleavage on $\{111\}$ may be preferred. Future microscopic experiments and/or quantum or empirical molecular mechanics studies are anticipated to enable a more unique determination of strengths of possibly active slip, twin, and fracture modes in single crystals of AlON.

Mesoscale Model

The mesoscopic length scale is treated using parallel, three-dimensional finite elements with microcracks explicitly represented on the grain boundaries using cohesive interface laws allowing investigation of crack nucleation, growth, and coalescence. The basis of our model is the Lagrangian approach and finite element meshes representing computational microstructures are constructed using Voronoi tessellation and a Monte Carlo-based grain growth approach [25,26,27].

The volume-meshed microstructures consist of grains, which are treated as separate bodies in a multi-body contact/interface algorithm. Currently, only isotropic linear elasticity is being used for the bulk grain material. In the future, anisotropic linear elasticity and crystal plasticity, discussed earlier, will be used based on results of density functional theory calculations of AlON for elastic constants. Microcracks are modeled using cohesive interface laws, where a relationship exists between traction and separation of two surfaces at an interface. Numerically, the imposed stress distribution eliminates the stress singularity at the “real” crack tip by imposing tractions across a “virtual” crack tip, acting to close the crack. The imposed distribution relates the crack opening displacement and tractions and is referred to as a cohesive law. In this work a linear-decreasing cohesive law is used.

For the 50-grain simulations, specimens were loaded with a range of constant strain rates. During the initial stages of building the three-dimensional computational framework, the microstructures were loaded so that the top boundary of the mesh was moved at a constant velocity of 0.2 m/s, or $\dot{\varepsilon}_{nom} = 0.20 \text{ m/s} / 0.002 \text{ m} = 100 \text{ s}^{-1}$. Since a sudden velocity impulse is imposed on the microstructure, this corresponds to a shock loading. Other boundary conditions could be applied as needed, such as confinement loading. Fig. 12 shows the engineering stress-strain response for 50 grain loading in tension and compression. As expected, when loaded in tension the failure strength is approximately 307 MPa (a model input). In contrast, the peak compressive strength is 871 MPa at $\dot{\varepsilon}_{nom} = 100 \text{ s}^{-1}$. This is an interesting result because Paliwal et al. [28] measured 720 MPa at quasi-static loading rates ($\dot{\varepsilon}_{nom} = 10^3 \text{ s}^{-1}$).

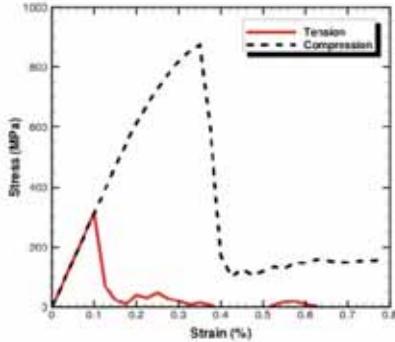


Fig. 12. 50-grain simulation in tension and compression.

Contour plots of stress in the Y-direction (loading axis) of the compression simulation at various times are shown in Fig. 13. At 27.66 μ s, stress concentrations at grain boundaries and triple junctions are pronounced until 32.45 μ s when a multiple cracks are activated and begin to open. Once cracks are activated and begin to propagate, it is not until 35 μ s, or 2.55 μ s later that the compressive peak strength is reached. It is interesting to note that at peak stress (which would occur somewhere between 34.58 and 35.64 μ s in the shown contour plots) the maximum crack density (all grain boundaries fractured) is not reached. Fig. 13(b) shows an image of the microstructure at 35.64 μ s rendered transparent to show how most of the grain boundaries are still carrying load (have high stress, colored red). This is also evident in Fig. 13(c), which shows a cross section of the microstructure also at 35.64 μ s.

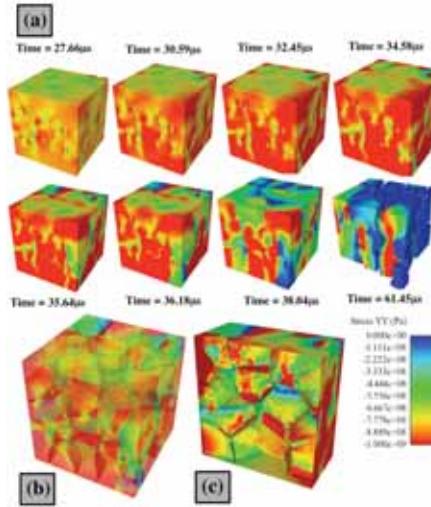


Fig. 13. Stress contour results in a 50-grain simulation.

CONCLUSIONS

This paper has provided an overview of an ongoing Army program which uses an integrated computational materials engineering (ICME) approach to model the multiscale constitutive and failure response of aluminum oxynitride. Critical for the success of this approach are experimental observations at each of the spatiotemporal scales shown in Fig. 1 that can be used for validation of the computational models developed at that scale. More specifically, interfacial grain boundary properties and estimated quasi-static strengths of slip and twin systems (Table 2),

can be quantitatively determined using FIB/SEM tests on AlON single and bi-crystals. QM and MD models were used to predict the cubic elastic constants of AlON, yet validation of these models awaits experiments on large single crystals of AlON. This work demonstrated 3-D mesoscale simulations with fracture explicitly represented using cohesive zone models; such models can be validated using CGS methods for measuring dynamic crack propagation rates and bifurcation phenomena. Although the individual models for the hierarchical multiscale model for AlON are still being combined into a coherent framework, this work established the feasibility of the multiscale ICME approach and the process for development of a virtual failure model for brittle materials (Fig. 12). Future work is aimed at development of a fully-concurrent multiscale model for brittle materials for “top-down” optimal design of armor ceramics.

Critical Gaps and Barriers

This research has identified a number of generalized gaps and barriers to the full realization of using an ICME approach for modeling materials subjected to extreme dynamic environments; these are listed below:

- A team of computational and experimental experts is needed for development and validation of multiscale material (constitutive) and failure models for *specific* materials (Fig. 1).
- Computational models should be validated using carefully controlled experiments which span the same spatiotemporal scales as the individual computational models depicted in Figure 1.
- Since the computational models at each scale (quantum to continuum) are governed by different sets of governing equations, an important challenge is to develop algorithms that will concurrently (two-way) link these sets of equations across the scales.
- Code concurrency is vital for optimal material design, particularly in those instances where local-scale, time-evolving microstructure and defects influence the global material response; here classical homogenization (hierarchical) methods are insufficient to account for the time evolution of internal boundaries.
- The evolution of new internal boundaries can occur on multiple length and time scales, and therefore a special challenge is to formulate consistent computational schemes for coarse-graining localization phenomena (e.g. fracture and flow) in a concurrent fashion.
- It is foreseen that for the near future, limitations in computational horsepower will necessitate a top-down approach for optimal material design; top-down approaches are also favored in the multi-material optimal design of structures which are subjected to dynamic loads at the global scale!

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MULTISCALE MODELING TO PREDICT PROPERTIES OF THERMOPLASTIC NANOCOMPOSITES

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Keywords: Concurrent coupling, Multiscale Modeling, Nanoclay, Polymer Matrix Composites, MD

ABSTRACT

Recent mechanical characterization experiments on thermoplastic nanocomposites have indicated significant improvements in compressive strength and shear strength in comparison with baseline thermoplastic properties. While the synergistic reinforcement of nanoparticles is evident, a simple rule-of-mixtures approach fails to quantify the dramatic increase in mechanical properties. Consequently, there is an urgent need to investigate and understand the mechanisms at the nanoscale that are responsible for such unprecedented strength improvements. It is envisioned that a better understanding of the mechanisms at the nanoscale will lead to optimization of materials processing variables at the macroscale, which, in turn, will lead to a more efficient and lower cost manufacture of nanocomposites. In this paper, an innovative and efficient method is proposed to model nano-structured components in a thermoplastic composite by employing a large-deformation hyperelastic constitutive model. Effort is directed toward finding fundamental answers to the reasons for significant changes in mechanical properties of nanoparticle-reinforced thermoplastic composites, and then using this knowledge to optimize processing variables to further improve the targeted properties of the nanocomposites. The proposed method involves a concurrent simulations approach in which the information from molecular dynamics (MD) is seamlessly exchanged with continuum mechanics based method using the embedded statistical coupling method (ESCM). Simulation results are presented, followed by a discussion of the gaps and barriers to the application of concurrent coupling in integrated computational materials engineering (ICME).

INTRODUCTION

The bottleneck for introducing new and improved polymer matrix composites (PMC) is the overwhelming amount of testing required to incorporate new materials into the Design allowable database (DAD). This extensive testing is a direct consequence of the system designer's need to address uncertainty and reduce risk; specifically, how variations in the constituent materials, the manufacturing process, and end use scenarios propagate into performance and failure of a component. The development of the DAD requires evaluation of multiple batches of composites with the associated construction of very large mechanical and other physical property databases. Also, to quantify uncertainty in the structural performance, (i) numerous subcomponents may have to be fabricated requiring expensive tooling and (ii) expensive tests must be performed on these elements to determine their long-term performance. Moreover, additional time and cost are incurred if there are any complications (which are typical) such as tooling rework, large error bands in mechanical properties, or processing complications.

In this context, ICME provides a methodology to support materials development without recourse to the expensive trial-and-error approach to materials fabrication and characterization. As described in greater detail in other chapters of this book, the key links in ICME are process-structures-properties-performance relationships. The motivation for the work presented in this chapter is that design requirements and knockdown factors are limiting our ability to exploit advanced composite and nanostructured composite materials for system-level payoffs. The challenge in achieving these goals stems from our current inability to accurately predict end-of-life properties, damage tolerance, and durability of multi-functional PMCs. A multiscale physics-based modeling approach, in which individual roles of constituent materials and their interfaces are recognized, is necessary to accurately represent the material anisotropy and damage evolution to the level of fidelity required for predicting the response of PMC structural components.

In recent years, numerous efforts have been directed toward modeling nanocomposites in order to better understand the reasons behind the improved mechanical properties, even by a slight addition (a few weight percent) of nanoparticles ([1-4], [7-13]). In studying molecular systems, however, a multiscale and multi-physics simulation approach is considered computationally more viable since relying on a single time or length scale require tremendous computational resources and can potentially lead to inaccurate results. There are two unique choices in multiscale modeling, namely, the hierarchical and concurrent simulations. In the hierarchical approach, the physical system is studied in isolation to far-field stimuli and the results are translated to a continuum response using curve fits and/or statistical averaging. Employing the hierarchical approach, Valavala et al. [1] used the energy equivalence of continuum and atomistic models of polymer systems to characterize the nonlinear stress-strain response of polymers (in particular, polycarbonate and polyimide). Burchyachenko et al. [2] used the Eshelby and Mori-Tanaka methods to determine the effective properties of nanocomposite materials. Riddick et al. [3] used equivalent modeling of carbon nanotubes (CNTs) in polymers to study the fracture toughness of PMCs with carbon nanotubes embedded in them. Awasthi et al. [4], employed MD simulations to determine the force-displacement curves between nano inclusions (CNT) and the polymer system.

In the concurrent modeling approach, several computational approaches are linked together in a combined model in which different scales of material behavior are considered concurrently and they communicate using a “handshaking” procedure. Currently, work published in the literature on concurrent coupling of polymeric systems is relatively limited. Muller [5] used a soft, coarse-grained model in the atomistic simulation and a time-dependent Ginzburg-Landau approach for the continuum description in order to study phase transformation and ordering in polymer blends. Melchionna [6] developed a concurrent multiscale technique based on MD and Lattice Boltzmann in stochastic formulations for the modeling of DNA translocation through nanopores in a biopolymer. To our best knowledge, the application of concurrent coupling to predict macroscale mechanical response for polymer nanocomposites has not been attempted.

In general, it has been observed that the strengthening behavior observed in nanocomposite materials due to nanosized inclusions can only be explained using theoretical formalisms that are based on fundamental physics of interactions at nanometer length scales. True material behavior cannot be accurately simulated through effective or “smeared” continuum analysis since these techniques, by definition, do not explicitly take into account the existence of a material interface. Consequently, the “smeared” analyses fail to capture local details, such as favorable surface energy interactions, which are responsible for the stiffness and strength improvements at the nanoscale. It is evident that the stress-strain response of the system is a function of localized mechanical behavior, and that the strength improvement is primarily due to attenuation of internal damage due to the complex interaction of voids/stress concentrators with the nanosized inclusions in the material. It is for this reason that standard continuum-based multiscale models, such as the

Mori-Tanaka method, can predict linear elastic stiffness accurately, but are unable to predict the material response of nanocomposites in the nonlinear regime (damage initiation to failure progression). However, from a design standpoint, it is imperative to be able to describe the material response from damage initiation to failure progression under all loads and ambient conditions.

Advances in computational tools have made it possible to study small scale phenomena using atomic scale classical techniques such as MD or Monte Carlo (MC) simulations, and macro-scale responses using continuum level simulations. In MD simulations, the dynamics calculations are conducted in a deterministic, time-dependent manner through numerical integration of Newton's equations of motion. In MC approach, simulations are not time-dependent but it explores the conformational phase-space of the material system by accepting or rejecting proposed configurations based on a specified algorithm [7]. In general, MC simulations are often used for polymeric systems as they permit more rapid exploration of the available conformational space due to their ability to make large changes in the structure of a complex molecule in a single step.

Figure 1 shows the length scales involved in a typical nanoparticle reinforced fiber composite. The nanoparticle (nanoclay) reinforcements are nanometer ($\sim 10^{-9}$ meters) size particles that interact with the polymer molecules to provide strengthening of the polymer matrix at the nano-scale. The size of the intercalating polymer molecules are roughly on the order of the nanoclay thickness, depending on the degree of polymerization. Moving up the length scale, carbon fiber diameter is usually on the order of 5 to 10 microns; although its length may extend up to several meters. The composite (matrix reinforced with fiber) is in the macro or engineering scale of analysis. The combination of fiber reinforcements in the polymer matrix gives the macro-scale composite orthotropic properties. The nanoscale interaction between polymer molecules and nanoclay is a key factor in determining the macro-scale strength of the composite.

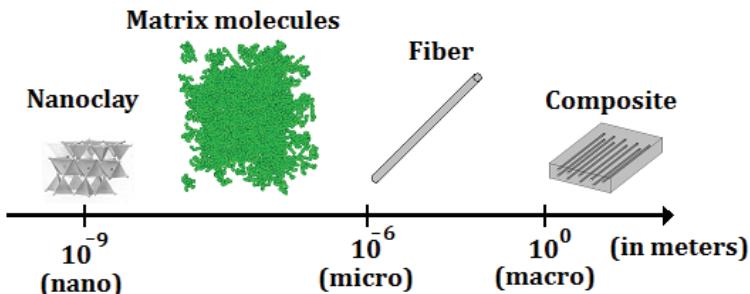


Figure 1: Length scales involved in multiscale modeling

Due to limited computer resources and the inefficiency and inaccuracy involved in using a single method to analyze large (or small) scale phenomena coupling of two (or more) methods of analysis have become common. For example, the continuum method (e.g. Finite Element Analysis (FEA)), can be used to solve the governing continuum field equations subject to given traction and displacement boundary conditions. Then apply the forces and tractions from its analysis are applied as boundary conditions to the region described by atomic interactions. By taking advantage of this synergy between these vastly different methods, we get the appropriate resolution to examine extremely localized phenomena such as crack initiation, dislocations, etc.

However, the challenge is to simultaneously process all information available from both length scales and efficiently pass this information across both time and length scales in a continuous way. Concurrent simulations have the unique advantage that it can tie local events at nanoscale to stimuli from a larger time and length scale during real time simulation. One of the earliest

forays into concurrent coupling was by Abrahams et al. [8] in their scheme, MAAD. The scheme involved simultaneous coupling of tight-binding (TB), MD and FEA. The scheme was successfully applied to study fracture behavior of silicon systems. However, the method had some shortcomings in it in that it was limited by the time-step of the tight-binding step (on the order of 10^{-15} seconds) which made the procedure computationally demanding. Ogata et al. [9] used FEA concurrently coupled with Density Function Theory (DFT) to study the surface oxidation of silicon system. Some of the more recent efforts in multiscale concurrent simulations has been the bridging-scale technique ([10-11]) and the MD-MPM (material point method) coupling technique by Ma et al. [12]. In Ref [12], the atoms within the handshake region of the MD domain are coupled point-wise to MPM particles. The continuum is hence refined down to atomic sizes and the boundary material points are assumed to overlap with boundary atoms of the MD zone at all times. The outcome of this refinement is that the MD domain induces spurious high frequency oscillations into the continuum domain as the simulation proceeds. Recently, Saether et al. [13], proposed a statistical averaging technique to overcome the high frequency vibrations, in their concurrent coupling scheme to study grain boundary structures in aluminum.

There have been many attempts to model standard solid lattice structures and to couple them to various continuum methods. But to our best knowledge, large scale concurrent coupling of nanoparticle reinforced polymer systems has not been attempted due to the complexity involved in modeling polymers. Under ambient conditions the polymer model is amorphous and lacks specific ordered structure. Further, a polymer MD model takes longer time to equilibrate as compared with an ordered lattice. In our approach, we propose to couple the Generalized Interpolation Material Point Method (GIMP, continuum scale) and MD (discrete scale) in simulating atomic interactions in polymer systems using the statistical averaging technique proposed by Saether et al. [13]. We envision that the work in this paper will contribute towards the understanding of nanoscale interactions in nanostructured composite materials.

MATERIAL POINT METHOD

The Material Point Method developed by Sulusky et al. [14], was proposed as an alternative to conventional Finite Element Method (FEM) to solve issues typically involved with large deformations (such as mesh entanglement). It belongs to a class of meshless methods originally developed as a subset of Particle-In-Cell (PIC) techniques at Los Alamos National Laboratories. In MPM, two descriptions are used to solve the problem – a collection of Material Points (Lagrangian) embedded in a stationary background (Eulerian) grid. The material points carry the information (velocity, acceleration, material property etc.) of the material that constitutes the continuum, which are then interpolated to the background grid at every time-step where the governing equations for the problem are solved in an updated-Lagrangian (UL) scheme. This solution is then extrapolated back to individual material points to simulate the macro-scale response of the body. Through this description, we have the material points “flow” over a stationary grid as time progresses, hence avoiding mesh entanglement or spurious physical behavior of the material points.

The primary advantage of MPM over FEA is that the particle state is updated through a single valued velocity field. Further, the particle character of the method ensures that the material does not penetrate into itself as time progresses. This property of the algorithm is especially useful in finite deformation simulations. A particular advantage that MPM has over other meshless methods is that the material point neighbors (i.e., the nodal points on the grid), the support for the material points on the grid are automatically determined from the interpolation function. This property is due to the compactness of the basis functions employed in MPM. Needless to say, this unique quality of MPM helps save computational time in comparison to other meshless

techniques such as the RKPM (ref [15]) where at each time-step the neighbors have to be identified through a nearest neighbor search.

Recently, Bardenhagen and Kober [16] resolved cell crossing issues in MPM using the GIMP. In GIMP, particle shape and volume are tracked during deformation. The finite size and shape of the particles enable the statistical coupling of the continuum domain to the atomistic domain as discussed in sections below.

MOLECULAR DYNAMICS

Because it is now well-established that the complex interactions at molecular level can only be understood by numerical methods which appeal to theoretical formalisms at the nano-scale, we look to use MD to analyze and understand small-scale phenomena. The ability to simulate large number of atoms (atomic systems simulated by MD are typically much larger ab-initio methods, see Khare et al. [17]) allows us to have better statistical estimates of system thermodynamic properties such as thermal conductivity and mechanical properties such as the Young's modulus. By retaining the level of detail required to describe the structure of atomic systems coupled with the selection of proper force-field parameters to accurately describe the various molecular interactions (see e.g. Allen and Tildesley [18]) we can closely simulate the necessary bulk properties of any system.

For a N atom, molecular system, we have the equation of motion of atom 'i' as,

$$m_i \ddot{\mathbf{x}}_i^t = -\frac{\partial V(\mathbf{x}_1^t, \mathbf{x}_2^t, \dots, \mathbf{x}_N^t)}{\partial \mathbf{x}_i^t} \equiv \mathbf{F}_i^t \quad (i=1,2,\dots,N) \quad (1)$$

Where m_i is the mass of the i^{th} atom, \mathbf{x}_i^t is the position of the i^{th} atom, $\ddot{\mathbf{x}}_i^t$ is the acceleration of the i^{th} atom, V is the inter-atomic potential, and \mathbf{F}_i^t is the inter-atomic force vector. In MD, the atomistic structure at initial time (\mathbf{r}_i^0) is imbedded in the algorithm with the required force fields chosen to describe the various atomic interactions. The internal force exerted on any atom i , \mathbf{F}_i is computed from the energy potential (V) chosen by the user (Eq.1). The interaction behavior is completely defined by the choice of these interaction potentials. The system is then allowed to evolve under imposed pressure, temperature and choice of boundary conditions (which is usually chosen to be periodic). Equation 1 illustrates the equation of motion for an atom 'i' in the atomistic system. As can be seen, the resulting equations of motion are non-linear, since the velocities and accelerations of the atom depend on the atomic positions of all the atoms (including itself) in the system (eq.1). A solution scheme commonly employed in predicting molecular trajectories is the Verlet integration scheme [18]. In our approach, we use the MD code Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [19] to simulate the molecular system and to ultimately couple it with our continuum (GIMP) model. The atomistic model will be simulated under free boundary conditions with constant number of particles (N) in the system. This implies that the system will exchange energy but not particles with the larger continuum scale system.

THE EMBEDDED STATISTICAL COUPLING METHOD IN GIMP

One of the most challenging issues involved in coupling the two methods (MD and GIMP) is the vastly different length as well as time scales in the two procedures. The response times for classical MD are typically on the order of 1 ps (10^{-12} sec) while conventional continuum methods are on the order of microseconds in timescale. The length-scale issues involved in coupling the two methods cannot be ignored either. While typical atomic system sizes are on the order of a few nanometers (10^{-9} m), the resolution for continuum scale only extends to a few micrometers, at the most. Hence, for seamless transition of information from the molecular domain into the continuum (or macro-scale) domain, the response from the smaller domain is time-averaged over a predetermined number of computational cycles and the time-averaged response is passed to the larger domain of computation (Saether et al. [13]).

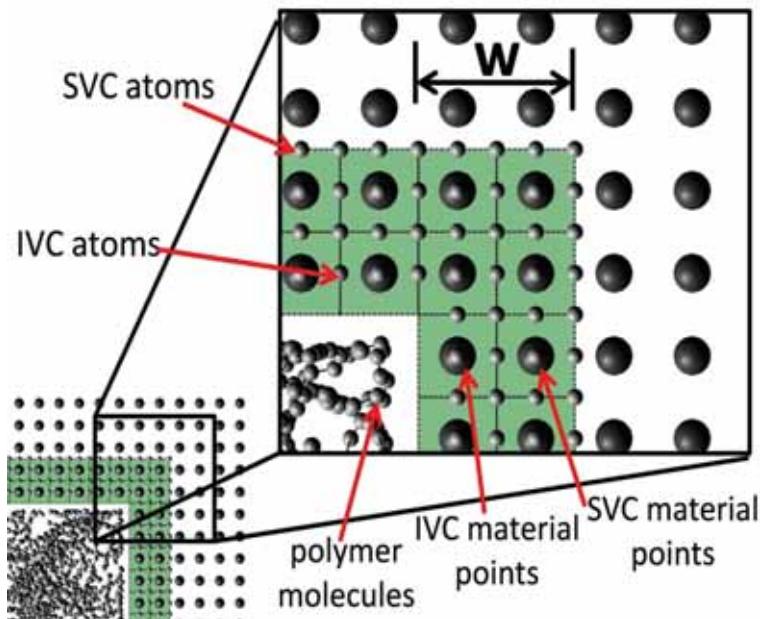


Figure 2: Spatial discretization of analysis zones: MD surrounded by an intermediate handshake region which is surrounded by a continuum region. The magnified view shows the transition region

Figure 2 shows the coupling or “hand-shake” region, where the continuum domain overlaps with the molecular region. One of the most critical problems encountered in MD/Continuum coupling, as highlighted in [8],[11]-[13], is the high frequency thermal vibrations that are transmitted out of the MD zone due to the direct coupling of atom to continuum domain and the coarse nature of the continuum mesh at the MD boundary. However, Saether et al. [13] formulated a multiscale approach that naturally smoothes out these high frequency vibrations using statistical coupling. The general idea of the coupling is to embed a localized region of molecular system within an overall continuum region. The response of the MD zone subjected to traction displacement boundary conditions will be communicated to the continuum region (or vice versa) through the interface (handshake) region (see Fig. 2). In order to achieve this, Interface Volume Cells (IVCs) are constructed around the material points that exist inside the transition zone. In Saether et al. [13] the IVCs are created using a Voronoi cell construction (e.g., O’Rourke [20]), such that the nearest atom neighbor of the transition node is a member of its IVC.

In GIMP, particle shape and volume are tracked during deformation. It follows that in a continuous deformation field the contiguous particle domains remain contiguous even after deformation. In this manner, the setup of IVCs is internal to GIMP and does not require a specialized algorithm. In the current coupling algorithm, the material point IVC is used to calculate time-averaged displacements (referred to, here on, as $\Delta\mathbf{u}_p^{IVC}$) of the atoms within each IVC. The GIMP algorithm uses this time averaged IVC deformation field to determine the internal forces on the background nodes (which is the divergence of material point stresses). Following the GIMP update, the total force on the IVC material point is equally distributed and applied as an external force on each atom within the IVC. The purpose of the Surface Volume Cells (SVC) is to prevent the atoms within IVC from becoming unstable due to internal forces from the continuum. In this manner it prevents the degradation of the outermost surface layer of the MD domain. The construction of the SVC domain is similar to that of the IVC. In the following paragraphs, the embedded statistical coupling technique is extended to GIMP (henceforth referred to as ESCM-GIMP), and presented in an algorithmic form.

Initialize discrete time-step of MD algorithm $\Delta t = \frac{\Delta T}{N}$ where, ΔT is the coarse (continuum) time-step and N is the number of MD steps for each coarse time-step. The coupling algorithm begins with the continuum update using GIMP. As mentioned, at the beginning of the GIMP time-step, we have the time-averaged IVC values at each material point. These time-averaged displacement values are updated as follows,

$$\mathbf{x}_p^T = \mathbf{x}_p^{T,old} + \Delta\mathbf{u}_p^{IVC} \quad (2)$$

Where, $\mathbf{x}_p^{T,old}$ is the position of the IVC material point at the beginning of time-step ‘T’. During the time update in GIMP, the total force on the background grid ($\mathbf{f}_i^{tot,T+\Delta T}$) is updated. Next, the update of the MD region follows the continuum update. The IVC atoms will be under the influence of the internal force on the neighboring nodes of the IVC material points, i.e. \mathbf{f}_a^{IVC} . The average external force on an atom ‘a’ in the neighbor list of the IVC material point ‘p’ is calculated as,

$$\mathbf{f}_a^{IVC} = \frac{\sum_i^{N_n} S_{ip} \mathbf{f}_i^{tot,T+\Delta T}}{N_a^{IVC}} \quad (3)$$

Where, S_{ip} is the GIMP interpolation function between IVC material point ‘p’ and node ‘i’ and N_a^{IVC} is the number of atoms in this IVC. Further, we also determine the velocities and accelerations of the SVC atoms from the updated nodal momentum and force of the background grid. As described in the previous section, a scalar function ‘V’ is chosen to simulate the energy of interaction between the atoms in the discrete MD system. For example, in a simple Leonard-Jones system, $V = \epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$ where, $r=|\mathbf{r}_{ij}|$ the distance between atoms i and j.

In this coupling scheme, the Langevin (see, e.g. [18]) technique is used to maintain the temperature of the atomic zone. As per its formulation, a damping force \mathbf{f}_a^τ is applied on the

atom ‘a’ such that the overall temperature of the system is maintained at ‘ τ ’ (temperature units). The total force on the atom in the interior zone of MD (indicated here with the superscript INT) and IVC zones are,

$$\mathbf{f}_a^{INT} = -\nabla_{\mathbf{x}'} V + \mathbf{f}_a^{\tau=\Gamma} \quad (4)$$

$$\mathbf{f}_a^{IVC} = -\nabla_{\mathbf{x}'} V + \mathbf{f}_a^{\tau=0} + \mathbf{f}_a^{IVC} \quad (5)$$

Where, $\nabla_{\mathbf{x}'}$ is the spatial (gradient) derivative along the three orthogonal space directions. In the above equations ‘ Γ ’ is the temperature of the interior atomic zone. Further, as can be seen from the above equations, the IVC atoms are maintained at zero temperature to damp out the long wavelength phonons from the interior atom zone. In order to negate the effect of short wavelength phonons, displacement averages within each IVC is calculated as follows,

$$\Delta \mathbf{u}_p^{IVC} = \frac{1}{N} \sum_{t=t_0}^{t_0+N\Delta t} \sum_{a=1}^{N_a^{IVC}} \frac{(\mathbf{x}_a^{t,IVC} - \mathbf{x}_a^{t_0,IVC})}{N_a^{IVC}} \quad (6)$$

APPLICATION OF ESCM-GIMP TO STUDY CRACK PROPAGATION

The coupling scheme for ESCM-GIMP introduced above was used to study mode I (opening mode) crack propagation in amorphous polypropylene. In this example, the internal atomic zone (i.e. amorphous polymer) is modeled using a coarse grained polypropylene structure with pair, bond order potentials etc. chosen from [21]. The continuum is simulated using a hyperelastic material model given by Valavala [1] to model thermoplastic polymer systems. The strain energy potential (W) for this system is given as,

$$W = c_1(I_3 - 1)^2 + c_2 \left(\frac{I_1}{I_3^{1/3}} + \frac{I_2^3}{I_3^2} - 30 \right) \quad (7)$$

The Cauchy stress in the body is then derived from the above potential as,

$$\boldsymbol{\sigma} = \frac{1}{J} \left\{ \left[6c_1 I_3 (I_3 - 1) - c_2 \left(\frac{I_1}{I_3^{1/3}} + 6 \frac{I_2^3}{I_3^2} \right) \right] \mathbf{I} + 2c_2 \left(\frac{1}{I_3^{1/3}} + \frac{3I_1 I_2^2}{I_3^2} \right) \mathbf{B} - 6c_2 \frac{I_2^2}{I_3^2} \mathbf{B}^2 \right\} \quad (8)$$

Where, J is the determinant of the deformation gradient \mathbf{F} (see e.g., [22]) I_1 , I_2 and I_3 are the invariants of the left Cauchy-Green tensor \mathbf{B} ($=\mathbf{F}\mathbf{F}^T$). The material constants are $c_1 = 34.3$ MPa and $c_2 = 9.59$ MPa, while the density of amorphous polypropylene is 0.85 g/cc. The simulations were carried out at $\Gamma=300$ K. Pressure barostatting was not used in these simulations.

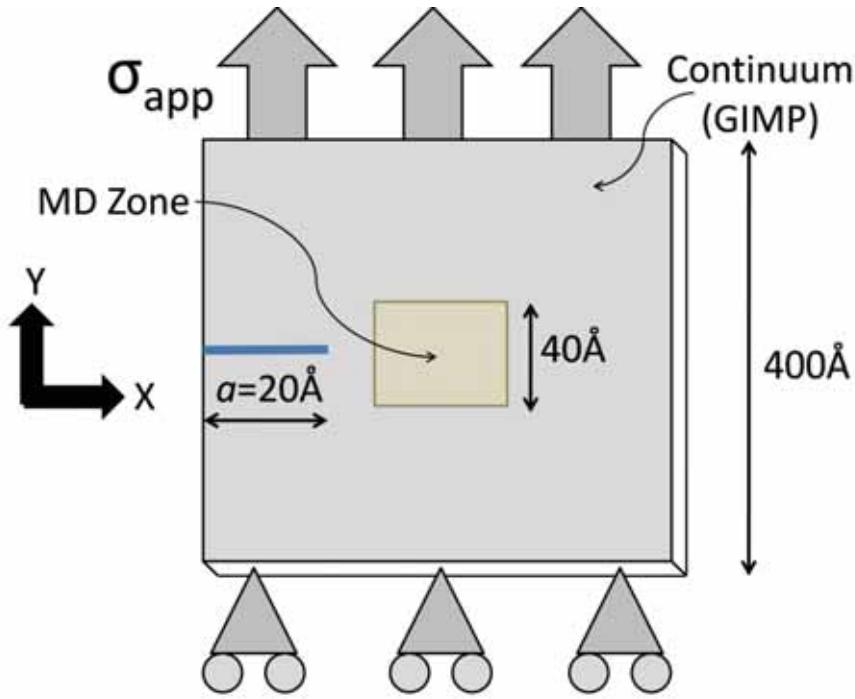


Figure 3: A schematic view of crack propagation problem

The crack propagation in the continuum region was accomplished using the Virtual Crack Closure Technique (VCCT) described in Nairn [23]. For the case of simplicity a pre-determined crack path was assigned in the problem. The VCCT was employed to determine the energy release rate at the crack tip, and crack propagation in GIMP. An arbitrary choice of $G_{lc} = 1 \times 10^{-7}$ J/m² (critical strain energy release rate) was made in order to propagate the crack. Figure 3 gives a schematic view of the MD/GIMP coupled model showing boundary conditions. For the example considered, $d_{MD} = 4$ nm. The initial length of the pre-existing crack is $a = 2$ nm. The atoms within the volume cells interact with the interior atoms through non-bonded pair potentials. The coarse time-step for the problem (ΔT) was chosen as 1.0 fs (1 fs = 10^{-15} sec). For each GIMP continuum update step, there were $N = 50$ steps of MD. Figure 4 shows the initiation and dynamic propagation of the mode-I crack in the continuum into the MD zone over a time period of 80 ps. The displacement gradient contour plot shown in Figure 4 indicates the deformation of the MD zone as the crack is propagated into the MD region. In order to show the effectiveness of the coupling scheme, in Fig. 5 the opening displacement (v) of the ESCM-GIMP material points and MD atoms are plotted along the z-axis. Note that the MD atoms show instantaneous large displacements due to atomistic thermal vibrations. The use of a suitable metric, such as the dynamic J-integral, to quantify the influence of nano-particle reinforcement on fracture toughness is described in the following paragraph.

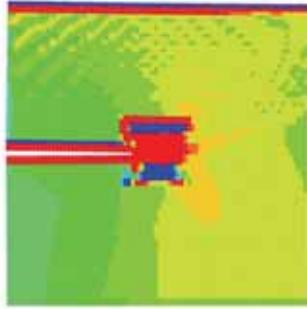


Figure 4: Displacement gradient (dv/dy) contours in coupled Polypropylene model at $T=80ps$

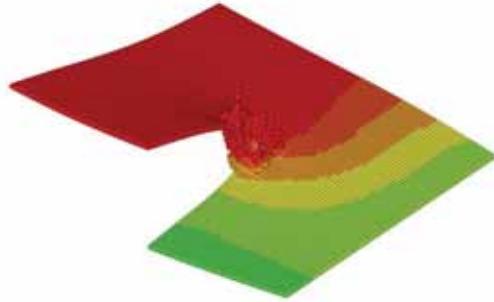


Figure 5: Vertical displacement (v) of the coupled model at $T=80ps$, with displacements plotted along the z -axis

Figure 6 shows the concurrently coupled GIMP/MD simulation of a dynamic Mode-I crack propagating from the continuum into the MD zone through the handshake region. The color contours indicate deformation gradients. While the current fracture coupling simulation was performed without an embedded nanoparticle, it is feasible to embed a nanoparticle as schematically depicted in Fig. 6. However, there is a need for quantification of the effect of the introduction of nanofillers on fracture toughness and/or energy release rate of the polymer nanocomposites. In this context, the dynamic J-integral around a contour in the continuum domain as shown in Fig. 6 may be computed using the following relation (for $m=1, 2$),

$$J_m = \int_{\Gamma} \left[(W + K)n_m - \sigma_{ij}n_j \frac{\partial u_i}{\partial x_m} \right] d\Gamma + \int_{A(\Gamma)} \left[\frac{\partial^2 u_i}{\partial t^2} \frac{\partial u_i}{\partial x_m} - \frac{\partial u_i}{\partial t} \frac{\partial^2 u_i}{\partial t \partial x_m} \right] dA \quad (9)$$

Where, indicial summation is implied on the repeated indices ‘i’ and ‘j’, σ_{ij} is the stress tensor, ρ is current mass density, n_i is the unit vector normal to the contour Γ (or Γ_ε), while $\partial u_i / \partial x_m$, $\partial u_i / \partial t$ and $\partial^2 u_i / \partial t^2$ are the displacement gradient, velocity and acceleration, respectively. W ($=\sigma_{ij}d\varepsilon_{ij}$) and K ($=\rho\dot{u}_i\dot{u}_i / 2$) are the stress-work density and kinetic energy density, respectively. For static problems, the area integral on the right hand side of eq. (9) drops out and the integral becomes path independent. This path independence is lost for dynamic problems, because the transmission of energy to different paths depends on the time stress waves reach the path, thereby necessitating the computation of the area integral [24]. It is feasible to compute the area integral over the MD domain through the use of numerical integration after smoothing of velocity and acceleration data. It is envisioned that a comparison of the values of dynamic J between the baseline polymer and the nano-filler reinforced polymer should provide a methodology to quantify the influence of nanoparticle dispersion and orientation on the fracture toughness.

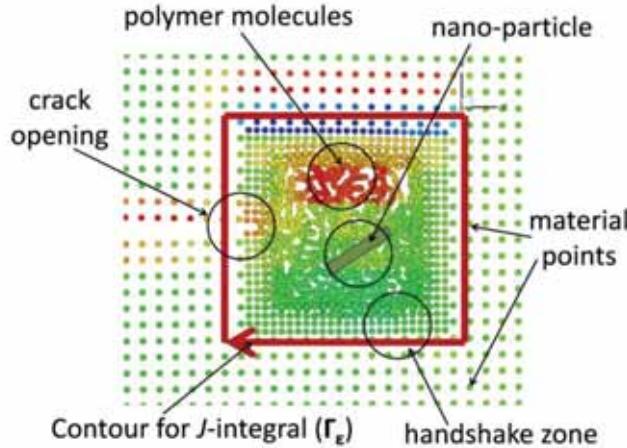


Figure 6: Concurrently coupled simulation of Mode-I crack growth in a polymer system

CURRENT GAPS AND BARRIERS

There are two main barriers that need to be overcome to fully utilize the potential of concurrent coupling within the framework of ICME. First is the scaling of the computational cost, and the second is the accuracy and reliability of the concurrent simulation in predicting material properties [7]. There are two key factors that come into play in determining the computational cost. First, the size of the time-step in MD simulations tend to be very small (~ 1 fs) in order to maintain numerical stability of the system as the equations of motion are integrated to update each atom. Secondly, a large number of time-steps must be taken to ensure that all of the statistically relevant configurations of ensemble atoms have been sampled to produce a meaningful set of ensemble averaged thermodynamic properties for a polymer system. Violation of the second factor will produce inaccurate results due to inadequate sampling of the thermodynamic phase space during the simulation. It is observed that coarse-grained atoms can help achieve larger time-steps by ignoring (or numerically freezing) the high frequency bond vibrations within the molecule during atomistic calculations. A related implication of coarse-graining is that the degrees of freedom in the system are reduced, which makes the atomistic simulation numerically faster and simpler to implement. However, a disadvantage of coarse-graining is its inability to accurately simulate chemical reactions that typically occur at the atomic scale. Accuracy and reliability of the concurrent simulation in predicting material properties depends primarily on the correctness of the potential energy function that is used to describe both the bonded and non-bonded the interactions between atoms. For polymeric systems for which the

classical form of the potential energy function is adequate, a key factor in determining accuracy is the quality of the force field parameterization, i.e., establishing numerical parameters for the various terms in potential energy function. Developing these parameters for a polymeric system is an iterative and labor intensive task, and therefore, transferability of parameters between similar molecules and atoms is frequently presumed. The robustness and applicability of these force fields have not been widely investigated. Given the current interest in research of novel materials such as polymer nanocomposites for structural and other multi-functional applications, the force-fields have to be “tuned” such that the atomistic model of the physical system strongly correlates to experimental and “real” world observations.

To summarize, the two key gaps hindering greater application of MD simulations are: (a) the difficulty in developing new force field parameters for a new polymeric system, and, (b) reliable transferability of the parameterization between chemically analogous molecules.

Methods such as parallel tempering [25] and generalized ensemble sampling [26] are currently being employed to overcome the issue of accuracy and reliability of the concurrent simulation in predicting material properties. It is envisioned that the advent of ever more powerful computer clusters will eventually address the issue of scaling of the computational cost in the not-too-distant future.

CONCLUSIONS

ICME provides a methodology to support materials development without recourse to expensive trial-and-error approaches to materials fabrication and characterization. It is envisioned that a better understanding of the mechanisms at the nanoscale will lead to optimization of material processing variables at the macroscale, which in turn will lead to the manufacture of nanocomposites in a more efficient and cost-effective way. The proposed concurrent coupling analysis will help provide insight into the nanoscale interactions that are responsible for strengthening and toughening mechanisms in thermoplastic polymer nanocomposite systems. The work presented in this paper could serve as the basis for the simulation of mechanical responses of nanoparticle-modified carbon-fiber reinforced polymer composites within the overarching framework of ICME.

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SOME KEY ISSUES IN MULTISCALE MODELING OF THERMOSET NANOCOMPOSITES/COMPOSITES

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ABSTRACT

Key issues in the development of a multiscale modeling strategy for thermoset composites and nanocomposites are addressed, with a focus on vinyl ester matrices reinforced with vapor-grown carbon nanofibers. Molecular dynamics (MD), computational micromechanics, and global finite element simulations are proposed, within an Integrated Computational Materials Engineering (ICME) framework, to determine composite material behavior from the molecular to global structural scales. Novel MD calculations were performed to assess the potential for the formation of a distinct interphase region at the pristine nanofiber/matrix interface. Based upon the calculated equilibrium redistribution of liquid resin monomers, a thin styrene-rich layer forms at the nanofiber surface that may dictate nanofiber/matrix interfacial properties after the resin is cured. An innovative crosslinking algorithm is being developed for vinyl esters that accounts for key aspects of free radical polymerization. After crosslinking, MD nanofiber pullout simulations will be performed to determine nanocomposite interphase properties and interfacial strengths for use in higher length scale models. Materials property data generated using MD simulations will feed directly into micromechanical calculations within the NASA MAC/GMC temporally concurrent, spatially sequential multiscale analysis framework. Progressive failure analyses will be performed that aim to establish structure-property relationships over a wide range of length scales, which account for the morphologies and geometries of real heterogeneous materials.

INTRODUCTION

Establishment of structure-property relationships for polymers [1], polymer composites [2], and polymer nanocomposites [3], which account for relevant irreversible processes manifested at fundamentally different spatial and temporal scales, is increasingly becoming a focal point in materials modeling and simulation efforts. Development of a coherent integrated multiscale analysis framework is crucial for determining the effect of microstructural features in polymers [4–6] and nanoscale reinforcements in polymer nanocomposites on micro-, meso-, and macroscale material behavior [7–12]. This is particularly true when describing lower length scale phenomena not amenable to direct observation or physical measurements. The efficient transfer of scale-specific model data in computations performed at successively higher or lower length scales is one key challenge in multiscale composites modeling [7]. Specification and validation of an appropriate “handshake” protocol linking calculations performed at disparate spatial or temporal scales has posed a serious obstacle in multiscale material model development for polymer nanocomposites [7]. These difficulties are mainly due to the complex nature of these materials and poor knowledge about the key mechanisms influencing the material behavior at different time and length scales. Establishment of a robust Integrated Computational Materials Engineering (ICME) framework for polymer composite design and analysis requires seamless integration between high fidelity scale-specific models.

In this work, key issues in the multiscale modeling of thermoset vinyl ester (VE) matrices reinforced with pristine vapor-grown carbon nanofibers (VGCNFs) are addressed. The issues

raised here will apply generally to thermoset nanocomposites of all types. VGCNF/VE nanocomposites are relatively low-cost material systems with promising mechanical properties for use in nano-enhanced continuous fiber structural composites [13-16]. A combination of molecular dynamics (MD) simulations, micromechanics, and hybrid finite element calculations is being used to determine nanocomposite material behavior spanning the molecular, nano-, micro-, meso-, and macroscales (Figure 1). Because of the relatively high surface-area-to-volume ratio associated with nanoreinforcements, MD simulations are being performed to investigate the formation of a distinct interphase region at the VGCNF/VE interface. Nanoreinforcements are mixed with a liquid resin and then the resin is cured to form the nanocomposite. Prior to curing, the redistribution of liquid monomers (characterized in terms of the local monomer mole ratio) can occur near the nanoreinforcement's surface, which can generate an “interphase” region [17] in the cured nanocomposite. This will be the primary focus for the MD results presented here. In the future, MD simulations will be used to generate the crosslinked resin network employing a knowledge of monomer reactivity ratios, chemical regio-selectivity, and growing radical concentrations. Then, the VGCNF/VE interphase properties and interfacial strengths will be estimated based upon VGCNF pull-out simulations. Also, the resin mechanical and dynamic mechanical properties will be calculated [18-20].

Appropriately averaged VGCNF/VE interphase properties and interfacial strengths developed using MD simulations will be employed in analytic and/or computational micromechanics models aimed at determining effective material properties of VGCNF/VE nanocomposites. A parametric study investigating the effect of interphase properties on bulk nano-phased matrix properties was previously performed by Yu et al. [21] and is briefly summarized in this work. That study accommodated both hollow and wavy nanofibers. The NASA special-purpose composite failure analysis code, MAC/GMC (Micromechanics Analysis Code with the Generalized Method of Cells) [22], is being used in conjunction with the ABAQUS [23] finite element solver to simulate progressive failure of composites at the micro-, meso-, and macroscale in a temporally concurrent, spatially sequential fashion.

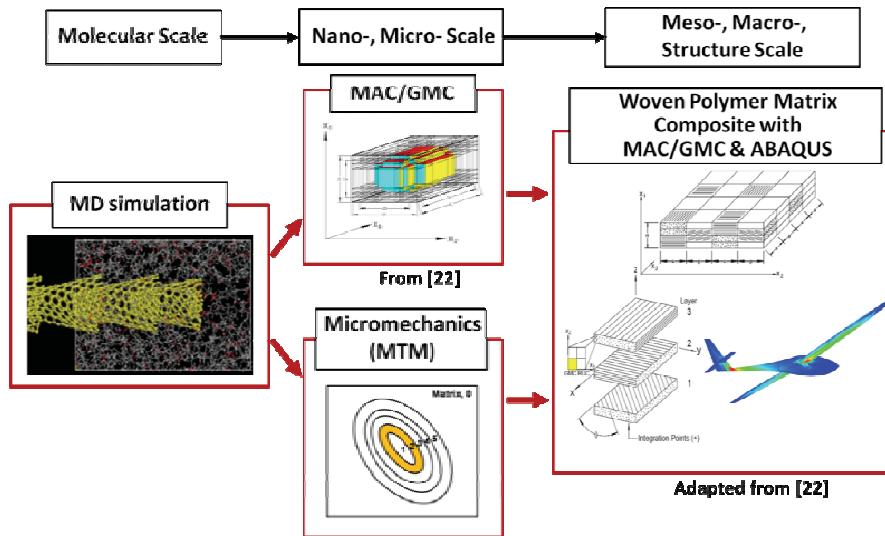


Figure 1: Multiscale modeling in composites (Adapted in part from [22])

MOLECULAR DYNAMICS SIMULATIONS OF VGCNF/VE NANOCOMPOSITES

MD simulations may be used to generate a wealth of information for use in higher length scale models. For example, polymer nanocomposite glass transition temperature [18], stress-strain responses [24], interfacial properties [25], Poisson's ratios, densities and local morphologies, all as a function of temperature or pressure [18-20], can be calculated in a representative simulation cell (computational volume) using MD simulations. One or several of these properties can be used as a direct input from the lower scale, depending on the fidelity of higher length scale models. In this study, the interphase and interfacial properties of VGCNF/VE nanocomposites will be used as input parameters for use in higher length scale computational models.

Interphase formation in polymer nanocomposites is driven by molecular interactions at the nanofiber-polymer interface. The interphase may be regarded as a distinct region with properties different from those of the bulk polymer [26]. This has been studied for thermoplastic matrices with various nanoreinforcements [27] and extensively so for continuous fiber reinforcements. Thermoplastic interphases can extend hundreds of nanometers from the reinforcement surfaces based on crystalline lamellae directional formation, but such thick interphases have not been observed for thermosets. During thermoset nanocomposite fabrication, the molecular interactions between liquid resin monomers and carbon nanofibers in the pre-curing (liquid resin) stage of nanocomposite fabrication could lead to different interfacial region monomer mole ratios versus those of the bulk resin. Rapid monomer equilibration will occur generating different mole ratios near and at the surfaces. This could lead to a different three-dimensional (3D) crosslinked network, as well as different crosslink densities and matrix microstructure in the interphase during resin curing. Therefore, gradients would be produced in the local matrix properties [28] leading to distinct interfacial properties. Given the high surface-area-to-volume ratios associated with VGCNFs, a relatively small interphase volume fraction could significantly affect bulk composite properties. Hence, knowledge of the interphase structure and properties should be considered in multiscale modeling of nanocomposites [29].

MD simulations of VGCNF/VE nanocomposites in the pre-curing stage were performed because of the inherent difficulty in experimental measurement of the interphase formation in thermoset polymer nanocomposites [30]. The liquid resin was modeled based on a commercial grade of VE resin: Derakane 441-400 (Ashland Co.). This resin is a mixture of VE dimethacrylates with an average molecular weight of 690 g/mol [31]. It has an average of 1.62 bisphenol-A groups ($n = 1.62$, where n is the number of bisphenol-A groups) in the dimethacrylate backbone [31]. A mixture of dimethacrylates with $n = 1$ (designated as VE1) and $n = 2$ (designated as VE2) yielding an average value of $n = 1.62$ was used in the simulation corresponding to a VE1/VE2 mole ratio of 37/61. VGCNFs exhibit stacked-cone (Dixie cup) or bamboo-like structures [32]. The pristine VGCNF surface was idealized using two fixed, overlapping flat graphene sheets closely resembling the region of stacked nanocones along the outer surface of the VGCNF (Figure 2). All MD simulations were performed using Materials Studio® v5.0 software [34] using a simulation cell size of $60 \times 50 \times 60 \text{ \AA}^3$ with 3D periodic boundary conditions. VE resin monomers (VE1, VE2, and styrene) were randomly packed around the graphene sheets at 300 K to yield a final simulation cell density of 1.18 g/cm^3 . The total number of monomer molecules and their weight fractions are given in Table 1.

The Condensed-Phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) force field, widely used for polymeric systems involving organic and inorganic molecules, was used in this study [35]. Geometry optimization (10,000 iterations) was carried out using the conjugate gradient method to partially relax the molecular structures [30]. The simulations of monomer equilibration consisted of several steps including the gradual increase of the simulation cell temperature to 600 K and then 1000 K, dynamics simulations at each

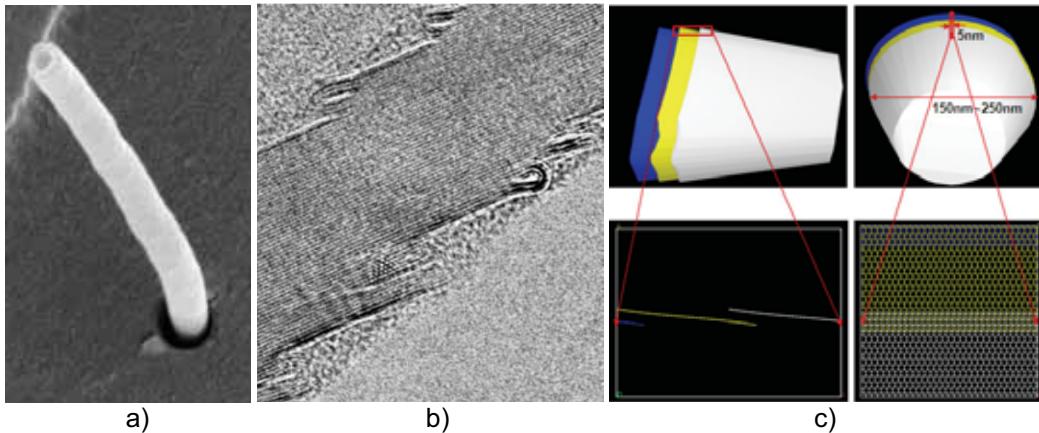


Figure 2: a) View of a single carbon nanofiber, b) cross section of the stacked nanocone structure of a VGCNF with shingled graphene sheets (adapted from [33]), and c) a schematic of overlapping graphene sheets along the outer edge of VGCNF stacked nanocones [30].

temperature, gradual cooling of the simulation cell to 300 K and running dynamics simulations for a total cumulative time of \sim 13 ns. An NVT ensemble (constant number of atoms, N; constant volume, V; and constant temperature, T) and a time step of 0.5 fs were used throughout. The MD simulations were conducted using the following protocol. (1) The temperature was increased from 10 K to 50 K and then to 600 K in increments of 50 K with 1 ps of dynamics simulation at each intermediate temperature except for 300 K, where the simulation time was 100 ps. (2) The simulation was run for a total time of 4 ns at 600 K and then the temperature was increased to 1000 K in 50 K increments (intermediate simulation times were 1 ps). (3) The MD simulation was run for a total time of 4 ns at 1000 K followed by system cooling to 300 K by two cooling procedures: 10 K (designated as C1) and 50 K (C2) decrements (intermediate simulation times were 1 ps). (4) Two separate dynamics simulations following cooling procedures C1 and C2 ran for a total time of 5 ns at 300 K. The elevated temperatures were used to speed up the equilibration process. Figure 3 shows two snapshots of the simulation: one after the geometry optimization step and the other at the end of the simulation run following the first cooling procedure C1 (total run time, \sim 13 ns). Complete wetting of the graphene surface by monomers at the end of the simulations can be seen in contrast to the initial randomly packed structure.

Table 1 Total number and weight fractions of vinyl ester resin monomers [30].

Resin monomer	Number of molecules	Mass (u)	Weight %
VE1 ¹	37	512.599	18.8
VE2 ²	61	796.954	48.2
Styrene	320	104.152	33.0

¹The dimethacrylate with $n = 1$, where n is the number of bisphenol-A groups in the dimethacrylate's backbone.

²The dimethacrylate, where $n = 2$.

Concentration profiles were generated for different monomers as a function of the y-coordinate, as defined in Figure 3 (roughly orthogonal to the graphene sheets), to analyze the distribution of liquid resin monomers at the nanofiber resin interface. The simulation volume was divided into a set of 1 Å thick sub-volumes using a series of cutting planes perpendicular to the y-axis. A set of relative monomer concentrations (for styrene, VE1, and VE2) within each subvolume was then defined using the atoms belonging to each specific monomer. The dimensionless relative concentration of a set of atoms contained in a given subvolume (belonging specifically to each of the individual monomers) is defined by the ratio of the number of atoms per unit subvolume to

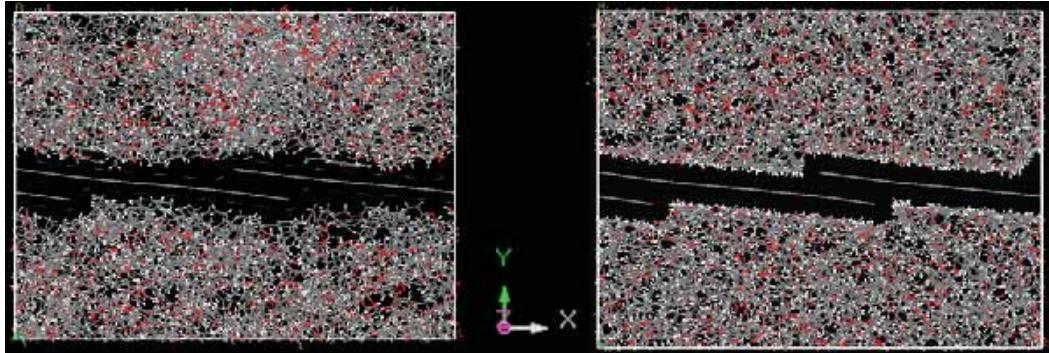


Figure 3: Snapshots of the initial frame after geometry optimization (left) and final frame after dynamics simulation for a total time of ~ 13 ns (cooling procedure C1).

the number density of atoms in the system volume [36]. The sum of all attractive and repulsive interactions of the different liquid resin monomers with the nanofiber surface and all of the monomer-monomer interactions will evolve towards a minimum system energy leading to an equilibrium arrangement of the molecules. This equilibrium determines the gradients in the final monomer distributions in the vicinity of the carbon nanofiber surface. Time-averaged concentration profiles for styrene and other monomers were used as the basis for checking the system's equilibrium status [30]. The relative concentrations were determined every 50 ps and then time-averaged over each successive 1 and 2 ns interval for the total simulation time of 4 ns performed at 1000 K. The spatial and temporal evolutions of the concentration profiles were monitored, and the profiles were compared with each other to ensure that equilibrium was reached before cooling the system to 300 K. Upon cooling, the system must re-equilibrate. The time-averaged concentration profiles for all resin monomers were determined over 5 ns at 300 K following each cooling procedure. Since the effect of cooling protocol on the equilibrium distribution of monomers at 300 K was minimal, the monomer concentration profiles obtained following cooling protocols C1 and C2 were averaged together.

The final monomer distribution represents the amount of each monomer available for free radical polymerization during the crosslinking reaction as a function of perpendicular distance from the graphene sheets. The relative concentrations were averaged over both sides of the overlapping graphene sheets to obtain a more realistic estimate of the monomer distributions roughly perpendicular to an actual carbon nanofiber surface (Figure 4a). Furthermore, the average relative concentration ratios of the monomers (i.e., styrene/VE1, styrene/VE2, styrene/(VE1+VE2), and VE1/VE2) were also calculated (Figure 4b). The average relative monomer concentration ratios versus distance from the surface show how these concentrations (ratios) deviate locally from the relative concentration in the bulk resin. For reference purposes, a relative concentration ratio of unity means that the local monomer distribution is the same as that for the bulk resin.

The styrene/VE1 relative concentration ratio starts to increase about 10 Å away from the graphene surface and reaches a peak relative concentration ratio that is 4.5 times that of the bulk value near the fiber surface. The styrene/VE2 relative concentration ratio reaches a peak of 2.5 near the fiber surface. Thus, the relative concentration ratio of styrene to the sum of both VE monomers is higher at the interface, while the VE1/VE2 ratio is a relative minimum. These simulations suggest that increased styrene accumulation will occur in an approximately 5 Å thick region adjacent to the fiber surface. If the matrix composition produced by free radical-initiated curing incorporates the monomers in their concentration ratios found in the 5-10 Å liquid region adjacent to the graphene surfaces, the cured matrix composition resulting in that region will differ substantially from that of the bulk matrix structure. A styrene-rich interphase leads to a more

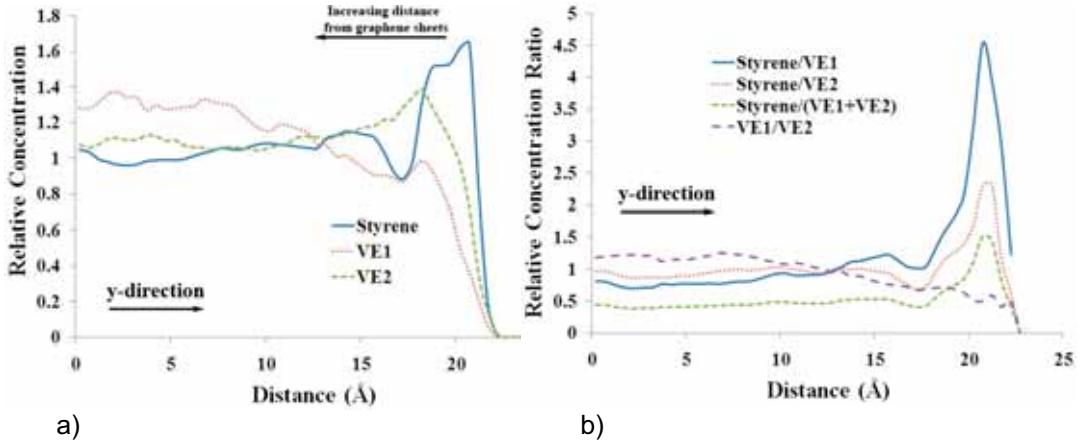


Figure 4: (a) Concentration profiles for styrene, VE1, and VE2 and (b) monomer relative concentration ratio. Simulation results were time averaged over 5 ns at 300 K and then spatially averaged over both sides of the graphene sheets [30].

compliant matrix layer, since styrene acts as a chain extender in the crosslinking reaction leading to fewer crosslink points and hence, a more flexible interphase. One substantial effect of such a thin soft interphase layer might be modified interfacial shear strength. Since styrene is strongly attracted to the graphene surface, higher interfacial shear strength may be anticipated compared to a more highly crosslinked resin region with a smaller styrene content. The simulations here were performed on a pristine VGCNF. The effect of VGCNF surface oxidation on possible nanocomposite interphase formation is also being studied.

Once the equilibrium concentrations of the liquid resin monomers are determined, the system must be crosslinked to evaluate cured nanocomposite properties. Optimal characterization of the VE curing reaction using MD simulations requires thorough understanding of the key aspects of the free radical polymerization such as regio- (head-to-tail) selectivity, determination of the appropriate reaction distances, monomer relative reactivity ratios, and growing radical site concentrations. These criteria should be integrated into an algorithm that crosslinks the system in a manner similar to the real VE resin curing process. Though several crosslinking algorithms have been proposed for epoxies [37-39], no such algorithm exists yet for VE resin that would include the real chemistry of the crosslinking reaction. A robust VE crosslinking algorithm is now under development as part of this work. Once the VE resin is crosslinked, the effective interphase, interface, and other properties of interest will be determined using MD simulations. The nanofiber/matrix interfacial shear strength will be determined at this stage using nanofiber pull-out simulations similar to those performed using carbon nanotubes [40]. MD-based estimates for nanocomposite interphase properties and interfacial strengths may be validated using novel experimental results from the literature [41,42]. Such data may be used in higher length scale calculations involving multitudes of nanofibers and other structures.

As an aside, several major factors affect the requisite simulation cell size and computational times associated with MD modeling of solid thermoplastics, thermosets, and their nanocomposites. High molecular weight thermoplastics with large entanglement densities and thermosets with extended chemical structures both require relatively large MD simulation cell sizes to properly represent the bulk polymer behavior. Macromolecular systems with slow diffusion rates may require extended equilibration times in MD calculations. In addition, real nanoinclusions are large in comparison to easily tractable simulation cell sizes. Thus, a nanofiber may be represented as

passing through the periodic MD simulation cell, which approximates an infinitely long nanofiber. Such an idealization can drastically increase computational times in comparison with simulations involving finite nanofiber lengths [18]. Moreover, huge differences in calculated elastic properties can result. Finally, optimal characterization of real polymeric and polymer composite systems, which are frequently not at full equilibrium as prepared, is a serious challenge. Such factors drive up the computational costs associated with MD modeling of polymers and polymer nanocomposites.

Despite all of these issues, with carefully designed large scale MD simulations, it is possible to predict polymer glass transition temperature, temperature dependent stress-strain curves and densities, Poisson's ratios, as well as storage and loss moduli. The effect of a variety of nanoreinforcement surface chemistries (including the number of surface-to-matrix covalent or ionic bonding sites per unit area) on interfacial shear strength can readily be probed using MD simulations.

MICRO- TO MACROSCALE SIMULATIONS OF VGCNF/VE NANOCOMPOSITES

One key challenge in predicting the effective properties of polymer nanocomposites is to account for the role of the nanofiber-matrix interphase properties and interfacial strength on bulk composite properties. While several researchers have performed novel nanofiber pull-out experiments [41, 42], interphase and interfacial properties are very difficult to experimentally measure because of the inherently small nanoreinforcement sizes. In addition, such properties may play a key role in nanocomposite failure given the relatively high surface-area-to-volume ratio associated with typical nanofibers. Hence, MD simulations may provide one means for generating nanoscale material properties and strengths for use in micromechanical material models. Of course, the nanoreinforcements should be sufficiently large so that they are amenable to a local continuum description.

A number of mean field micromechanics approaches have been developed for predicting effective heterogeneous material properties, particularly for composites containing low volume fractions of reinforcements in an elastic matrix. These include the Mori-Tanaka method (MTM) [43-44], the self-consistent method (SCM) [45], and various coated inclusion techniques [46, 47]. These approaches are based upon the classic Eshelby solution [48] for the stress and strain field due to the presence of an ellipsoidal inclusion in an infinite domain subjected to uniform far-field loading. Mean field approaches have been used to investigate the effect of solid nanofibers or nanoplatelets on bulk nanoreinforced matrix properties [49, 50], and have been modified to account for the effect of varying degrees of nanofiber waviness [50]. As part of the current study, Yu et al. [21] developed MTM and SCM models for predicting effective elastic properties for nanocomposites containing *hollow* wavy nanofibers surrounded by an arbitrary number of interphase layers. A parametric study was performed investigating the effect of hollow nanofiber wall thickness, nanofiber-matrix interphase thickness and elastic properties, and degree of nanofiber waviness on effective nanocomposite properties. The interphase modulus was expressed as a fraction of the matrix modulus (i.e., E_i/E_m) since no experimental data (or MD-based estimates of interphase properties) were available. Also, a normalized nanofiber modulus (E_F/E_m) consistent with VGCNF/VE nanocomposites was used. Figure 5a shows a plot of the effective longitudinal modulus, E_L , from [21] as a function of normalized interphase thickness (t/R) for straight hollow fibers (aspect ratio, $L/D = 100$; volume fraction, 0.63 v%) based upon the MTM. The interphase properties were varied over the range $0.5 \leq E_i/E_m \leq 20$ in order to encompass both relatively compliant and stiff interphases. A normalized nanofiber wall thickness, $R_i/R_o = 0.3$, was assumed where $R = R_o$ and R_i are the nanofiber outer and inner radii, respectively. As the average thickness (and volume fraction) of the interphase was increased, there was a significant increase in the predicted effective composite modulus. This underscores

the importance of the contribution of the interphase to overall composite properties. Similar results were obtained when calculating the effective transverse modulus [21].

The results shown in Figure 5a suggest that the use of very small amounts of VGCNFs (0.63 v%) results in a substantial improvement in the predicted effective longitudinal modulus of the nanoreinforced matrix. Improvements in experimentally measured moduli, however, typically are less profound [51]. The discrepancy between measured and predicted results may be attributed to nanofiber waviness, poor nanofiber dispersion, poor fiber-matrix adhesion, and/or the presence of nanofiber agglomerates in the actual composite specimens. Using the approach developed by Brinson and colleagues [50], Yu et al. [21] performed effective modulus calculations for composites containing solid ($R_i / R_o = 0$) and hollow ($R_i / R_o = 0.3$) nanofibers with varying degrees of fiber waviness and 0.63 v% of solid carbon. Two different fiber aspect ratios were considered ($L/D = 10, 50$). Figure 5b contains a plot of the effective nanocomposite longitudinal modulus, E_L , as a function of the nanofiber waviness ratio (h/λ) as defined in [50], where a nanofiber-matrix interphase is present ($t/R = t/R_o = 0.3$, $E_i/E_m = 10$). Note that for a given nanofiber aspect ratio, the use of *straight* hollow fibers ($h/\lambda = 0$) led to substantially higher modulus values than for straight solid fibers ($h/\lambda = 0$, $R_i/R_o = 0$) with the same volume fraction of solid carbon (0.63 v%). This issue is discussed at length in [21]. As the fiber waviness ratio

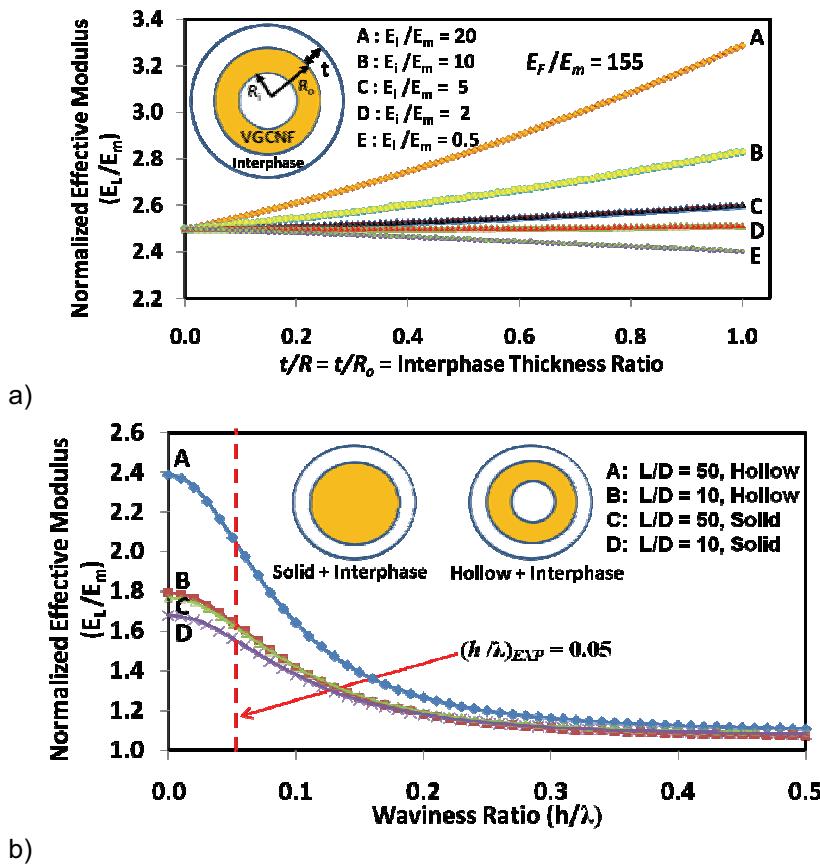


Figure 5. Effect of interphase thickness on effective longitudinal modulus for nanocomposites containing a) hollow straight nanofibers ($R_i / R_o = 0.3$, $L/D = 100$, $0.5 \leq E_i/E_m \leq 20$) and b) solid and hollow wavy nanofibers ($L/D = 10$ & 50 , $t/R = t/R_o = 0.3$, $E_i/E_m = 10$) at 0.63v% VGCNF [21].

increased to a modest level ($h/\lambda = 0.1$), the predicted modulus for all four cases decreased substantially. For higher degrees of fiber waviness ($h/\lambda > 0.3$), the nanofibers ceased to make a significant contribution to the effective longitudinal modulus. Figure 5b includes the experimentally determined mean fiber waviness ratio, $(h/\lambda)_{EXP} = 0.05$, obtained from transmission electron microscopy (TEM) imaging of VGCNF/VE specimens [52]. Given the two dimensional nature of the TEM images and the fact that the sections contained portions of actual nanofibers, the reported value likely represents a *lower bound* on expected h/λ values. The actual mean fiber waviness ratio may be somewhat greater than $h/\lambda = 0.05$, resulting in a significant decrease in the effective modulus in comparison with the straight nanofiber case.

Computational micromechanics techniques, however, may be used to simulate progressive failure and evolution of structure within a representative volume element (RVE) or repeating unit cell (RUC). For example, the method of cells [53,54] is an approximate analytical theory for predicting composite properties and failure based on the assumption that composites are comprised of periodic micro- or mesostructures. Subsequently, the generalized method of cells (GMC) [55-57] extended the method of cells to account for inelastic thermo-mechanical responses, variable fiber configurations, and the presence of an interphase. In the GMC, a RVE or RUC containing an arbitrary distribution of heterogeneities is discretized into a number of finite subvolumes (or cells). Continuity of displacements and tractions are imposed along subvolume boundaries as well as along the RVE (or RUC) boundary. Local evolution of structure in each cell is determined iteratively in a computationally efficient fashion, based upon the uniform prescribed RVE (or RUC) boundary conditions. Effective composite properties, which account for progressive failure within the RVE (or RUC), are obtained using standard homogenization techniques. The GMC may be used to accurately predict macroscale nonlinear composite material behavior and failure as a function of the properties, shapes, orientations, and distributions of constituents manifested at multiple lower length scales (i.e., micro- and mesoscales). In addition, the lower length scale progressive failure predicted using the GMC as a function of macroscale applied load history can be used to provide crucial information on the local internal stress and strain distributions leading to scale-specific damage mechanisms.

The GMC may be coupled with traditional macroscale continuum-based computational solid mechanics techniques to predict progressive failure of both component and global scale structures subjected to variable thermo-mechanical loadings. For example, NASA Glenn Research Center developed the special-purpose multiscale composite failure analysis software, the Micromechanics Analysis Code with the Generalized Method of Cells (MAC/GMC) [22], based upon the GMC theory. MAC/GMC may be used to perform coupled rate-dependent multiscale analyses, design/optimization, computational micromechanics analyses, and life predictions for structures made of multiphase composite materials. MAC/GMC uses a robust local-to-global iteration scheme where a hierarchy of RUCs may be used to explicitly model the composite material structure and morphology over a wide range of length scales. The code may be readily coupled with the ABAQUS [23] finite element (FE) solver. MAC/GMC [22] can be used to predict local field quantities within each RUC; homogenized material properties at the highest length scale are then calculated at each FE integration point [22]. The effect of local damage or failure at the constituent level is automatically propagated at each load or time step to the global FE scale through the change in homogenized stiffness properties. MAC/GMC is well suited to simulate polymer matrix composites containing woven fiber tows [58], unidirectional fiber tows, traditional short fibers and particulate reinforcements.

One goal of the current work is to extend MAC/GMC's temporally concurrent, spatially sequential multiscale analysis capabilities to include nanoreinforcements using the code's multi-step homogenization procedure. It is envisioned that key materials data generated using MD simulations will feed directly into nano- or microscale RUC calculations within MAC/GMC's

multiscale framework. An essential requirement is to employ an appropriate spatial and temporal averaging strategy for materials data when transitioning between scales, i.e., establish a “handshake” protocol between MD and local continuum level simulations.

CONCLUSIONS AND RECOMMENDATIONS

In this work, key issues in the development of a multiscale modeling strategy for thermoset composites and nanocomposites are addressed within an Integrated Computational Materials Engineering framework, with a focus on thermoset vinyl ester matrices reinforced with vapor-grown carbon nanofibers. Integrated molecular dynamics (MD), multiscale computational micromechanics, and global finite element simulations are proposed to determine composite material behavior from the molecular to global structural scales. Novel MD calculations were performed to assess the potential for the formation of a distinct interphase region at the nanofiber/matrix interface, which account for the complex physio-chemistry between the liquid resin and carbon nanofiber surface. In the MD simulations, the nanofiber surface was idealized using a pair of overlapping graphene sheets. Based upon the calculated equilibrium redistribution of liquid resin monomers, a thin styrene-rich layer forms at the nanofiber surface that may dictate nanofiber/matrix interfacial properties once crosslinking occurs. An innovative crosslinking algorithm is being developed for vinyl ester that accounts for regio-selectivity, monomer relative reactivity ratios, and other key aspects of free radical polymerization. After crosslinking, MD nanofiber pullout simulations will be performed to determine nanocomposite interphase properties and interfacial strengths for use in higher length scale models.

Appropriately averaged materials property data generated using MD simulations will feed directly into local continuum-based nano- or microscale calculations within the NASA MAC/GMC temporally concurrent, spatially sequential multiscale analysis framework. Progressive failure analyses will be performed that aim to establish structure-property relationships over a wide range of length scales, which account for the morphologies and geometries of real heterogeneous materials. This investigation aims to facilitate the development of engineered multiscale materials design by providing insight into relationships between nanomaterial fabrication/processing, chemical and physical characteristics, and interaction and evolution of structure across disparate spatial scales that lead to improved macroscale performance.

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A GENERALIZED FRAMEWORK FOR QUANTIFYING MATERIAL STRUCTURE-PROPERTY RELATIONSHIPS AND UNCERTAINTIES: APPLICABILITY TO ICME

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INTRODUCTION

Integrated computational materials engineering (ICME) is driven by an industrial need to reduce the time and cost required for the development and validation cycle for new materials [1],[2]. Accelerating the insertion of materials through physics-based computational models and databases that span from alloy design to material processing to material structure to part performance can have a tremendous impact on the way that materials are designed and selected for parts and structures. However, the vision of ICME does not come without many challenges and barriers [3], one of these being that there are multiple components required to fully develop an integrated physics-based analytical representation of materials. For instance, simulations and experiments over multiple length scales are required [4], as are a large amount of codes and scientists from different disciplines. While the focus of this book is on ICME, this chapter focuses on a generalized framework for quantifying material structure-property relationships and uncertainties for inclusion in ICME models that aim to design polycrystalline materials for improved functionality and performance. Here, while the focus is on interatomic potential development and grain boundary structure-property relationships, this generalized framework is also readily applicable for describing other mechanisms observed experimentally.

The multiscale modeling framework is the backbone of ICME, which incorporates information from relevant length and time scales in a hierarchical or concurrent manner to accurately represent material behavior at the structural level. For a historical review, Horstemeyer [5] outlines the various perspectives regarding multiscale materials modeling. In one example, multiscale models have been able to accurately capture mechanical behavior in single crystal aluminum [6] using computational simulations ranging from electronic structure to discrete dislocation dynamics to continuum finite element. However, in polycrystalline materials, passing grain boundary structure-property information from the nanoscale to higher-order computational models has not been adequately addressed in a multiscale framework. In the absence of constitutive relations describing nanoscale structure-property relationships, grain boundaries in finite element models are typically represented through continuity relations between elements in the two adjoining grains or simply as a different type of element. In discrete dislocation dynamics simulations, grain boundaries are typically represented as impenetrable line defects. Neither of these representations gives insight into the structure-dependent properties of grain boundaries or interfaces from the nanoscale. In order to pass information from the nanoscale scale to mesoscale, microscale and macroscale models, a generalized framework that addresses a number of questions needs to be developed. For example, what metrics or degrees of freedom are appropriate for characterizing grain boundary structure? What grain boundary characteristics need to be simulated to adequately represent the array of polycrystalline grain boundaries? What macroscale constitutive relationships are appropriate for capturing structure-property relationships for grain boundary structures? In the absence of constitutive models, what sort of information should be passed to higher scale models?

The reason that many of these questions have yet to be answered is that there is no generalized framework for linking observed mechanisms to physical properties, such as the relation between grain boundary degrees of freedom and grain boundary properties. For instance, even the Read-Shockley dislocation model for grain boundary energy breaks down for high misorientation angles. An additional complication is that the five-dimensional grain boundary space is vast and contains cusps in behavior related to certain low index boundary normal directions, low coincident site lattice boundaries, or other boundary characteristics (tilt versus twist, low angle versus high angle, *etc.*). While difficulties exist with probing grain boundary space at the nanoscale to develop an understanding of grain boundary structure-property relationships, these kinds of issues have been addressed to some extent in prior literature. This current work builds upon that literature and previous work that explored dislocation nucleation from grain boundaries to understand how grain boundary structures affect the deformation mechanisms of nanocrystalline materials [7-10].

This chapter discusses a generalized framework for addressing the aforementioned questions along with current research assessing material structure-property relationships and associated uncertainties. Figure 1 shows a schematic of the generalized framework used to quantify grain boundary structure-property relationships at the nanoscale for use in multiscale models. Much of the focus here is on nanoscale simulations, which are crucial for sampling the wide range of grain boundary degrees of freedom. There are three components that are required: interatomic potential development, grain boundary structure databases, and grain boundary property databases. This chapter is organized as follows. First, an overview of the current state of research into grain boundary structure-property relationships is presented. Then, current research at the nanoscale is presented. Last, gaps and barriers to inclusion of grain boundary structure-property relationships into ICME are discussed.

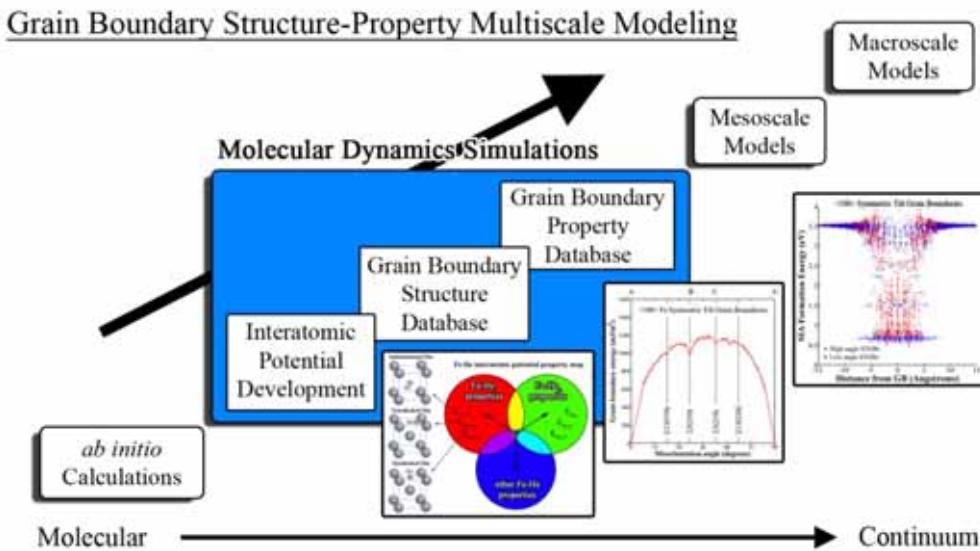


Figure 1: Schematic of models at multiple length scales for quantifying grain boundary structure-property relationships.

OVERVIEW OF THE CURRENT STATE

In this section, a brief overview of the current state is given for nanoscale calculations of grain boundary structure-property relationships. For an overview of atomistic modeling of interfaces

and their impact on microstructure and properties in a number of different areas, the reader is referred to the recent overview of Mishin *et al.* [11].

The design methodology for interatomic potentials for specific applications is still being developed. There are a number of different multi-objective optimization techniques for developing interatomic potentials, ranging from unconstrained simplex routines to genetic algorithms to constrained conjugate gradient routines. There is still some debate as to what properties constitute the best objective function for potential optimization, *e.g.*, solid-liquid properties, force-matching properties, phase stability and energies, or stacking fault energies. In many cases, the optimal potential may change depending on the weighting of each property. In addition, there is not a unified format for interatomic potential at the nanoscale.

As the applications for atomistic simulations steadily increase for particular materials systems, often a single potential fitted for a specific purpose is used for simulations outside of the intended purpose. In part, this explains why there are multiple potentials in the literature for a particular material system. Moreover, if a potential is used outside of its intended purpose, this will affect the physical mechanism studied. In many cases, a researcher is restricted to evaluating existing potentials from the literature for their specific purpose. This dilemma motivates the development of Knowledge-base of Interatomic Models¹, which will test the property predictions of an interatomic potential database to assess each potential's validity for a specific purpose. However, clearly, there is also a need for a generalized framework for developing interatomic potential design maps that addresses the aforementioned problems. This chapter will discuss some current work that explores a generalized framework for developing interatomic potential design maps, similar to Ashby property maps [12].

A cyberinfrastructure containing databases of grain boundary structures for use in assessing properties is not currently available. In many instances, a researcher has to develop the database prior to assessing grain boundary properties. These simulations can be tedious, which in part may explain the lack of studies that adequately probe a wide range of grain boundary structures to assess properties. Much of the early work of Wolf and colleagues [13-15] examining the correlation between grain boundary structure and energy has not been replicated to this extent with other properties, despite the increases in computational power over the last few decades. The closest example may be the recent work of Olmsted *et al.* [16],[17] that investigated 388 Ni grain boundaries to examine the variability in grain boundary mobility, where application of atomistic simulations is appropriate. At the scale of electrons, calculations are often limited to a single grain boundary, because of the computational demands of *ab initio* simulations. However, for many atomistic simulations, often the grain boundary property simulations are not limited by computational ability, but rather by the availability of grain boundary structures. Future work into increasing the accessibility of grain boundary structure databases for researchers to use to explore grain boundary properties may in turn impact our understanding of grain boundary structure-property relationships at the nanoscale.

CURRENT WORK IN ICME

Integrated computational materials engineering models that aim to capture the influence of material microstructure on material properties require nanoscale structure-property relationships. Nanoscale simulations are essential for modeling these structure-property relationships. The following section details current work towards developing a generalized framework to quantify material structure-property relationships, with an emphasis on grain boundaries.

¹ <http://openkim.org/>

Interatomic Potential Development

Development of empirical or semi-empirical interatomic potentials is required to accurately model structure-property relationships at the nanoscale. Here, the focus is on a generalized framework for (i) developing interatomic potential design maps, (ii) validating developed potentials for a specific purpose, and (iii) highlighting the importance of such a framework in developing structure-property relationships. Figure 2 shows a schematic that outlines some important aspects of some current work in this area.

As an initial example, an Fe-He interatomic potential with the modified embedded atom method (MEAM) [18] formulation is developed within this framework to show its profound effect. The Fe-He system is chosen because helium interactions in Fe systems play an important role in the mechanical behavior of steel alloys. In a fusion reactor environment, the fuel cladding materials are exposed to a high flux of He generated by transmutation reactions under radiation, which can lead to He bubble formation, void swelling, and subsequent material failure. Molecular dynamics simulations with various potentials have shown that He and He cluster formation affects physical properties in iron [19-23]. While recent work [24] has examined how different Fe-He potentials affect properties, there has not been a comprehensive study to examine the limits of a single interatomic potential formulation for these observed behaviors or quantify the uncertainty associated with the interatomic potential development process.

Hence, a generalized framework that addresses these issues is important. The generalized framework described herein is outlined in Figure 2(a). While this framework is initially applied to the iron-helium (Fe-He) system [25], this framework is not limited to development of Fe-He and can be extended to develop single- and multiple-element interatomic potential design maps. The difficulty of fitting many-element potentials with traditional methods may be overcome by utilizing this framework. This framework is grouped into two stages: a global approach and a local approach. The global approach is used as a coarse refinement of the interatomic potential. The local approach then constructs the interatomic potential design maps, which are used to locally optimize the interatomic potential for the design space. There are a number of steps for each stage, but for the sake of brevity we will concentrate on a few important steps herein.

Accurate development of analytical relationships are critical for probing the interatomic potential design space to produce different potentials for different purposes. The *Analytical Model Generation* step fits a higher-order polynomial regression model that provides an analytical representation of the relationship between potential parameters and He formation energies. Figure 2(b) shows the polynomial analytical surface that accurately represents the formation energies for single He that were calculated using nanoscale simulations. For instance, if the purpose is to investigate the interaction between a few He atoms and the Fe matrix, obtaining analytical models for He formation energies are important. Later, other analytical expressions can be developed for different purposes. This is illustrated in Figure 2(c), which shows an interatomic potential property map for the Fe-He system. The ideal interatomic potential should perform well in all properties. However, there are often tradeoffs in fitting the interatomic potential for specific purposes as well as the degree of accuracy for describing physical mechanisms. This demonstrates the need for a robust framework for interatomic potential development.

Interatomic Potential Development

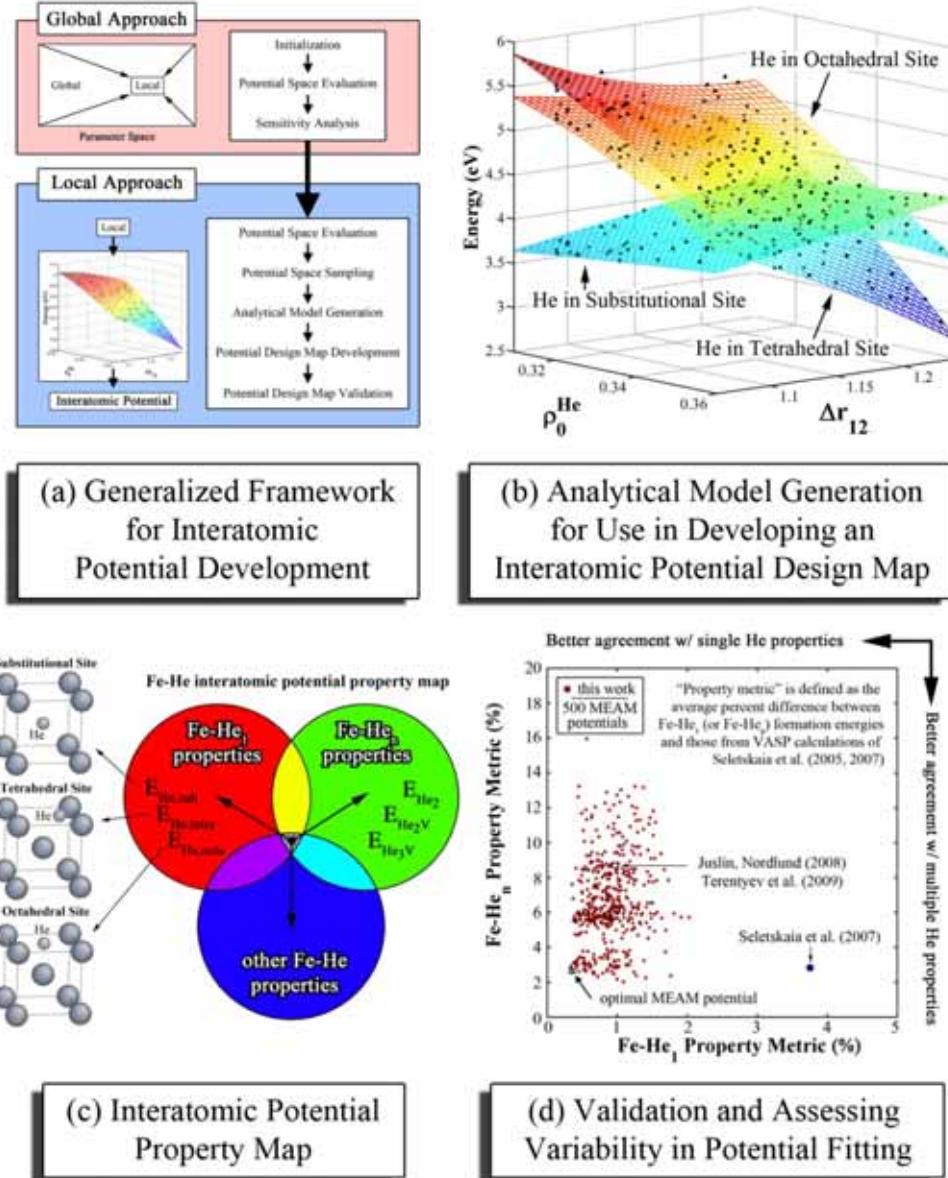


Figure 2: Development of interatomic potentials at the nanoscale.

Finally, assessing the variability due to the fitting process is shown in Fig. 2(d). This variability can be important for addressing the tradeoff in properties due to the fitting process. As an example of the potential of this framework, a $\pm 2\%$ uncertainty in the single He *ab initio* formation energies [26] was included to show the effects of formation energies on multiple He atoms in Fe lattice. Figure 2(d) shows the property metrics calculated using the developed potentials as well as property metrics calculated for some previously-developed Fe-He potentials [25]. A number of the Fe-He modified embedded atom method (MEAM) interatomic potentials

perform well when compared to previously-developed potentials. The formation energies for the optimal Fe-He MEAM potential from this study is shown as a triangle in Fig. 2(d). In these results, a $\pm 2\%$ variation in the *ab initio* formation energies caused $\pm 12\%$ differences in multiple He property metric in the optimized potentials.

Grain Boundary Structure Database

Generating a database of grain boundary structures that can be accessed to evaluate properties is also required for assessing grain boundary structure-property relationships at the nanoscale. Current research extends previously-developed methodology for generating grain boundaries to a large number of grain boundary types. Figure 3 shows a schematic that outlines some important aspects of work in this area.

First, the computational methodology used to generate a single grain boundary is discussed. In this work, a parallel molecular dynamics code, LAMMPS [27], was used to probe the nanoscale behavior and properties. For each individual grain boundary, the crystallography of the two adjoining single lattices are first determined for the bicrystal simulation cell. The use of periodic boundaries means that low index directions are preferred, since fewer atoms are required. After generating the atom positions for each lattice, an energy minimization routine is used to find the minimum energy structure at the boundary. However, previous work has shown that this configuration may not be the global minimum energy structure without trying different translations [28], atom removal techniques [29],[30], or annealing schedules [31],[32]. Previous work [28-30] has shown that the minimum energy structure for some boundaries is obtained very infrequently ($<1\%$) and this accessibility² decreases with increasing Sigma value or complexity of the boundary (*e.g.*, symmetric versus asymmetric). Therefore, it is important to sample a large number of starting configurations to obtain the minimum energy structure. The minimum energy structure is similar to the limited number of high-resolution transmission electron microscopy (HRTEM) images of grain boundary structure in the literature, *e.g.*, compare the nanoscale grain boundary structures of the 9R phase in Tschopp and McDowell [29],[7] with HRTEM images in Ernst *et al.* [33]. If a grain boundary structure is chosen at random without sampling multiple configurations, it is possible that a higher energy non-equilibrium configuration is chosen.

Second, this methodology is extended to generate grain boundaries over a wide range of grain boundary degrees of freedom. Understanding the material physics related to the grain boundary structure and how this affects the macroscopic polycrystalline material requires a representative sample of grain boundary degrees of freedom. This representative grain boundary sample may include low and high angle boundaries, symmetric and asymmetric boundaries, twist and tilt boundaries, as well as low Σ and high Σ grain boundaries. Currently, it is not clear as to how many grain boundaries or what types of grain boundaries constitutes a representative sample for grain boundary property evaluation, but the framework presented here is a methodical investigation into these types of questions. Figure 3 shows an example of how the grain boundary energy changes with respect to misorientation angle for 50 $\langle 100 \rangle$ symmetric tilt grain boundaries. The structures for the two $\Sigma 5$ grain boundaries is also shown, where the structures are viewed along the $\langle 100 \rangle$ tilt axis and the atoms on consecutive $\{200\}$ planes are shown as black and white. The structural units have been outlined for the two boundaries.

² Accessibility is defined as the percentage of the time that a particular minimum energy grain boundary structure is obtained via an energy minimization routine.

Grain Boundary Structure Database

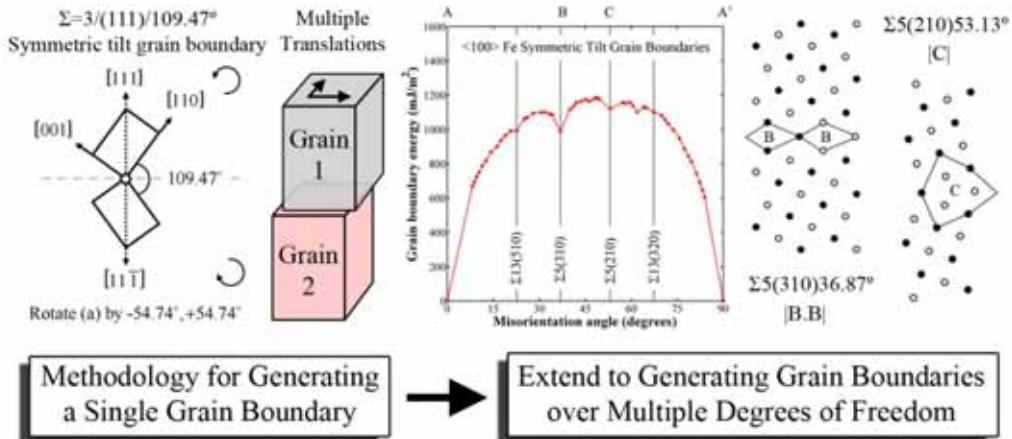


Figure 3: Generation of a grain boundary structure database at the nanoscale.

The strategy for exploring structure-property relationships using nanoscale simulations requires sampling a range of grain boundaries that is a sufficient representation of grain boundary space. Sampling too few grain boundaries or all grain boundaries of the same type may yield results or correlations that are not representative of grain boundaries in a polycrystalline material as a whole. Experimental studies that measure the five-parameter grain boundary character distribution in terms of both misorientation angle and grain boundary plane [34],[35] may provide guidance as to what the representative makeup of boundaries are in the material system of interest.

Grain Boundary Property Database

Generating a database for grain boundary properties related to structures in the grain boundary structure database is then used to quantify the nanoscale grain boundary structure-property relationships. Figure 4 shows a schematic that outlines some important aspects of work in this area [36].

First, a grain boundary property model for a single grain boundary is developed. For instance, Fig. 4(a) shows the calculation of formation energies for vacancies and self-interstitial atoms at multiple grain boundary sites for each boundary. For a single boundary, performing this calculation shows that formation energies for vacancies and interstitials are lower at the grain boundary. In fact, relative to the formation energy in the bulk (white), the interstitial formation energy is much lower than vacancies. However, in the context of all the possible grain boundary degrees of freedom present in a real polycrystalline material, these $\Sigma 5$ grain boundaries represent only a very small fraction of a representative grain boundary sample. Hence, extending these calculations over a representative sample within the grain boundary structure database gives more confidence in results and provides the distribution of properties that occurs due to variability in grain boundary structure.

Second, the grain boundary property model is applied to all grain boundaries within the grain boundary structure database. For example, in Fig. 4(b) and 4(c), we have shown a grain boundary property model for vacancy/interstitial formation being extended to 50 <100> symmetric tilt grain

boundaries. Figure 4(b) shows evolution of the self-interstitial atom (SIA) formation energy as a function of distance from the grain boundary for all 50 boundaries. This conclusively shows that the majority of formation energies within 5-8 Angstroms of the grain boundary are lower than in the bulk. Interestingly, through examining a large range of structures, it was found that the majority of interstitial formation energies near bulk values within 5 Angstroms of the boundary occur in single crystal regions between dislocations for low angle boundaries. Figure 4(c) shows that grain boundary binding energy for vacancies and self-interstitial atoms for each site for all 50 boundaries. The large amount of binding energies above the line indicates that the system energy is decreased more through interstitials occupying grain boundary sites, rather than vacancies. Hence, over a large range of grain boundary structures, this plot shows that there is an energetic driving force for interstitials to segregate to grain boundary sites over vacancies, which is important for microscale and mesoscale models that account for grain boundary interactions with point defects, *i.e.*, for the design of radiation-resistant nuclear materials.

Grain Boundary Property Database

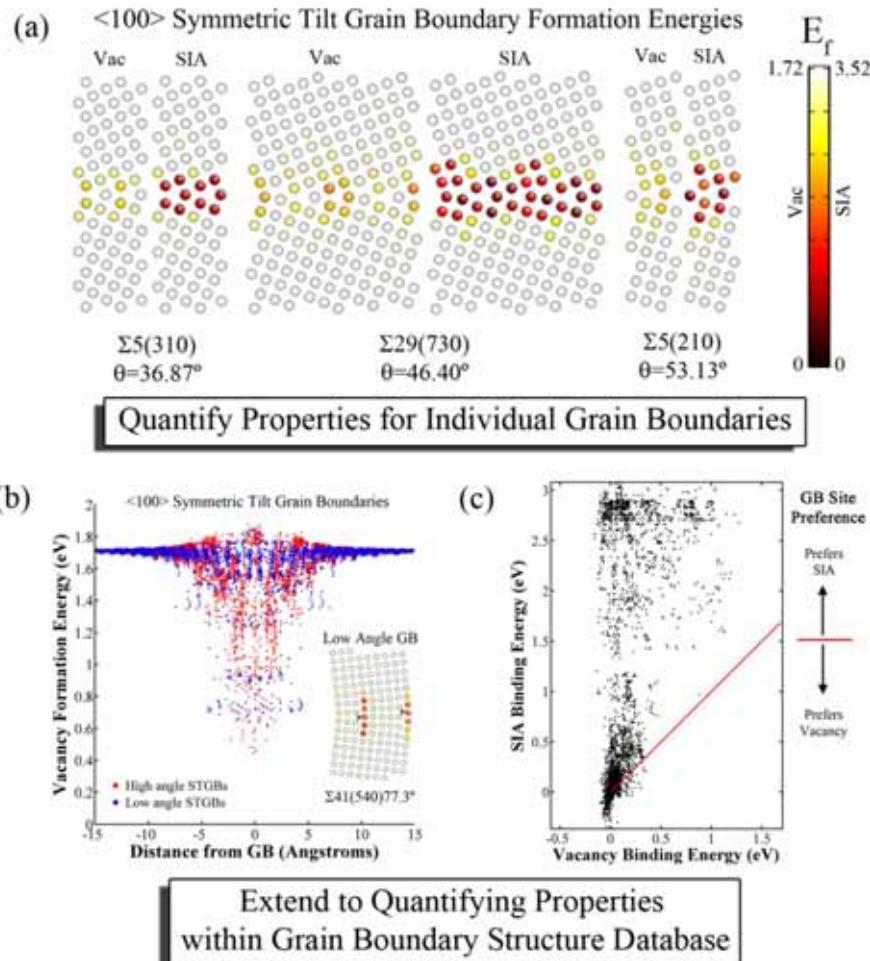


Figure 4: Generation of a grain boundary property database at the nanoscale.

GAPS AND BARRIERS

There are still a number of gaps and barriers for inclusion of grain boundary structure-property relationships into integrated computational materials engineering.

1. ***Bridge from Electronic Structures Scale to Higher Scales.*** The focus here is how information is passed from *ab initio* calculations is still an open area. This includes how to best construct interatomic potentials, as was discussed earlier. Several open questions remain. For instance, what are the best optimization techniques since there are several objectives? What are the most important properties? Do these vary with specific applications? What is the sensitivity of properties to various potential parameters? What is the best way to evaluate and validate interatomic potentials? Are there formats that better incorporate the physics from the electronics structure scale?
2. ***Bridge from Lower Scales to Macroscale Models.*** The focus here is how to pass information from nanoscale simulations to higher length scale simulations in the context of macroscale requirements. Clearly grain boundaries can affect plasticity, damage progression/fracture, and fatigue, which are then guides for lower length scale simulations. The question then is how to make the bridge between the length scales. Whether average or extreme value statistics of structures and properties are required will depend on the macroscale application. For example, stochastic averaging might be used for plasticity, but extreme structure characteristics might play a role in fatigue. A good example of using averaged quantities is that from Warner, Sansoz, and Molinari [37] who employed continuum finite element models that assigned a distribution of grain boundary properties (informed by nanoscale calculations) to examine the influence of grain size in the nanocrystalline regime. Such approaches may be adequate as a first approximation for passing grain boundary structure-property relationships into higher scale models in lieu of constitutive relations. However, can information be passed through analytical expressions, average responses with uncertainty, or distributions of structures and properties? How are mechanisms from nanoscale simulation results incorporated into the macroscale constrained equations? Are top-down approaches clearly defining the requirements for the bottom-up approaches for incorporating the relevant cause-effect relationships?
3. ***Quantifying Uncertainty in Structure-Property Relationships at the Nanoscale.*** The focus here is on how to quantify uncertainty in structure-property relationships at the nanoscale, in particular uncertainties associated with the potential fitting process, with material structure (*e.g.*, grain boundaries), and with loading and boundary conditions (*e.g.*, strain rate). Can the framework outlined in Figure 2(a) be used to propagate uncertainty from *ab initio* simulations to molecular dynamics simulations and then on to mesoscale models? What is the uncertainty in properties at the *ab initio* scale? What frameworks or techniques are available for sampling error (*e.g.*, Bayesian error estimation of interatomic potentials [38] and DFT calculations [39])?
4. ***Validation Simulations/Experiments.*** The focus here is how to validate the grain boundary structure-property relationships at the nanoscale. Validation of some mechanisms may require *in situ* HRTEM experiments or other critical small-scale experiments, which are often time-intensive, cost-intensive, and difficult to conduct. Additionally, validating the properties of individual grain boundaries provides challenges as well. On the other hand, validation simulations may be less difficult. One question might be whether validating higher-scale models that includes nanoscale grain boundary structure-property relationships constitutes validation at the lower scale.

5. **Cyberinfrastructure.** The focus here is developing the cyberinfrastructure for research pertaining to grain boundary structure-property relationships at the nanoscale. Open access to codes, input scripts, grain boundary structure/property databases and experimental data can further research to the community at-large in this critical area and help truly integrate grain boundary structure-property relationships into ICME approaches.

DISCUSSION

While this book chapter has focused on grain boundary structure-property relationships at the nanoscale as a common theme, there is nothing inherent to the concepts described herein that is specific only to grain boundaries and the examples described within. For instance, the methodology for interatomic potential design can just as easily be used to develop potentials for mechanics-related problems using stacking fault energies, Peierls' stresses, and dislocation properties rather than the interstitial He properties used here. Additionally, while grain boundaries have been the focus of the *Grain Boundary Structure Database* and *Grain Boundary Property Database* sections, this section could also have discussed sampling the cohesive strength (or other properties) from a single crystal database that contains a large number of crystallographic orientations with varying concentrations of defects or impurities. Another example might have been to discuss how grain boundary character impacts grain boundary deformation mechanisms, such as dislocation nucleation, dislocation transmission, or grain boundary sliding. The examples shown are not meant to be all-inclusive, but rather to be a concise view of the applicability of simulations at the atomistic scale in the context of ICME and multiscale modeling. Moreover, the gaps and barriers identified are not an all-inclusive list, nor does this list encapsulate the progress that has been made with respect to individual items. However, *integrated* computational materials engineering suggests that not only is progress necessary in these areas, but it is also necessary to make tackling these barriers routine such that integrating the solutions for these barriers becomes a viable option for computational materials engineering of future materials.

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MULTI-SCALE MODELING APPLIED TO NON LINEAR CONSTITUTIVE EQUATIONS

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ABSTRACT

Several multi-scale approaches have been developed at Onera in order to describe as accurately as possible the non linear behavior of materials with complex microstructures. These developments are conducted in conjunction with experimental observations that are more and more sophisticated leading to very precise information at the local scale. The interaction between the modeling and the experimental techniques facilitate the identification of material parameters.

Two main ways are proposed to perform the multi-scale analysis. The first one called “integrated approach” consists to compute the macroscopic response and the local one at the same time using an imbricated finite element scheme. The second way called “sequential approach” consists to establish macroscopic constitutive equations from a multi-scale technique generally based on a mean field approach. This way is close to a phenomenological one but is richest allowing the possibility to determine the local fields in the microstructure using post-processing tools.

INTRODUCTION

In the field of the mechanics of materials, a multi-scale approach consists to propose macroscopic constitutive equations taking into account the local behavior of each sub-phase in the Representative Volume Element (RVE) which must be adequately defined. The real difficulty is to establish a theoretical formalism linking macroscopic and microscopic scales when one or several sub-phases are nonlinear.

From the past decades a wide range of nonlinear multi-scale models have been proposed which can be classified in three main categories: mean field approaches, based on the linearization of Eshelby’s solution [1], integrated approaches computing at each time step the global equilibrium of the structure taking into account the microstructure (no macroscopic behavior is necessary [2]) and sequential approaches proposing macroscopic phenomenological constitutive equations based on a multi-scale approach performed on the discretized RVE.

Today, only few of these approaches are really able to perform, in a reasonable time, a multi-scale structure analysis helping industrial partners to manufacture and design real components. The proposed approach presented here totally fits within the scope of the Integrated Computational Materials Engineering (ICME) purpose. The goal of the model is to introduce more physics in the description of the non-linear behavior of materials taking into account the complexity of their micro-structure and to analyze the impact of some pertinent local parameters on the overall behavior. To achieve this purpose, the paper is divided in several sections described below.

Section 2 presents the theoretical framework of the approach that seems the more relevant in elasto-viscoplasticity. This approach is an improvement of the method called Transformation

Field Analysis (TFA) proposed by [3] and [4] where the RVE is decomposed in a given number of sub-phases with uniform eigenstrains inside each of them.

Section 3 presents the introduction of damage in the formalism as a new eigenstrain in order to avoid the calculation of some tensors each time the damage evolves and saving huge calculations when the number of sub-phases is important. This model was initially developed to describe the damage evolution at the interface of a fiber reinforced metal matrix composite. It is based on a cohesive zone model [5] which has been generalized to a classical continuum damage model (CDM).

The complete sequential approach in elasto-viscoplasticity coupled with damage based on the TFA formalism leading to a macroscopic model built up from this multi-scale analysis is detailed in section 4.

Finally, section 5 presents one application of the fully coupled approach proposed in the previous section to analyze the nonlinear behavior of a reinforced engine turbine disk. The structure consists of a long fiber metal matrix composite material reinforcing the circumferential direction of the turbine disk in order to be capable of withstanding the centrifugal force. This section will show that the macroscopic model obtained from the multi-scale approach completed by a new proposed post-localization technique [6] provides a set of numerical tools used to accurately predict the nonlinear behavior of complex structures avoiding heavy finite element calculations.

MICRO-MECHANICAL ANALYSIS IN ELASTO-VISCOPLASTICITY

Generally, a micromechanical model is based on relations (the localization relations) between the microscopic and macroscopic scales for the mechanical total strain or stress fields. In elasticity, such relations are bijections, both scales linked by the fourth order strain $\underline{\underline{A}}$ or stress $\underline{\underline{B}}$ localization tensor:

$$\begin{aligned}\underline{\underline{\varepsilon}} &= \underline{\underline{A}} : \underline{\underline{E}} && \text{for the strain} \\ \underline{\underline{\sigma}} &= \underline{\underline{B}} : \underline{\underline{\Sigma}} && \text{for the stress}\end{aligned}\tag{1}$$

where $\underline{\underline{\varepsilon}}$, $\underline{\underline{\sigma}}$ and $\underline{\underline{E}}$, $\underline{\underline{\Sigma}}$ are respectively the microscopic and macroscopic fields.

Tensors A and B generally depend on the geometry and on the mechanical properties of the microstructure. They are directly involved in the definition of the macroscopic stiffness (L_z^{hom}) or compliance (S_z^{hom}) from:

$$\begin{aligned}L_z^{\text{hom}} &= \left\langle L : \underline{\underline{A}} \right\rangle \\ S_z^{\text{hom}} &= \left\langle S : \underline{\underline{B}} \right\rangle\end{aligned}\tag{2}$$

Symbol $\langle \rangle$ represents the volume average over the RVE.

These localization relations are exact in elasticity with a linear relation between the macroscopic and microscopic strain or stress fields. Severe thermo-mechanical loads will induce nonlinear evolutions on the behavior of some phases constituting the microstructure of the material. These

evolutions are determined by introducing internal variables in the theoretical formalism that must be included in the localization relations with no particular rules.

Among some multi-scale approaches proposing this link between scales, it is possible to distinguish three main categories related to:

1. Pure analytical approaches, mostly based on the work performed by [7] in elasticity. Within this framework, nonlinear materials are modeled through the linearization of Eshelby's inclusion problem. This linearization can take the form of a tangent formulation [8], a secant formulation [9], an affine formulation [1, 10, 11 and 12] or with a particular interaction law as proposed recently by [13] using the regular anisotropic tangent modulus.
2. Integrated approaches, in which the final goal is to describe as close as possible the real microstructure of the RVE without macroscopic constitutive equations. This category includes the multilevel Finite Element approach, FEⁿ, where n defines the number of separated scales in the analysis [2] or the methods based on the FFT approach [14, 15 and 16]. Many other theories are proposed in the literature being able to describe at the same time the local fields and the macroscopic ones. Among them, two formulations emerge, the Non-uniform TFA (NTFA) proposed by [17 and 18] and the High Fidelity Generalized Method of Cells (HFGMC) proposed by [19].
3. Sequential approaches [20 and 21] generally performed in two steps described in detail in this paper.

TFA formalism

In the early 90', Dvorak proposed a formalism called TFA consisting in decomposing the RVE in a number of sub-phases, considering the inelastic part of the strain, ε_r^i uniform over each sub-phase. The localization relations become as follows:

$$\underline{\varepsilon}_s(y) = \underline{A}_s(y) : \underline{E} + \sum_{r=1}^N \underline{D}_{sr} : \underline{\varepsilon}_r^i \quad \text{for the strain field}$$

(2)

$$\underline{\sigma}_s(y) = \underline{B}_s(y) : \underline{\Sigma} - \sum_{r=1}^N \underline{F}_{sr} : \underline{L}_r : \underline{\varepsilon}_r^i \quad \text{for the stress field}$$

The first term in the second member of Eq. (2) is the elastic relation and the second term is the perturbation induced by the nonlinear behavior. Fourth orders tensor \underline{D}_{sr} are the strain influence tensors giving the influence of the inelastic strain $\underline{\varepsilon}_r^i$, located in the sub-phase r, on the total strain $\underline{\varepsilon}_s$ in the sub-phase s. \underline{F} are the corresponding influence stress tensors that are correlated to \underline{D} .

The number of sub-phases that defines the RVE, N, is an important parameter inducing more or less accuracy in this approach: for a RVE containing one inclusion, the minimum value for N is two, i.e. one sub-phase for the inclusion and one for the surrounding matrix.

This particular case is similar to a classical mean field approach with uniform mechanical fields inside each sub-phase. The advantage is the possibility to determine the localization and influence tensors analytically from Eshelby's formalism if the inclusion is ellipsoidal, but the

inconvenient is to deal with an overall too stiff behavior induced by the elastic accommodation. When the local RVE is decomposed in several sub-phases, tensors must be determined numerically with the same tools used in the homogenization of periodic media technique assuming periodic boundary conditions.

INTRODUCTION OF DAMAGE EFFECTS

Theoretical framework

Unlike the plastic flow, damage evolution (as well as temperature) influences material parameters, like elastic stiffness for instance, having a repercussion on the localization relations that can be rewritten as:

$$\underline{\varepsilon}_s(y) = \tilde{A}_{\tilde{s}}(y) : \underline{E} + \sum_{r=1}^N \tilde{D}_{\tilde{s}r} : \underline{\varepsilon}_r^i \quad (3)$$

where $\tilde{A}_{\tilde{s}}$ and $\tilde{D}_{\tilde{s}r}$ are the effective tensors affected by the damage (or temperature). Instead of being determined once at the beginning of the calculation, these tensors need to be evaluated each time the damage evolves in the microstructure, increasing drastically the computation time. This kind of procedure is inconceivable for a real structure analysis.

An alternative way has been developed in order to determine the localization tensor $\underline{\mathcal{A}}$ and influence tensor \underline{D} at the beginning of the computation, as in the “classical” approach, introducing all the damage effects or/and temperature effects in a generalized eigenstrain. In that case, Eq. (7) could be rewritten in the following way as proposed by [20]:

$$\underline{\varepsilon}_s = \underline{\mathcal{A}}_s : \underline{E} + \sum_{r=1}^N \underline{D}_{sr} : \underline{\varepsilon}_r^g \quad (4)$$

where thermal and damage effects are included in the term $\underline{\varepsilon}_r^g$, as follows:

$$\underline{\varepsilon}_r^g = (\tilde{L}_{\tilde{r}}^{-1}(T, D, \dots) - \underline{L}_r^{-1}) : \underline{\sigma}_r + \underline{\varepsilon}_r^i \quad (5)$$

\tilde{L} and L are respectively the actual (affected by damage) and initial stiffness. In the same way, the macroscopic constitutive equation can be written introducing a generalized macroscopic eigenstrain:

$$\underline{\Sigma} = \underline{\mathcal{L}}_r : (\underline{E} - \underline{E}^g) \quad (6)$$

with the classical relations linking both scales: $\underline{E} = \langle \underline{\varepsilon} \rangle$, $\underline{\Sigma} = \langle \underline{\sigma} \rangle$ and also $\underline{E}^i = \langle \underline{B}_{\tilde{z}}^t : \underline{\varepsilon}^i \rangle$. The expression of \underline{E}^g is then given by:

$$\tilde{E}^g = \sum_{r=1}^N c_r \tilde{B}_r^T : [(\tilde{L}_r^{-1}(T, D, \dots) - \tilde{L}_r^{-1}) : \sigma_r + \varepsilon_r^i] \quad (7)$$

where σ_r can be replaced by the equivalent expression of Eq. (2) for the stress.

Working with Eq. (5) to (7) gives expressions of the macroscopic plastic strain and the influence of damage and thermal properties on the macroscopic stiffness, for example:

$$\tilde{E}^P = \sum_{r=1}^N c_r \tilde{B}_r^t : \left\{ \varepsilon_r^P - \left(\tilde{L}_r^{-1} - L_r^{-1} \right) : \sum_{k=1}^N \sum_{s=1}^N H_{sr}^{-1} : F_{sk} : \tilde{L}_k : \varepsilon_k^P \right\} \quad (8)$$

where the fourth rank tensor H has the form: $H_{sr} = [I_{sr} + F_{sr} : L_r : (\tilde{L}_r^{-1} - L_r^{-1})]$.

The macroscopic model can be solved as a classical viscoplastic one with a large number of internal variables if the number N of sub-phases is important. However, if the number of sub-phases reduces to only two, analytical expressions can be derived from the above relations, leading to a purely macroscopic model build up from micromechanics as it will be shown in the next section.

Application to a Metal Matrix Composite

This model has been applied to simulate the nonlinear behavior of a unidirectional metal matrix composite introduced in several aeronautical applications. More precisely, the titanium (Ti6242) matrix is reinforced with long SiC fibers (SM1140+ or SCS6), in a relatively regular array presented in Fig. 4a, leading to a strongly anisotropic material. Experimental tests performed on this composite show that the longitudinal direction (i.e. fiber direction) is dominated by the viscoplastic behavior of the matrix and the transverse direction (i.e. perpendicular to the fibers direction) is dominated by both viscoplasticity and damage. Damage is directly linked to the fiber/matrix debonding process induced by the weak carbon layer surrounding the SiC fiber as shown in Fig. 1. This thin carbon layer is considered as an interphase described with a Cohesive Zone Model (CZM) in which the initial slope characterizes its undamaged stiffness.

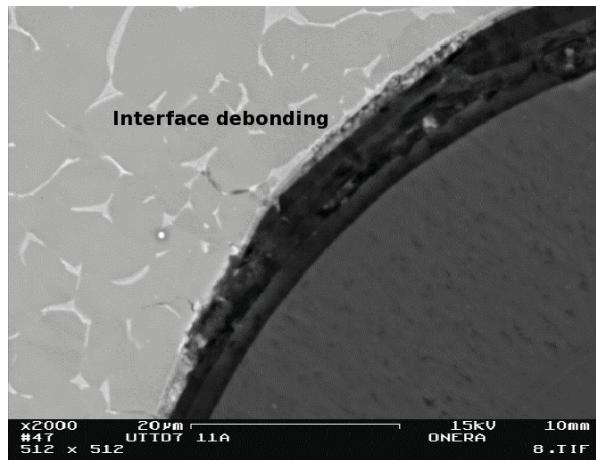


Figure 1: Micrography of the damaged interface between the titanium matrix and the SiC fiber

From this hypothesis, the damage formalism introduced in the TFA approach is based on the CZM proposed by [22] and [5] that describes the progressive debond of two surfaces for 3D problems. This local constitutive law links two initially superposed nodes of the matrix and the fiber defining two relative displacements, in the normal and tangent direction U_n and U_t , respectively, giving the evolution of a damage variable, λ , that combines tension and shear damages as follows:

$$\lambda = \sqrt{\left(\frac{U_n}{\delta_n}\right)^2 + \left(\frac{U_t}{\delta_t}\right)^2} \quad (9)$$

where adjustable parameters δ_n and δ_t represent characteristic lengths of the interface to be determined from micromechanical tests.

This damage variable varies from 0 (local safe state) to 1 (broken). A schematic evolution of the pure normal and tangential modes is represented in Fig. 2 showing the main differences between two extreme damaging conditions. For negative values of U_n , which is the case when fibers are transversely compressed by the matrix due to the residual stresses, the normal component does not induce any damage and this one is only influenced by the shear stress state. For positive values of U_n , both damages are active, increasing the evolution of the interface debonding. As it is pointed out in Fig. 2, the unloading/reloading path characterizes the irreversibility of the damaging process.

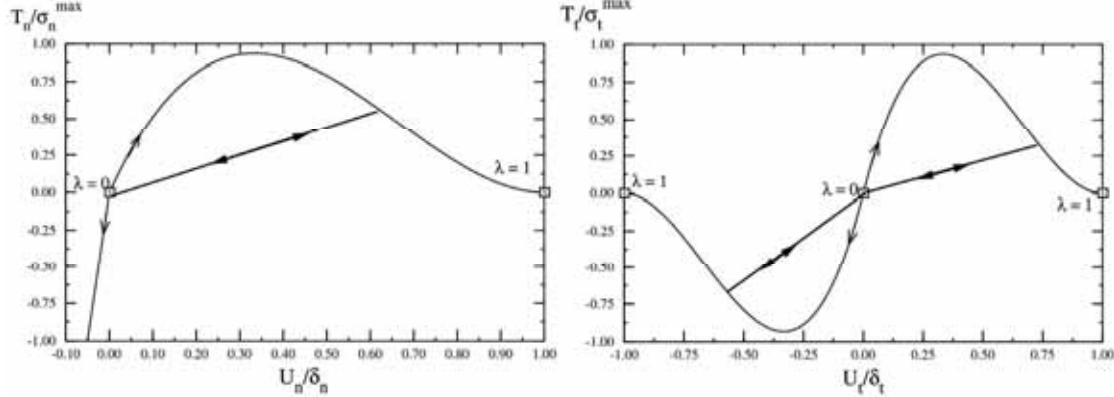


Figure 2: Schematic evolution of the normal and tangential behaviors of the cohesive zone model

When the RVE is divided in several sub-phases (more than two), the interaction between damage and constitutive equations must be introduced in sub-phases representing the interphase of the composite material, as presented in Fig. 3. Inside each sub-phase s , a scalar damage d_s is defined in the local space coordinates defining the local normal and tangential axes (see Fig. 3).

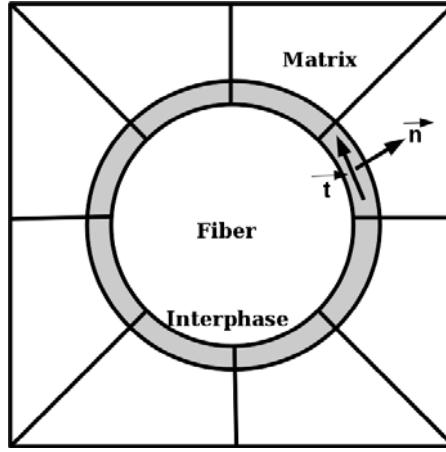


Figure 3: Sub-phases decomposition of the unit cell for the introduction of the interphase damage

SPECIAL CASE OF TWO SUB-PHASES

Elasto-viscoplasticity

If the analysis is performed with a two-phase unit cell, i.e. a cylindrical inclusion embedded in an infinite matrix, the macroscopic behavior is stiffer than the reference one obtained with a fine discretization of the RVE, as shown in Fig. 5. However, in order to avoid this problem and make a profit of this infinitely costless calculation, it is possible to introduce a correction term in the formalism. The correction proposed by [23] consists to overcome the fact that, influence tensors being averaged over the two sub-phases, the plastic gradients are underestimated. In this way, a fourth rank tensor which depends directly on the matrix properties is introduced in the strain localization relation as follows:

$$\underline{\varepsilon}_s(y) = \underline{A}_s(y) : \underline{E} + \sum_{r=1}^2 \underline{D}_{sr} : \underline{K}_r : \underline{\varepsilon}_r^p \quad (10)$$

The expression of the correction fourth rank tensor $\underline{\underline{K}}$ is determined combining Eq. (10), written for the matrix phase, with the asymptotic regime in which all the hardenings are saturated.

$$\underline{\underline{K}}_m = (\underline{\underline{I}} - \underline{\underline{L}}_m^{-1} : \underline{\underline{L}}_f) : (\underline{\underline{I}} - \underline{\underline{A}}_m)^{-1} : (\underline{\underline{A}}_m \underline{\underline{A}}_m^{-1} - \underline{\underline{I}}) : (\underline{\underline{I}} - \underline{\underline{L}}_m^{-1} : \underline{\underline{L}}_m)^{-1} \quad (11)$$

where $\underline{\underline{L}}_m$ is the matrix tangent operator and $\underline{\underline{A}}_m$ is the tangent asymptotic localization tensor.

This expression of the correction term does not introduce any new material parameter in the formalism.

The following application has been performed to illustrate and compare the results obtained with the sequential approach and the integrated one using the TFA technique. A unit cell representative of a periodic pattern of a long fiber reinforced matrix is loaded in the transverse direction (i.e. perpendicular to the fiber). Fig. 4a presents a micrography of a section of the

composite and Fig. 4b shows the geometry and the boundary conditions applied to the representative unit cell.

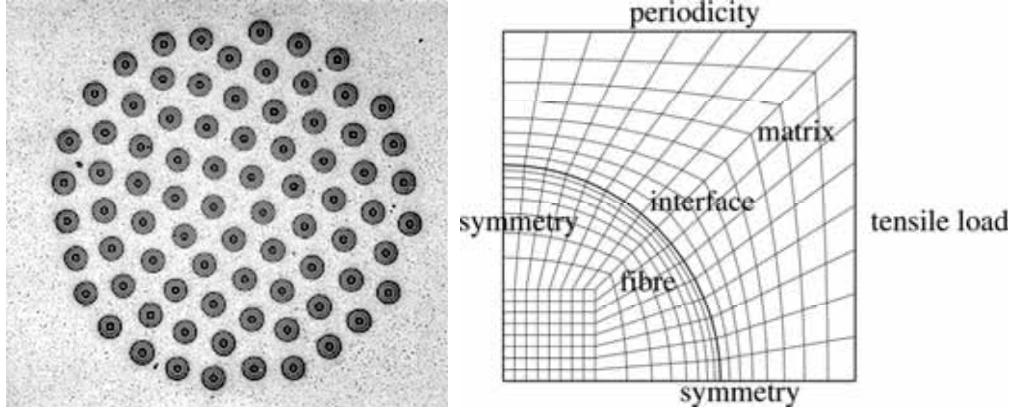


Figure 4: a) Micrograph of a section of a MMC b) Elementary cell and boundary conditions used to identify some mechanical properties

Hypotheses on the materials constitutive equations used in the numerical analysis are the following: The fiber is elastic orthotropic, the matrix is elasto-viscoplastic obeying to a Von Mises criterion:

$$\mathcal{J} = \sqrt{\frac{3}{2}(\underline{\sigma} - \underline{\chi})^t : (\underline{\sigma} - \underline{\chi})} - k$$

where $\underline{\sigma}$ is the deviatoric stress tensor, $\underline{\chi}$ a linear kinematic hardening and k the yield threshold:

$$\underline{\chi} = \frac{2}{3} C : \underline{\varepsilon}^p$$

The rate dependent inelastic behavior is described by a Norton's law.

$$\dot{p} = \left\langle \frac{\mathcal{J} - k}{K} \right\rangle^n$$

where \dot{p} is the cumulative plastic strain rate, K and n are material parameters characterizing the viscosity.

It is important to precise that material parameters, summarized on table 1, are not representative of a real material but they are used to run numerical tests and to perform comparisons between the proposed approaches.

Table 1: Material parameters of the elasto-viscoplasticity model

E (MPa)	100 000
ν	0.3
k (MPa)	600
C (MPa)	1000
K (MPa/s)	100
n	7

Fig. 5 resumes technical aspects discussed in this section, comparing macroscopic transverse tension simulations performed with the “classical” formulation and with the corrected one. As it is shown, the introduction of the correction tensor drastically improves the result, this one being very close to the reference calculation.

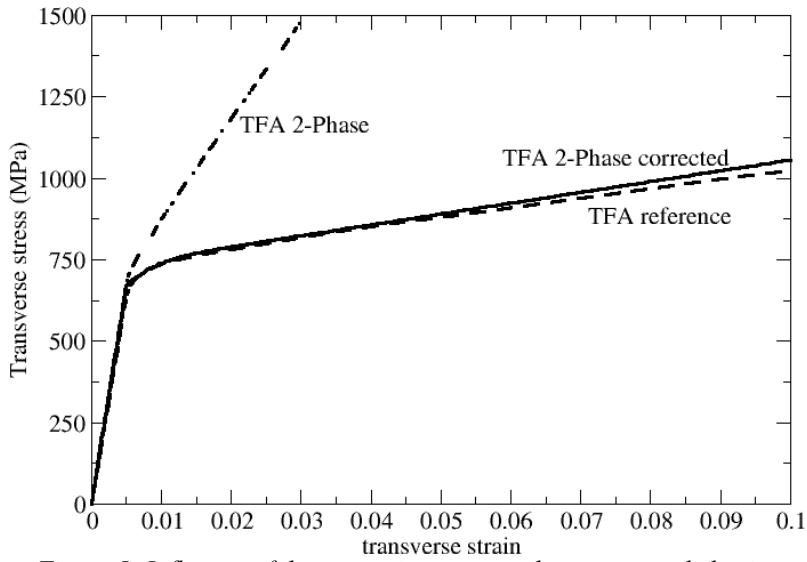


Figure 5: Influence of the correction term on the transverse behavior

Elasto-viscoplasticity and damage

In this specific geometrical configuration, authors have chosen to introduce all the damage effects in the constitutive equations of the inclusion (no viscoplastic effects are considered in the fibers avoiding to couple damage with viscoplasticity). Damage evolution is described by means of a set of scalar variables, as the one presented in the previous section, giving the possible damage activations in the plane of the fiber. The effective compliance matrix is written as follows:

$$\tilde{\tilde{S}} = \tilde{\tilde{S}}_0 + \sum_{s=1}^N d_s \tilde{\tilde{S}}_s^0 \quad (12)$$

where N is the total number of planes of normal direction \vec{n} inside the fiber able to develop damage in the normal and tangential directions. In order to reduce the number of parameters to identify, it was chosen to describe damage in only two directions:

0° , to take into account the damage induced by tensile loads and 90° to describe transverse effects like for example the cracks initiated in the loading direction during compression tests.

This fully coupled approach has been tested comparing the results with a finite element calculation performed with the same materials and on the same geometry presented in section 4.1 but a cohesive zone model is introduced at the interface between the fiber and the matrix in the mesh of the unit cell. Unlike in elasto-viscoplasticity, where the results of the model were predictions, the comparison has been used here to identify and adjust the parameters of the damage law.

The macroscopic behavior in the transverse direction is plotted in Fig. 6, which compares the proposed approach with the reference calculation obtained by FEM. As expected, results are very close but the CPU time is quite different: less than 12 seconds for the coupled TFA approach and 30 minutes for the reference Finite Element one.

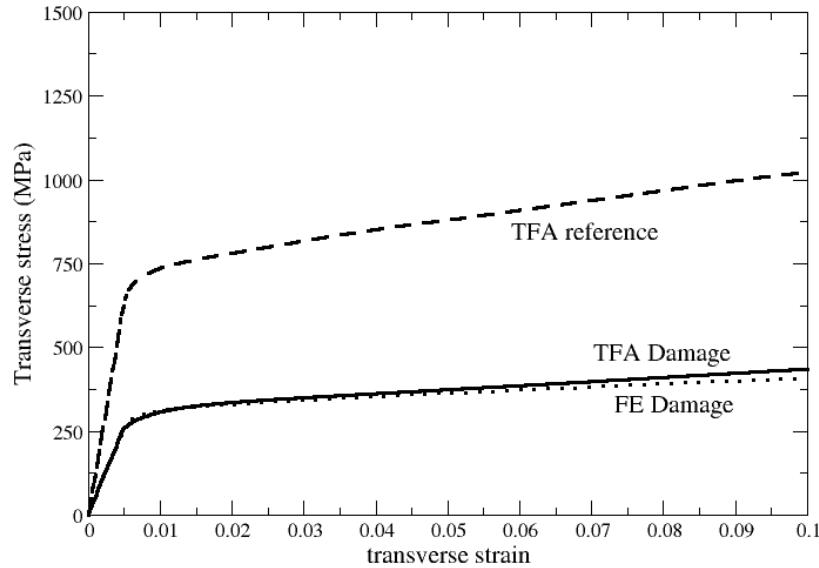


Figure 6: Comparison of the transverse behavior in viscoplasticity coupled with damage.

APPLICATION

The previous constitutive model has been applied to analyze several aerospace components like reinforced turbine disks, some parts of landing gears or low-pressure turbine shafts in order to determine the ultimate strength under cyclic or monotonic loads. Even if the geometries are very different, these structures have the particularity to be constituted with the MMC material, assuring the reinforcement, surrounded by the titanium matrix.

Fig. 7 presents a simplified geometry and the applied load of a reinforced turbine disk representative of a BLING (BLaded rING). The structure is not the geometry of a real component but it is sufficiently representative to allow performing the nonlinear analysis under a monotonic centrifugal load. As presented on figure 7, only half of the structure is meshed due to symmetry

conditions. The reinforced zone including the composite material is located in the dark zone and it is surrounded by titanium. The right zone represents the titanium turbine blade that is characterized with a particular behavior in order to take into account the fact that the blades are not continuous in the circumferential direction.

In the transverse direction, both the radial and axial stresses have relatively low values but have induced damage in the right end side and in the upper left corner of the reinforced zone as presented on figure 8 showing the contour of the damage developed in the radial direction. However, the multiaxial stress state remains dominated by the hoop stress reducing the influence of the interfacial damage.

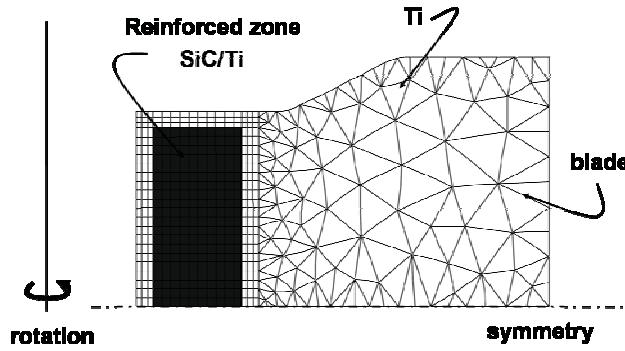


Figure 7: Geometry of the bladed disk

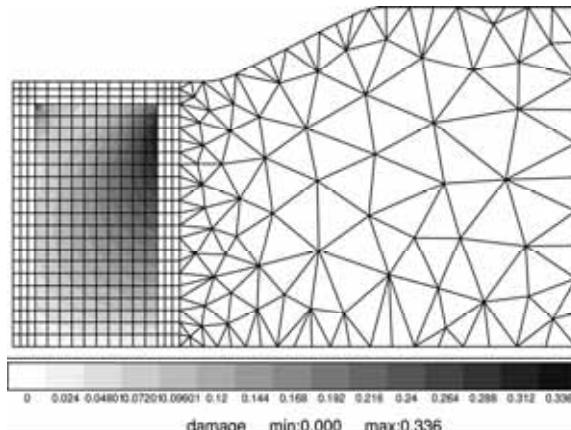


Figure 8: Contour of the damage in the radial direction

Post-localization procedure

One of the advantages of a multi-scale approach is the possibility to get at the same time the information at both microscopic and macroscopic scales using the localization relations. From the two-phase approach, as presented in the above example, only the averaged fields on each phase can be reached during the numerical analysis. However, it is possible to obtain more precise local information from a post-processing analysis. Actually, the macroscopic strain (stress) fields is used as a load input on a unit cell containing several sub-phases to determine the local fields using the appropriate constitutive equations. This post-processing analysis can be performed only in critical zones of the structure where the mechanical fields present a concentration, avoiding in this way long and costly numerical analyses. This approach, named here post-localization (but

also relocalization [6] or recovery procedure [24]), has been applied successfully to describe local fields, even when some basic assumptions of the homogenization technique are no longer verified, for example when the scales between the macroscopic and microscopic geometries are not separated (i.e. coarse grain microstructures) or in the loss of periodicity close to borders. The special procedures developed to analyze these particular situations allow to process to an extensive multi-scale analysis of complex structures with a complete set of sophisticated numerical tools.

Figure 9 presents the post-localization technique applied on a specific integration point in the reinforced material of the macroscopic structure. This figure shows the contours of the radial, axial and circumferential stresses and the differences between the averaged values and the local ones. The precision in this calculation allows to propose local criteria, like crack initiation, which can take into account overstresses underestimated otherwise.

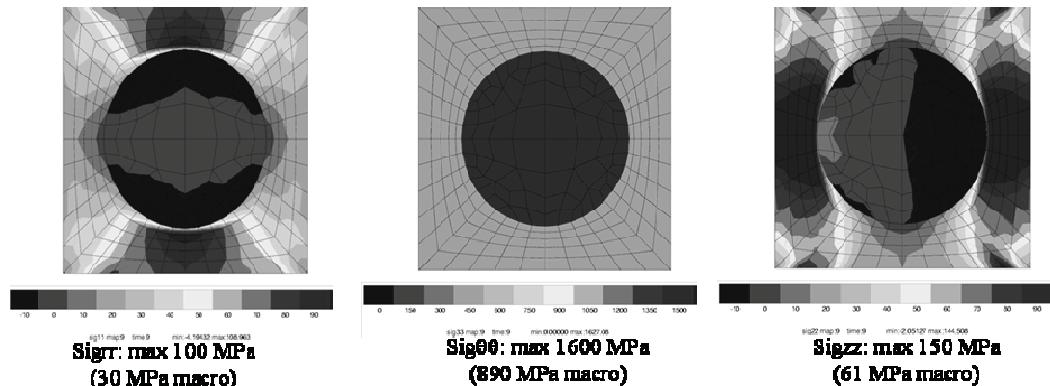


Figure 9: Contours of the radial, hoop and axial stress from the post-localization technique on a given integration point of the reinforced zone

CONCLUSION

Several multi-scale approaches have been developed at Onera for the purpose of performing the numerical analysis of aerospace components. Integrated approaches consist in solving the macroscopic problem classically with the FEM computing the global equilibrium of the structure but without using macroscopic phenomenological constitutive equations. Instead, composite material response derives from homogenization techniques performed on a periodic unit cell representative of the microstructure. Phenomenology is located at the microscopic level trying to describe as precisely as possible the behavior of the several constitutive materials. For strongly nonlinear problems, discretization of the unit cell must be very fine, for both TFA and FE2 approaches, leading to heavy computations time and memory. However, they may be considered as reference calculations and they are very useful to compare and to discriminate results from other theories. Sequential approaches consist in proposing analytical macroscopic constitutive equations which are determined from a previous multi-scale analysis. Among those, the two-phase TFA approach appears to be a clever choice. However, it has been shown that it is necessary to introduce a correction term in the proposed formalism in order to avoid the elastic accommodation problem which induces a too stiff macroscopic behavior. Results obtained on a RVE with this approach are in complete agreement with the reference ones, in elasto-viscoplasticity coupled with damage.

Using this methodology, we have shown how it is possible to achieve the same accuracy in the calculation as in the reference one and with light computation times.

Actually the phenomenology is introduced at the local scale to describe each behavior of the composite (the metallic matrix, the fibers or the interphase) using adequate experimental methods to identify material parameters. A challenge consists to find feasible solutions outside the limit of the conventional phenomenology in order to describe with more physics the origins and evolutions of local behaviors. For instance, plasticity can be described with classical crystalline models, at the scale of slip systems, or, more accurately, with the dislocation dynamics approach but in this case difficulties remain to perform a complete structure analysis linking the macroscopic scale to the local one describing the evolution of dislocations.

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A MULTISCALE, NONLINEAR, MODELING FRAMEWORK ENABLING THE DESIGN AND ANALYSIS OF COMPOSITE MATERIALS AND STRUCTURES

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Abstract

A framework for the multiscale design and analysis of composite materials and structures is presented. The ImMAC software suite, developed at NASA Glenn Research Center, embeds efficient, nonlinear micromechanics capabilities within higher scale structural analysis methods such as finite element analysis. The result is an integrated, multiscale tool that relates global loading to the constituent scale, captures nonlinearities at this scale, and homogenizes local nonlinearities to predict their effects at the structural scale. Example applications of the multiscale framework are presented for the stochastic progressive failure of a SiC/Ti composite tensile specimen and the effects of microstructural variations on the nonlinear response of woven polymer matrix composites.

Introduction

The use of advanced composites (polymer matrix composites (PMCs), ceramic matrix composites (CMCs), and metal matrix composites (MMCs)) provides benefits in the design of advanced lightweight, high temperature, structural systems by providing an increase in specific properties (e.g., strength to density ratio) when compared to their monolithic counterparts. To fully realize the benefits offered by these materials, however, experimentally validated, computationally efficient, multiscale design and analysis tools must be developed for the advanced, multiphased materials of interest. Furthermore, in order to assist both the structural analyst in designing with these materials and the materials scientist in designing/developing the materials, these tools must encompass the various levels of scale for composite analysis as illustrated in Figure 1.

These scales are the micro scale (constituent level), the meso scale (laminate/composite and/or stiffened panel level) and the macro scale (global/structure level), and they progress from left to right in Figure 1. One traverses these scales using homogenization (moves right) and localization (moves left) techniques, respectively (Figure 2 and Figure 3); where a homogenization technique provides the properties or response of a “structure” (higher level) given the properties or response of the structure’s “constituents” (lower scale). Conversely, localization techniques provide the response of the constituents given the response of the structure. Figure 3 illustrates the interaction of homogenization and localization techniques, in that during a multi-scale analysis, a particular stage in the analysis procedure can function on both levels simultaneously. For example, in Figure 3, the constituents X and Y at Level 1, when combined (homogenized) become the constituent V (on Level 2) which is subsequently combined with W to produce U (the effective structure at Level 3). The reverse process is known as localization, in which the constituent level responses (Level 1) are determined from the structure level (Level 3) results. Obviously, the ability to homogenize and localize accurately requires a sophisticated theory that relates the geometric and material characteristics of structure and constituents.

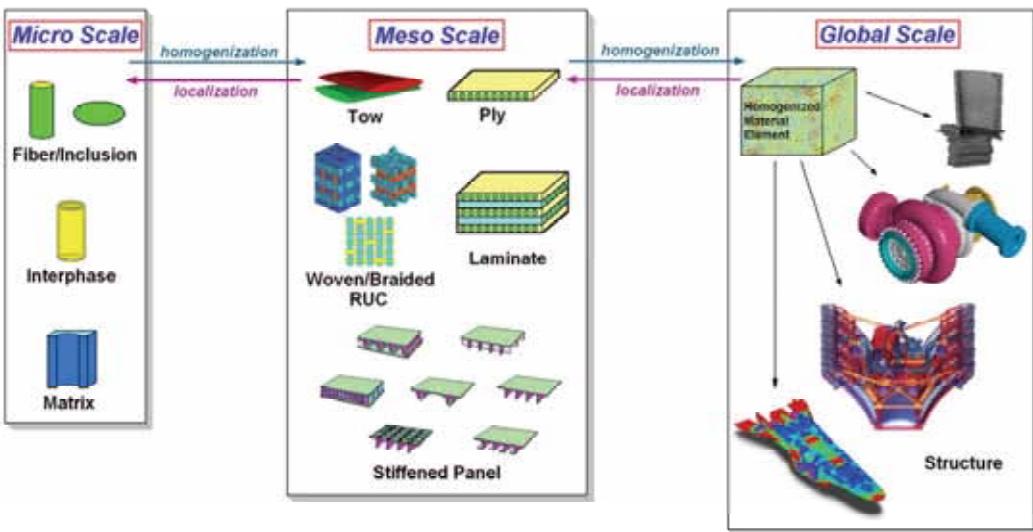


Figure 1: Illustration of associated levels of scale for multiscale composite analysis

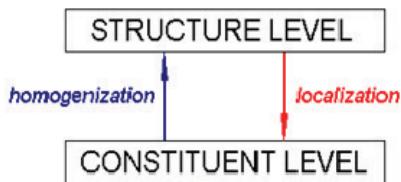


Figure 2: Homogenization provides the ability to determine structure level properties from constituent level properties while localization provides the ability to determine constituent level responses from structure level results

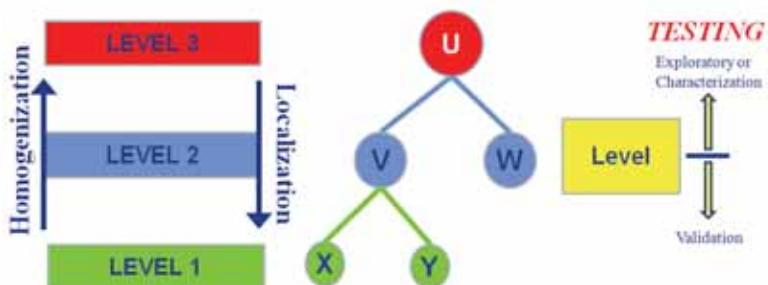


Figure 3: Multilevel tree diagram illustrating three levels of scale and the role of testing for both validation and characterization.

Additionally, Figure 3 illustrates that experiments (virtual or laboratory) performed at each level can be viewed either as exploratory or characterization experiments used to obtain the necessary model parameters for the next higher level. Alternatively, these tests can be viewed as/used to validate the modeling methods employed at the lower level. Figure 3 also illustrates the authors' view that the term "multiscale modeling" should imply consideration of at least two levels of

homogenization/localization or a minimum of three levels of scale. The rationale is that if analyses that consider only two levels of scale (rather than two homogenizations) are considered to be multiscale, many standard structural analyses would qualify. For instance, an elastic finite element model of a structure considers the materials with given elastic properties as Level 1 and the structural response as Level 2. Similarly, standard classical lamination theory considers the plies (with given elastic properties) as Level 1 and the laminate (with calculated ABD stiffness matrix) as Level 2. It is our position that the term “multiscale modeling” is intended to distinguish an analysis from such standard analyses that consider only two scales. Examining the recent literature in multiscale modeling revealed that a majority of authors have not applied this standard to their own work, as evidenced by the fact that 66% of the papers that were characterized by the authors as involving multiscale modeling considered only two scales [1].

Numerous homogenization techniques (micromechanical models) exist that can provide effective composite properties. These range from the simplest, analytical approximations (i.e., Voigt/Reuss) to higher fidelity, more involved methods (e.g., concentric cylinder assemblage, Mori-Tanaka, Eshelby, and Aboudi’s generalized method of cells) to finally, fully numerical methods that are the most general and the highest fidelity yet the most computationally intense (e.g., finite element, boundary element, Fourier series). Each has its realm of applicability and advantages, however, many are unable to admit general user defined deformation and damage/failure constitutive models for the various constituents (i.e., fiber or matrix) thus limiting their ultimate usefulness, especially for high temperature analysis where nonlinear, time-dependent behavior is often exhibited.

An alternative approach to modeling composite structures, which circumvents the need for micromechanics, involves fully characterizing the composite material or laminate experimentally, which has the advantage of capturing the in-situ response of the constituents perfectly. However, such full characterization for all applicable temperatures and configurations (e.g., fiber volume fractions, tow spacing’s, etc.) can be expensive. In addition, composites are almost always anisotropic on this scale (i.e., laminate). Thus some needed properties can be virtually impossible to measure, and the development of realistic models that capture the nonlinear, multiaxial deformation and failure can be challenging (due to the anisotropy). Clearly, the physics of deformation and failure occur on the micro scale (and below), and, by modeling the physics at the micro scale, models for the monolithic, often isotropic, constituents can be employed.

Recently, a comprehensive and versatile micromechanics analysis computer code, known as MAC/GMC [2] has been developed at the NASA Glenn Research Center based on Aboudi’s well-known micromechanics theories [3]-[6]. FEAMAC (the coupling of MAC/GMC micromechanics with the finite element analysis framework through user subroutines), HyperMAC (the coupling of MAC/GMC micromechanics with the commercial structural sizing software known as HyperSizer [7]), and Multiscale Generalized Method of Cells (MSGMC, the recursive coupling of micromechanics with micromechanics) have begun to address the truly multiscale framework depicted in Figure 1. This software suite, known collectively as ImMAC (available from NASA Glenn), provides a wide range of capabilities for modeling continuous, discontinuous, woven, and smart (piezo-electro-magnetic) composites. Libraries of nonlinear deformation, damage, failure, and fiber/matrix debonding models, continuous and discontinuous repeating unit cells (RUCs), and material properties are provided. To illustrate the multiscale capabilities of the ImMAC framework, this paper focuses on the application of FEAMAC and MSGMC to model the stochastic progressive failure of a SiC/Ti metal matrix composite tensile specimen and to investigate architectural variability on the nonlinear response of woven PMCs.

FEAMAC

As shown in Figure 4a, FEAMAC is the direct implementation of MAC/GMC unit cell analyses within structural finite element analysis (FEA). The software currently supports Simulia's commercial finite element software package Abaqus [8]. The coupling is accomplished utilizing the Abaqus user subroutines, which enable the MAC/GMC code to be called as a library to represent the composite material response at the integration and section (used for through-thickness integration in shell elements) points in any element within the finite element model. Two- and three-dimensional continuum elements, as well as shell elements, are supported. Any nonlinearities due to local effects (e.g., inelasticity or damage) in the fiber/matrix constituents at any point in the structure are thus captured and homogenized, and their effects on the structure are manifested in the finite element model structural response at each increment of loading.

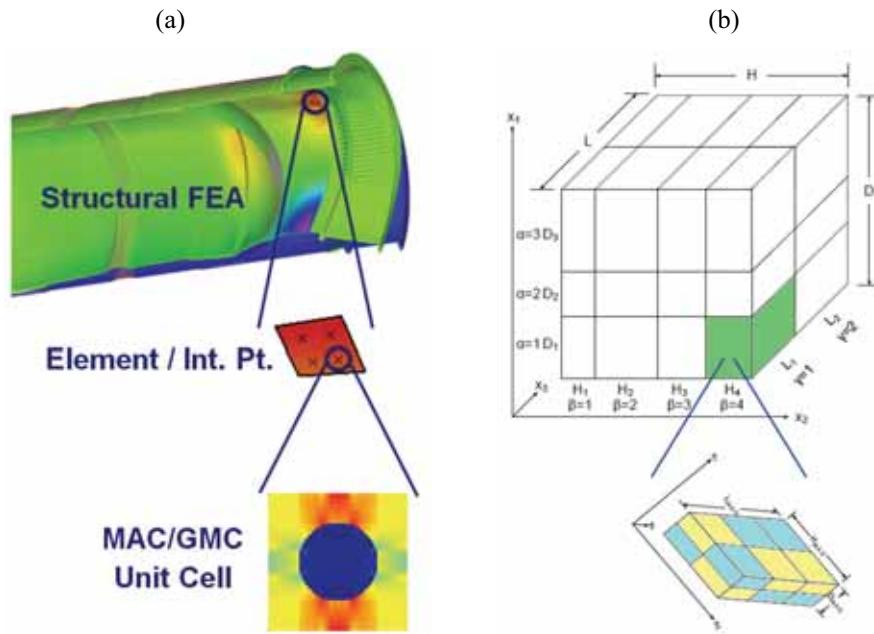


Figure 4 (a) FEAMAC couples MAC/GMC with finite element analysis. (b) MSGMC recursively calls the generalized method of cells (GMC) to represent the behavior within the subcells of a RUC operating at a given level.

MSGMC

As shown in Figure 4b, MSGMC [9] implements the three-dimensional generalized method of cells (GMC) to represent the behavior of the subcells within GMC repeating unit cells. This can be performed an arbitrary number of times to represent an arbitrary number of scales in an integrated multiscale analysis. The methodology is ideal for analyzing woven and braided composites, where the behavior of the tows can be modeled with GMC operating within a subcell in an RUC representing the weave or braid. Similar to FEAMAC, any nonlinearity occurring at the lower scales will affect the global scale response.

RESULTS AND DISCUSSION

Progressive Failure Analysis of a SiC/Ti Tensile Specimen

The stochastic analysis of the fiber breakage dominated progressive failure process in a longitudinally-reinforced SiC/Ti MMC structures is examined using FEAMAC. In particular, we consider perhaps the simplest (yet extremely important) composite structure: an experimental tensile test specimen, shown in Figure 5. Such test specimens are critical to both materials scientists and structural engineers because they are used to evaluate material quality during development of materials and to characterize material model parameters needed for structural analysis. The design of test specimens is also known to be critical so as to ensure a uniform state of stress and strain in the gauge section, as well as consistent failure within the gauge section.

The SiC/Ti test specimen was modeled with a one-eighth symmetry finite element mesh. A monotonic longitudinal tensile load was applied in the form of an applied uniform displacement in the direction of the longitudinal axis (x_1) of the specimen at a rate of 3×10^{-4} in/s. With a total of 300 Abaqus C3D8 (8-noded brick) elements in the mesh and eight integration points per element, the MAC/GMC micromechanics model is called as a user material (UMAT) subroutine 2400 times per time step in the FEAMAC simulation. This highlights the necessity for having such a computationally-efficient means as GMC of relating both the properties and the local stress/strain fields of the constituent phases of the composite to the effective properties and deformation response of its homogenized continuum representation. Note that, based on the mesh shown in Figure 6, along with the fiber diameter and composite fiber volume fraction, each element in the tensile specimen gauge section is sufficiently large to encompass approximately 25 fibers.

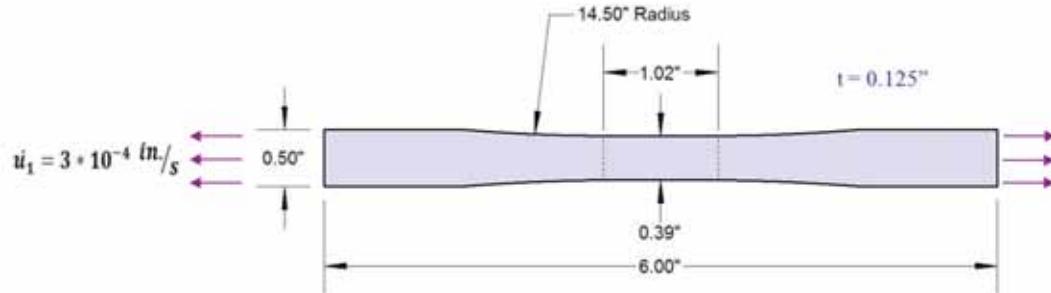


Figure 5: NASA GRC dog-bone test specimen.

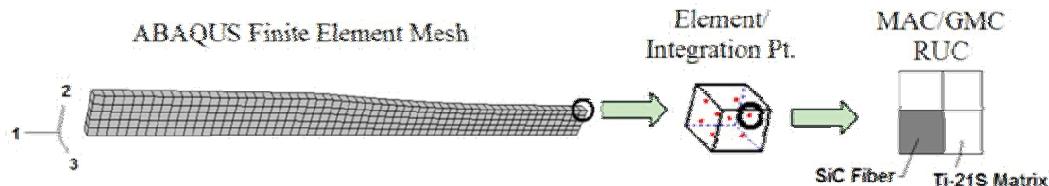


Figure 6: Abaqus finite element mesh of the dogbone specimen and MAC/GMC RUC operating at each integration point.

On the local scale within the MAC/GMC input files, which define the composite material details, in addition to the geometry of the composite RUC, material properties for the fiber and matrix are required. The SiC fiber is treated as linearly elastic and isotropic while the *TIMETAL 21S* matrix is treated as viscoplastic and was simulated using the Generalized Viscoplasticity with Potential Structure (GVIPS) constitutive model [10]. The material properties of the constituents are given in Table 1 and Table 2.

Table 1. SCS-6 fiber elastic properties.

Temperatur ϵ (°C)	E (GPa)	v	α ($1 \times 10^{-6}/^{\circ}\text{C}$)
21	393	0.25	3.56
316	382	0.25	3.72
427	378	0.25	3.91
538	374	0.25	4.07
860	368	0.25	4.57

Table 2. TIMETAL 21S material properties and GVIPS model parameters.

Temp (°C)	E (GPa)	α ($1 \times 10^{-6}/^{\circ}\text{C}$)	κ (MPa)	μ (MPa/sec)	B_0 (MPa)	$R\alpha$ (1/sec)	β
23	114.1	7.717	1029	667.6	6.908×10^{-5}	0	0.001
300	107.9	9.209	768.4	137.8	1.035×10^{-4}	0	0
500	95.1	10.70	254.2	1.45×10^{-3}	2.756×10^{-4}	1.68×10^{-7}	0
650	80.7	12.13	5.861	6.19×10^{-9}	5.870×10^{-4}	1.00×10^{-6}	0
704	59.7	14.09	0.756	1.13×10^{-11}	6.346×10^{-4}	6.01×10^{-5}	0

temperature-independent: $v = 0.365$, $n = 3.3$, $B_1 = 0.0235$, $p = 1.8$, $q = 1.35$

The final ingredient to the multiscale FEAMAC progressive failure analysis of the TMC specimen is the stochastic failure response of the SiC fibers, as shown in Figure 7. Two approaches to modeling this stochastic behavior will be investigated and compared. The first relies on the stochastic Curtin fiber failure model [11] and the second is based on a simple maximum stress failure criterion, which is deterministic when applied uniformly across the test specimen and stochastic when the strength is randomly distributed throughout the specimen. Both failure models are applicable only to the fiber subcell(s) within the RUC. The Curtin model predicts fiber stiffness degradation due to damage and complete failure of an effective, degrading fiber. Herein, upon complete failure using either the Curtin or maximum stress model, the fiber is given a negligible stiffness (0.0001 times its original stiffness). The employed Curtin model parameters (which are obtained from fiber strength statistics, see Figure 7) are the fiber gauge length, $L_0 = 1$ in. (25.4 mm), fiber diameter, $d = 0.0056$ in. (142 μm), characteristic strength, $\sigma_0 = 609$ ksi (4200 MPa), Weibull modulus, $m = 10$. The Curtin model requires one additional parameter, the fiber-matrix frictional sliding resistance, τ , which was taken as $\tau = 2.03$ ksi (14 MPa) at 650 °C based on the work described in [12]. This value was backed out of GMC simulations such that good correlation was achieved with test data. Thus, because these simulations were based on GMC simulations for a single material point at a specific temperature, the applicability of this τ value in the simulations of the entire tensile specimen and at temperatures other than 650 °C is questionable.

First let us consider a simulation with no fiber failure as shown in Figure 8a. The plotted von Mises stress field shows the stress concentrations that are inherent to dogbone type test specimens. Along the specimen edge, a strong minimum is observed at the start of the reduction section, whereas a milder maximum is present at the transition from the reduction section to the

gauge section. Because it is relatively mild, this maximum is difficult to see in the figure, but as indicated, it is an absolute maximum at node 67, which is just above the transition to the gauge section. It is this structural level concentration that can lead to specimen failure outside the gauge section, which is why a large reduction radius (14.5 in.) was employed in the NASA GRC specimen, thus making this concentration very mild. It has been shown that for smaller reduction radii, this concentration increases significantly [13], [14]. Even though the magnitude of this stress riser, as modeled, is only slightly higher than the stress magnitude in the gauge section, this will always be the location of simulated failure initiation if the fiber failure parameters are spatially uniform throughout the tensile specimen.

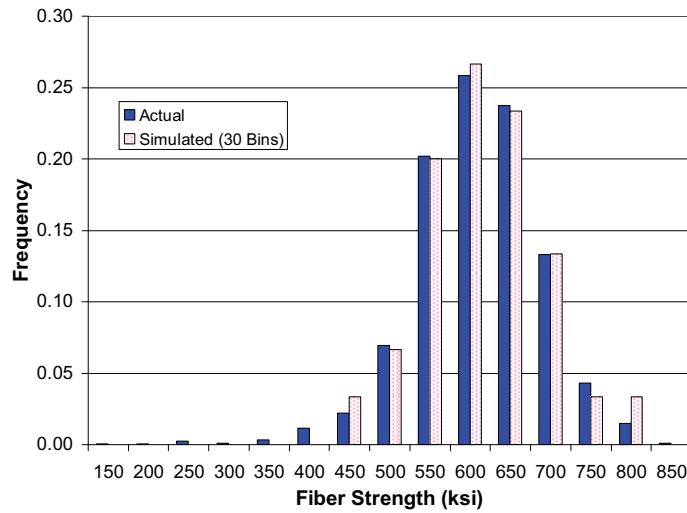


Figure 7: Fiber strength histogram for SCS-6 SiC fibers. The actual data is vendor-supplied [15], while the simulated data refers to the distributed characteristic strength. Note, the fiber gauge length: $L_0 = 1$ in. (25.4 mm) and diameter: $d = 0.0056$ in. (142 μ m) are vendor supplied.

The effect of the global stress riser can be seen in Figure 8b and c, where the fiber damage progression is shown for the max stress and Curtin model simulations. Note that the fiber damage is quantified as a fraction of fiber damage within the elements; a fiber damage value of zero corresponds to an undamaged state, while a fiber damage value of 1.00 corresponds to complete failure of all fibers within an element. For the case in which we use the maximum stress criterion, the failure simulation is fully deterministic as fiber failure initiates at the stress riser and no statistical data related to the fiber strength are employed. If one uses the Curtin model, failure still initiates at the highest global stress raiser, but now the stochastic nature of the fiber failure process is captured at the local level through the fiber strength statistics incorporated within the model. Both fiber failure models exhibit similar damage zones and both simulations exhibit complete failure of the specimen within 1/10,000th of a second after initiation of failure begins. This is despite the fact that the Curtin model simulates fiber stiffness degradation prior to failure while the max stress model does not. The Curtin model simulation does fail at a significantly lower overall stress than does that using the maximum stress criterion; see the composite stress-strain curves in Figure 9. However, these results are dependent on the chosen value of τ , the fiber-matrix frictional sliding resistance. A higher value of τ would shift the Curtin model failure predictions higher, closer to those of the max stress criterion. Note, the strain plotted in Figure 9 corresponds to a virtual extensometer measurement, that is, an average strain over the gauge length of the specimen as shown in Figure 8c (calculated as change in displacement divided by original length).

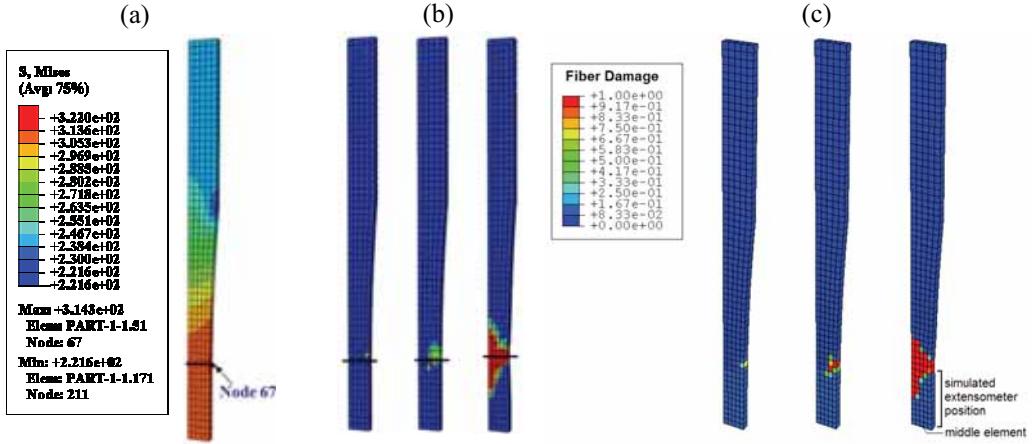


Figure 8: (a) Stress contours in the longitudinal 33% SiC/Ti-21S tensile specimen in a linear elastic simulation with no fiber failure indicating the maximum stress riser at node 67. Local fiber damage fraction as a function of time as fiber failure progresses within the longitudinal 33% SiC/Ti-21S specimen with spatially uniform fiber failure model parameters. (b) Max stress criterion, (c) Curtin model.

At this point it is worthwhile to summarize the process involved in the FEAMAC simulation results (see for example Figure 8 and Figure 10). Global incremental displacement loading is applied on the specimen, and Abaqus solves the structural problem to determine the stress and strain fields throughout the specimen. The strains and strain increments at each integration point are then passed to MAC/GMC (through the Abaqus UMAT subroutine), which performs a micromechanics analysis given the composite local geometry and constituent properties. Within MAC/GMC, the integration point strains are localized to the level of the fiber and matrix constituent subcells (see Figure 6), which allows determination of the viscoplastic behavior of the matrix and the damage/failure behavior of the fiber. The local response of the fiber and matrix subcells are then homogenized within MAC/GMC to obtain new stresses and a new stiffness matrix (which may have changed due to the imposed strain increment and additional damage accumulation) for the composite at each particular integration point. This information is passed back to Abaqus (through the UMAT subroutine), which then imposes the next increment of the applied global loading. This multiscale approach enables the effects of damage, failure, and inelasticity, and the associated redistribution of stresses within the RUC, to impact the global specimen response. When a particular integration point experiences fiber failure its stiffness is significantly reduced, which causes it to shed load to the surrounding integration points that remain intact and may cause failure to progress, as shown in Figure 8. It should be noted that complete fiber failure through the specimen, as depicted in Figure 8, does not truly represent complete separation in the simulation because matrix material subcells remain intact within the RUCs (see Figure 6). A matrix failure criterion could be added to the simulation within MAC/GMC to model complete failure. However, since the tensile failure of longitudinal SiC/Ti specimens is known to be dominated by fiber failure, this was not done here as the current results are expected to be representative.

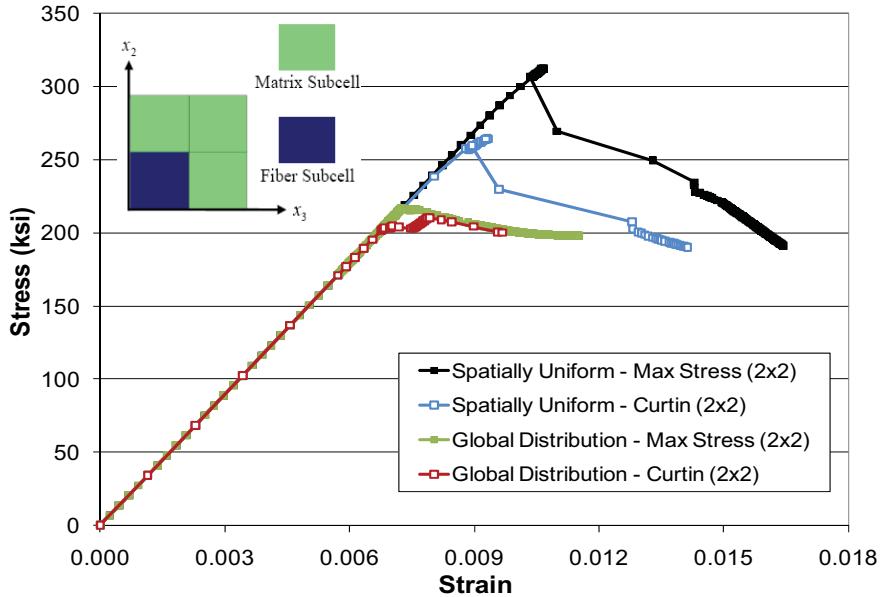


Figure 9: Stress-strain curves assuming both spatially uniform and spatially random failure strengths for unidirectional, 33% fiber volume fraction, SiC/Ti21S composite specimen.

It is clear from Figure 8 that the multiscale stochastic FEAMAC simulation of the SiC/Ti specimen has predicted failure outside of the gauge section, which does not typically occur with the NASA GRC MMC tensile specimen. This shortcoming is due to the inappropriate implementation of the fiber strength variability exclusively at the local level (i.e., uniform spatial variation of strength). In order to more realistically simulate the SiC/Ti tensile specimen progressive failure, it is necessary to account for the realistic fiber strength distribution on the structural level. This was accomplished by varying the max stress criterion in one case and the Curtin model parameters (an obvious choice being the characteristic strength, σ_0) in the other case, over the specimen geometry. Providing different elements with different values of these model parameters, in essence, enables the elements to damage and fail at different local fiber stress levels.

To distribute the characteristic strength spatially, 30 user materials were associated with the finite element mesh of the composite specimen. Each material was defined by a MAC/GMC input file with a different σ_0 value chosen according to the vendor-supplied fiber strength histogram shown in Figure 7. This was accomplished by determining the number of user materials having σ_0 values in each 50 ksi range (see the horizontal axis of Figure 7) in order to provide a good match with the actual fiber strength distribution (as shown in Figure 7). If only one material's σ_0 value was located within a particular 50 ksi range, the characteristic strength was chosen as the middle of that range. Otherwise, the characteristic strength values for the materials were evenly distributed within the applicable 50 ksi range. As shown in Figure 7, the 30 σ_0 values provide an excellent match with the actual fiber strength histogram. When considering the Curtin model, the other important parameter that must be considered to obtain the correct fiber strength statistics is the Weibull modulus, m , as this affects the shape of the fiber strength distribution. Immediately, one might consider using a constant value of m for all values of σ_0 , yet when summing over all fibers, this did not reproduce the correct overall fiber strength distribution. If however, each user material was allowed to have a distinct Weibull modulus value, one could obtain the correct

distribution. Consequently, a simple computer program was written to optimize the Weibull modulus values in order to provide the best correlation of the combined fiber strength distribution of all 30 user materials with the actual fiber strength distribution.

Now, with these 30 user materials (represented by 30 MAC/GMC input files) whose Curtin model data (or maximum strength criterion data, depending upon which failure model one chooses to employ) cumulatively represent the fiber strength statistics accurately, the 300 elements within the specimen were randomly distributed to the user materials (with ten elements per material, all ten having identical properties). The random distribution was accomplished via a simple computer program. The resulting distribution of maximum characteristic strengths (i.e., σ_0) over the specimen geometry is shown in Figure 10 (left most figure). This idealization (i.e. spatially varying fiber strength distribution) was subjected to the identical simulated tensile test considered previously in the non-distributed case. Results for the progressive failure simulation of the spatially distributed maximum fiber strength statistics specimen are given in Figure 10. In this simulation, failure initiated (see Figure 10 snapshot (a)) not at the stress concentration (i.e., node 67, see Figure 8a), but rather within the gauge section in an element that happened to be assigned a low characteristic strength (see the blue element in the left most Figure 10). Subsequently, progressive failure across the specimen occurred in 0.68 seconds (see snapshots (b) through (e) in Figure 10). The global stress-strain curve responses for both the Curtin and maximum stress model predictions are shown in Figure 9 for both uniform and spatially varying cases. Clearly, the peak stress value (ultimate strength) in both of these predicted stress-strain curves are significantly lower than the previous uniformly (or non-distributed) case; in that the distributed Curtin model simulation predicts an ultimate strength of 210 ksi (1451 MPa) compared to a value of 264 ksi (1822 MPa) for the non-distributed simulation, while the maximum stress criterion simulation predicts an ultimate strength of 217 ksi (1494 MPa) compared to a value of 313 ksi (2155 MPa) for the non-distributed simulation. Note how both spatially distributed simulations, regardless of the failure model used, provide similar (less than 3% difference) results; as both are now stochastic in nature due to the random spatial variation of fiber strength. Furthermore, random failure locations within the gauge length can be obtained by creating different actualizations (i.e., new random assignments of fiber strengths within the various 30 bins); which agrees qualitatively with numerous experimental results obtained at NASA GRC as shown in Figure 11.

To assess the quantitative accuracy via comparison with experimental results, three additional factors are accounted for in the FEAMAC simulation: (1) local fiber strength variation within the RUC, (2) incorporation of residual stresses due to specimen heat treatment/consolidation, and (3) shifted fiber strength due to fiber length scale. In order to account for the local fiber strength distribution within the RUC, an RUC containing 25 subcells (see insert in Figure 12) was utilized. Furthermore each fiber subcell was randomly assigned a different strength while maintaining that the average of these fiber strengths equals the specific fiber strength assigned to the RUC. Recall that the 30 RUCs (10 elements per RUC) are randomly assigned throughout the 300 element mesh in order to capture the global fiber strength distribution. This enables each integration point to experience a progressive failure which in turn enables an even more gradual failure evolution than if one utilizes only a global fiber strength distribution, with one fiber per RUC at an integration point. Incorporation of residual stresses (which are key for accurate predictions of metal matrix composites failure response) is accomplished by imposing the complete thermomechanical loading cycle for a given specimen. A 16 hour cool down from a uniform 900 °C (assumed stress-free) heat treatment temperature to room temperature (23 °C), was simulated followed by an unconstrained temperature rise to 650 °C over 5 minutes. The temperature was then held constant while a monotonic uniaxial tensile loading, at a displacement rate of 3×10^{-4} in/s, was applied until complete fiber failure was achieved. The predicted tensile response of a 25% fiber volume fraction SiC/Ti titanium matrix composite (TMC) test specimen

at 650 °C is shown in Figure 12, given the vendor supplied strength distribution of Figure 7, which is also shown as the black line ($\lambda = 1.0$) in the insert of Figure 12. Clearly, this curve agrees well with the experimental data provided, except it appears to suffer premature fiber failure since it significantly under predicts the specimen UTS.

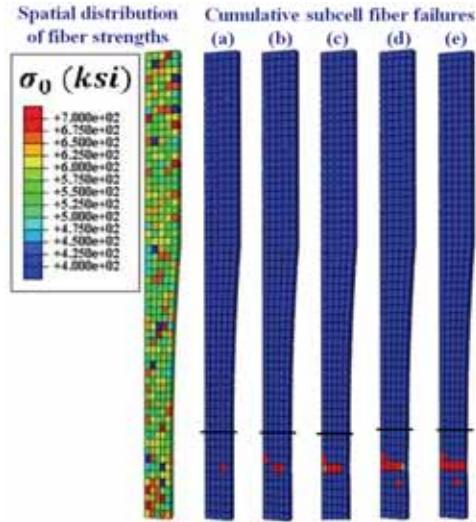


Figure 10: Global fiber strength distribution contour plot; (a)-(e) cumulative fiber subcell failure contours at simulation times of 63.40 s, 63.93 s, 63.95 s, 64.06 s, and 64.08 s, respectively (Note that the black lines denote the beginning of the transition region from the end of the gage section to the end of the specimen).

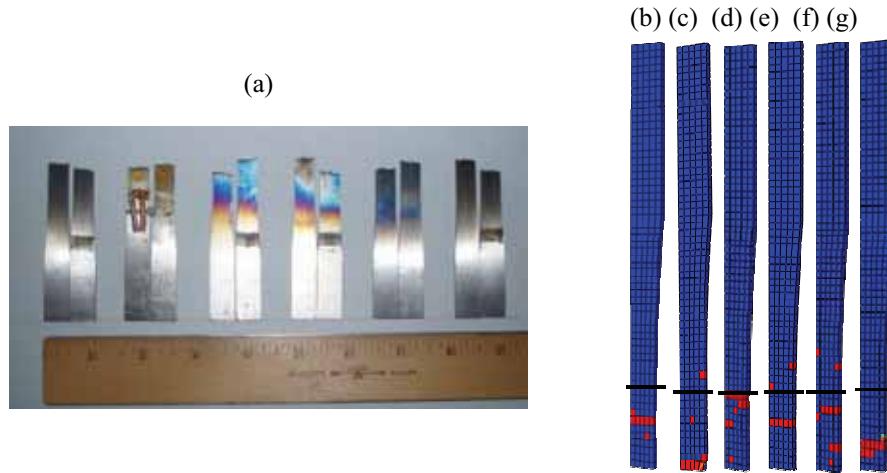


Figure 11: a) Picture of the failure location of six test specimens and (b)-(g) Cumulative fiber subcell failure contour plots showing probabilistic nature of the simulated fiber failure location from six separate actualizations (simulations). Note that the black lines denote the beginning of the transition region from the end of the gage section to the end of the specimen once again.

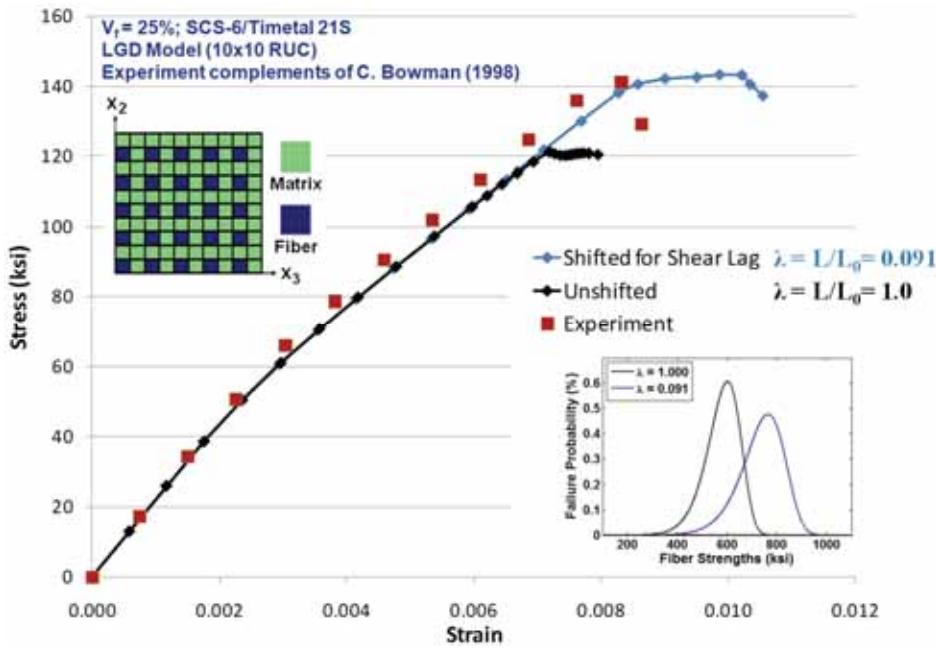


Figure 12: Composite stress-strain response for randomly distributed, maximum stress failure criterion simulations (black and blue lines) compared to experimental data (red square symbols) at 650 °C.

To compensate for this premature failure, we must account for the disparity between the gage length of the fiber specimens used to conduct the fiber strength tests ($L_0 = 1.0$ in) and the characteristic length needed to develop full fiber loading in the FE model (calculated to be $L = 0.091$ in. from shear-lag calculations [16], [17]). Consequently, a new set of fiber strength bins were generated using a modified Weibull distribution, shifted to account for this change in length ratio (this ratio is defined as lambda, or L/L_0 [11]):

$$p_f(\sigma) = 1 - \exp\left[-\frac{L}{L_0}\left(\frac{\sigma}{\sigma_0}\right)^m\right] \quad (1)$$

The original and shifted Weibull distributions (failure probability distribution) are illustrated in the lower right insert in Figure 12. These new fiber strength RUCs were then used to simulate the same thermomechanical loading cycle described previously, the result of which is depicted by the blue line in Figure 12. Clearly, this new simulation captures the experimental data response extremely well including the UTS of this test. Note however, that the strain to failure is over predicted; as expected since no failure criterion was applied to the matrix subcells, so that upon complete failure of the fiber subcells matrix inelastic flow is unconstrained.

Recursive Multiscale Analysis of a Woven Polymer Matrix Composite

In this study, MSGMC is used to examine the effects of architectural parameter variations on the response of woven PMCs. As illustrated in Figure 13, the analysis considers four physical length scales from the fiber/matrix constituents (microscale) to the RUC representing the tow (mesoscale) to the RUC of the weave (macroscale) to an assembly of nine RUCs (structural

scale). This would normally indicate three separate homogenizations to span the four scales, but actually, an additional intermediate homogenization is performed when using MSGMC to analyze woven or braided composites. This involves a separate through-thickness homogenization within the macroscale, which has been shown to improve the model's predictions (see [19] for details). Thus, the analyses at the structural scale involve four homogenizations while those at the macroscale involve three. The architectural parameters that were varied at the mesoscale (fiber packing arrangement and fiber volume fraction within the tows) and the macroscale (tow aspect ratio) are also shown in Figure 13.

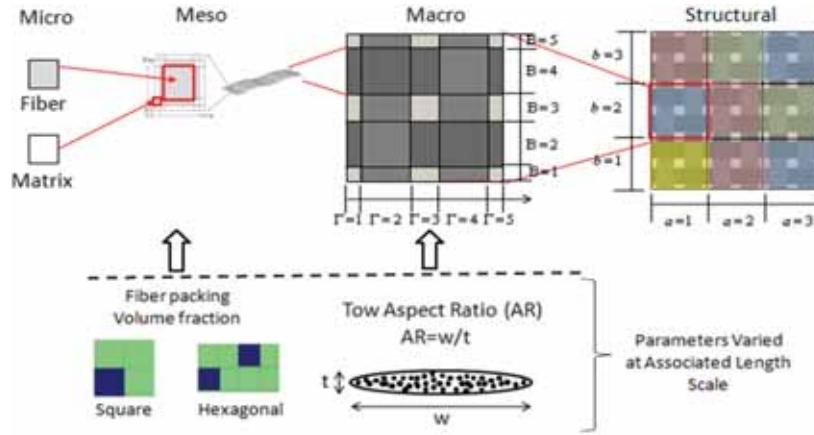


Figure 13: Multiscale analysis methodology with architectural effects being varied as shown at the meso and macro scales.

For these analyses an AS-4/3501-6 material system with an overall fiber volume fraction of 60% was assumed. The properties of the constituent materials are shown in Table 3. The fiber is treated as linearly elastic while the matrix is modeled as elastoplastic using classical plasticity with exponential isotropic hardening of the form,

$$\kappa(\bar{\varepsilon}_p) = \sigma_Y - \frac{H}{A} (e^{-A\bar{\varepsilon}_p} - 1) \quad (2)$$

where $\kappa(\bar{\varepsilon}_p)$ is the isotropic strain hardening rule, $\bar{\varepsilon}_p$ is the equivalent plastic strain, and the material parameters are σ_Y (yield strength), H (initial post-yield modulus), and A (exponent) (see [20] for details). To study the effects of architectural and material variation on the macroscale response, a full factorial set of numerical simulations were conducted. The parameters varied are shown in Table 4 and are depicted in Figure 13. The three architectural parameters varied are tow volume fraction, tow aspect ratio (width divided by thickness, as shown in Figure 13) and fiber packing arrangement. All other parameters in the analysis were kept constant. The tow volume fraction and fiber packing arrangement are both considered mesoscale attributes because their geometrical properties are involved in the mesoscale concentration matrix. The tow aspect ratio is considered a macroscale property because it is taken into account in the macroscale concentration matrices. The tow volume fraction was varied among 0.62, 0.65, and 0.70. These three values were chosen based on common experimental values for PMCs. The tow aspect ratio was chosen to be 9, 18, or 36. A value of 9 is typical of

CMCs, 18 is typical of PMCs, and 36 was chosen as an upper bound. Two different fiber packing arrangements were considered, square and hexagonal, as both exhibit different responses. Although most PMCs exhibit random packing, square and hexagonal packing are both reasonable approximations of this. The full factorial simulations were executed for both the tension and shear response and were also performed for two macroscale weave types: plain weave and 5-harness satin (5HS) weave (see Figure 14). The full factorial simulations for both responses and weave types resulted in a total of 72 cases analyzed. In each of these cases, the overall volume fraction of the woven composite was kept constant so that the results are comparable.

Table 3: AS-4/3501-6 constituent properties.

	E _A (GPa)	E _T (GPa)	v _A	v _T	G _A (GPa)	σ _Y (MPa)	a	H (GPa)
AS-4	225.0	15.0	0.2	0.2	15.0	N/A	N/A	N/A
3501-6	4.2	4.2	0.34	0.34	1.56	71	100	1.5

Table 4: Parameters varied in multiscale analyses.

Microstructural Parameter	Relevant Length Scale	Values
Tow Volume Fraction (V_{tf})	Meso	0.62, 0.65, 0.70
Tow Packing	Meso	Hexagonal, Square
Tow Aspect Ratio (AR)	Macro	9, 18, 36

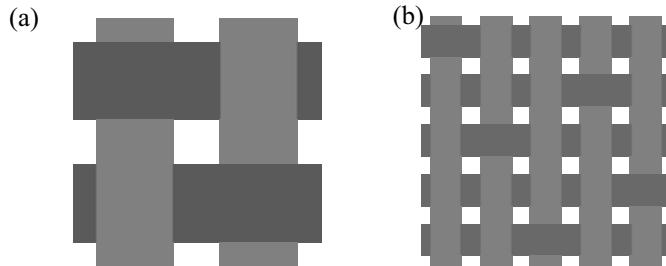


Figure 14: Weave macroscale RUCs, (a) plain and (b) 5HS.

The typical simulated stress-strain curves for a plain weave composite subjected to tensile and shear loading are shown in Figure 15 where a single RUC of the composite (i.e., macro response) has been considered. For illustrative purposes, only one architectural parameter, namely, the tow aspect ratio, was varied. Clearly this variation has a significant effect on the macroscale tensile response, but little effect on the shear response. The full factorial parameter variation results for the macroscale analyses are presented in Figure 16, with each curve on each chart representing a particular set of architectural parameters. It is apparent that there is a significant amount of variation at the macroscale caused by varying the architectural parameters even though the overall fiber volume fraction of the composite is kept constant. The architectural parameter variation caused approximately three times more macroscale variation in the composite tensile response compared to the shear response (as measured by standard deviation). However, the variation in the shear stress-strain curves was still appreciable. Further, examination of individual stress-strain curves revealed that decreasing tow volume fraction has the same effect as increasing tow aspect ratio, an increase in modulus and strain energy (area under stress-strain curve). Also, the hexagonal RUC at the mesoscale was more compliant and exhibited more plasticity than the square RUC for equivalent volume fractions.

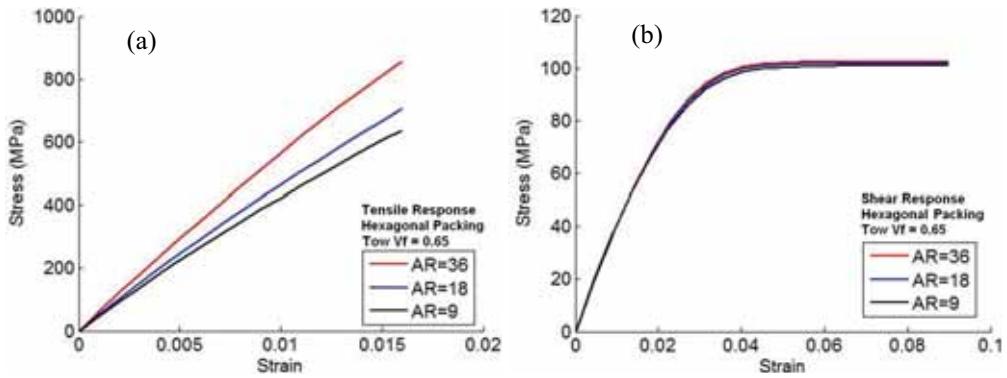


Figure 15: Typical macroscale (a) tensile and (b) shear deformation response for a plain weave composite, given a tow volume fraction of 65%, hexagonal fiber packing within the tows, and varying the tow aspect ratio from 9 to 36.

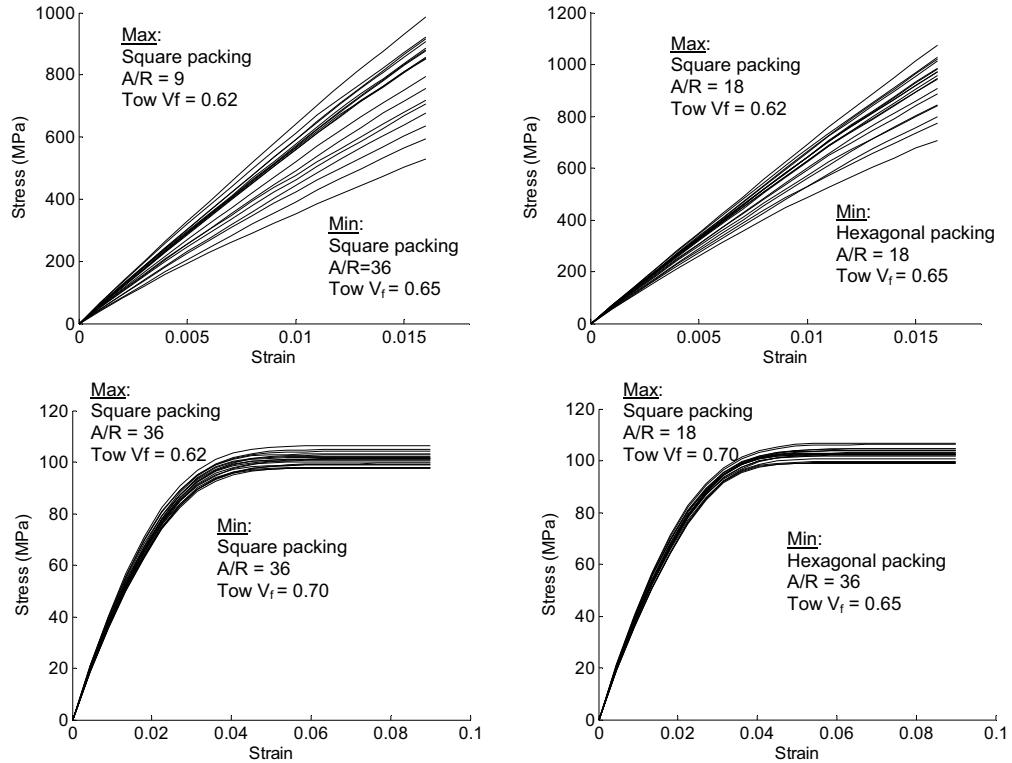


Figure 16: Macroscale tensile response (top row) and shear response (bottom row) for all architectural variations, for a plain weave (left column) and 5HS weave (right column).

To examine the structural scale, the effects of parameter variation on the response of nine (3×3) macroscale RUCs was studied (see Figure 13). Each of the RUCs composing the 3×3 RUC at the structural scale is comprised of a macroscale RUC with a set of architectural parameters chosen at random from the permutations considered in the macroscale architectural study. For example, one RUC might have a 62% tow volume fraction with an aspect ratio of 18 and square packing and another could be completely different. Each architectural parameter was randomly selected

for each RUC, without imposing any probabilities on the parameters. Thirteen cases (realizations) were run for each structural RUC in order to achieve a broad spectrum of combinations. The results for all 13 cases are shown in Figure 17. It is important to note that the variance is greatly reduced when compared to that observed in the macroscale plots. The maximum standard deviation at the macroscale was 15% compared to a mere 2% at the structural scale. Consequently, it appears that the effects of lower scale variations are diminished after one or two higher length scales of homogenization. Thus one must be cautious in attempting to draw conclusions regarding the impact of variability observed at a given scale on the behavior at higher scales.

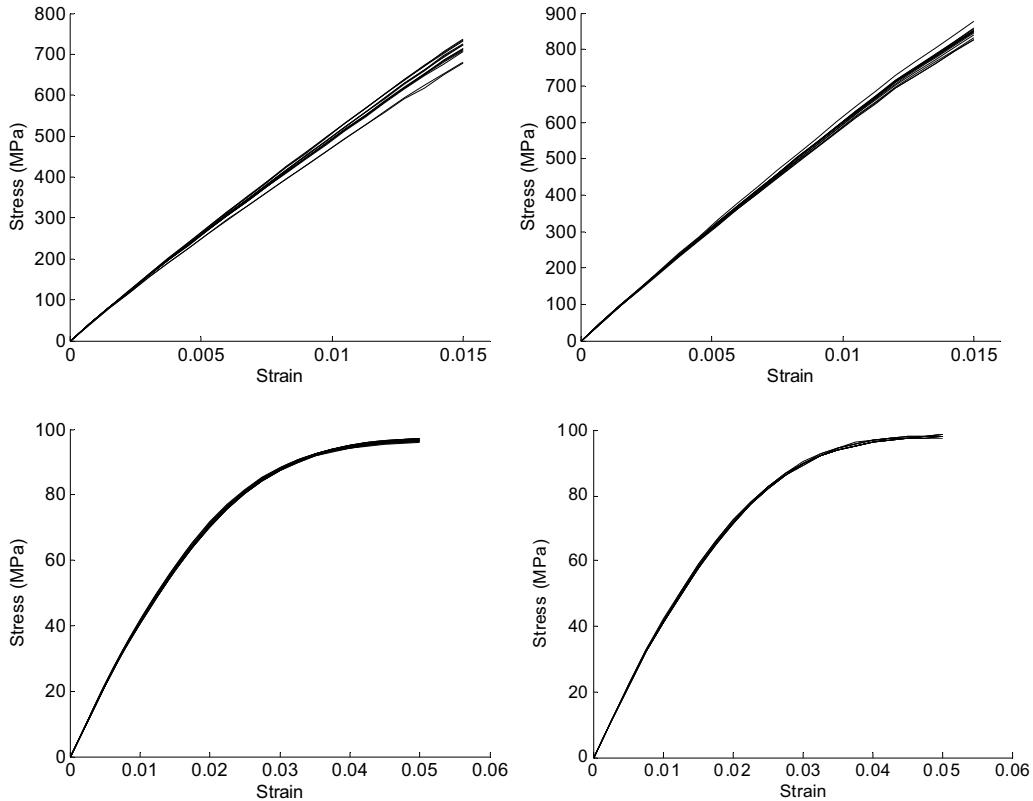


Figure 17: Structural (3x3 RUCs) tensile response (top row) and shear response (bottom row) for all architectural variations, for a plain weave (left column) and 5HS weave (right column).

CONCLUSIONS

NASA Glenn Research Center's ImMAC software suite provides an integrated multiscale framework for the design and analysis of composite materials and structures. FEAMAC calls the GMC micromechanics methods to represent the nonlinear composite constitutive response at the integration points (and section points) within an Abaqus finite element analysis. MSGMC calls GMC micromechanics recursively such that at any scale, the GMC subcells may be occupied by an effective composite material. GMC's ability to localize and homogenize extremely efficiently enables these types of integrated multiscale analyses where nonlinear deformation and damage models for the constituents drive the nonlinear response at the structural scale. Furthermore,

because the nonlinear deformation and damage is handled at the constituent scale, complex, multiaxial, anisotropic models, which would be needed at the composite scale, can be avoided.

Examining the response of a SiC/Ti tensile specimen using FEAMAC, it was shown that incorporating stochastic features at the proper scale (spatially random at the local/global level) enables the use of a simple failure model (e.g., max stress criterion). The model was shown to predict realistic gauge section failure and accurate deformation response and failure load level in the specimen. MSGMC was used to model the nonlinear deformation response plain weave and 5-harness satin graphite/epoxy composites. The effects of tow fiber volume fraction, tow fiber packing arrangement, and tow aspect ratio were shown to be significant when examining the nonlinear response of a single RUC. However, when the response of a structure (idealized with nine RUCs) is modeled, the effects of such variations are greatly reduced. It is also noteworthy that the presented structural MSGMC simulations involve four homogenizations across five levels of scale.

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CONCLUSION

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SUMMARY

This compilation of papers in this book represents approximately half of the works discussed at the MS&T 2010 symposium entitled “*Tools, Models, Databases, and Simulation Tools Developed and Needed to Realize the Vision of Integrated Computational Materials Engineering at Materials Science & Technology*” wherein five sessions comprised of 33 presentations was organized. The goal of the symposium was two fold

- To provide a forum in which current state-of-the-art methods for ICME (e.g., information informatics, experimentation, and modeling) could be openly discussed and critiqued by not only materials scientist but also structural engineers/researchers, component designers, industrial leaders and government program managers.
- To leave the symposium and in particular the panel discussion with a clear idea of the gaps and barriers (both technical, cultural and economical) that must be addressed in order for ICME to fully succeed.

The organizers felt that these goals were met, as particularly evident by the standing room only attendance during a lively panel discussion session at the end of the Symposium. However it is the firm belief of the editors of this book that this symposium was merely a start in the right direction, and that subsequent conferences/symposium (e.g., **First World Congress on Integrated Computational Materials Engineering** to be held July 10-14, 2011 at Seven Springs Mountain Resort in Pennsylvania) must work hard to ensure that a truly diverse, multidisciplinary, community of researchers and practitioners are present and have ample opportunity for interaction. This will ensure that a proper balance between push and pull disciplines and technologies is maintained so that this emerging focus area, Integrated Computational Materials Engineering (ICME), has the greatest potential for success and impact on “system-level” payoffs. Similarly, a pro-active approach is required to reform historical modes of operation in industry, government and the academic sectors so as to facilitate multidisciplinary collaboration and to clearly articulate the vision and scope of ICME.

[The ICME] goal is to enable the optimization of the materials, manufacturing processes, and component design long before components are fabricated, by integrating the computational processes involved into a holistic system. ICME can be defined as the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation. ... The emphasis in ICME is on the “I” for integrated and “E” for engineering. Computational materials modeling is a means to this end. [1]

The vision of ICME is compelling in many respects, not only for the value-added in reducing time to market for new products with advanced, tailored materials, but also for enhanced efficiency and performance. However, as articulated in the various articles contained herein, it involves much more than just enhancing the role of modeling and simulation in design and manufacturing processes. For example advances are needed in the following area:

:

- Computational materials science, micromechanics, and multiscale modeling strategies.
- High resolution materials characterization and *in situ* measurements at various levels of scale
- Informatics and information sciences (information theory, databases, digital interfaces, data visualization for decision support, web protocols).
- Decision theory and systems design (game theory, utility theory, multi-objective optimization).

While many of the papers in this book dealt with multiscale modeling, it is important to remember, as reminded by Dr. McDowell, that multiscale modeling is a means to an end and not equivalent to ICME. Lastly as indicated by various authors, although the challenges and barriers (both technical and cultural) are formidable; substantial cost, schedule, and technical benefits can result from broad development, implementation, and validation of ICME principles. Not only are there clear benefits for aerospace applications, as indicated by Dr. Cowles, et al., these benefits extend to materials producers, the automotive industry and also system customers such as the Air Force and NASA.

GAPS/ BARRIERS AND RECOMMENDATIONS

As put forth by the various authors in this compilation, there are many technical and non-technical challenges and barriers to broad development, implementation and acceptance of ICME. This section will extract and consolidate the over arching challenges, barriers and recommendations and categorized them into three broad areas. This consolidation of all the authors' challenges and recommendations will provide a backdrop for a few concluding recommendations detailed in the next section. Specific technical barriers will not be summaries here, but left to the reader to ponder and elaborate on in future articles.

Cyber-Infrastructure Challenges and Recommendations

As noted in the introduction to this book, the cyber-infrastructure developed for ICME is the road on which materials data and information will travel. It is essential that the infrastructure be carefully developed in order for ICME to succeed. Dr. Cowles et al. show a figure (reproduced below as Figure 1) of a possible ICME architecture which can be implemented in a company's local intranet system or on the internet to allow for collaboration between many different companies, universities and government agencies spread across various locations.

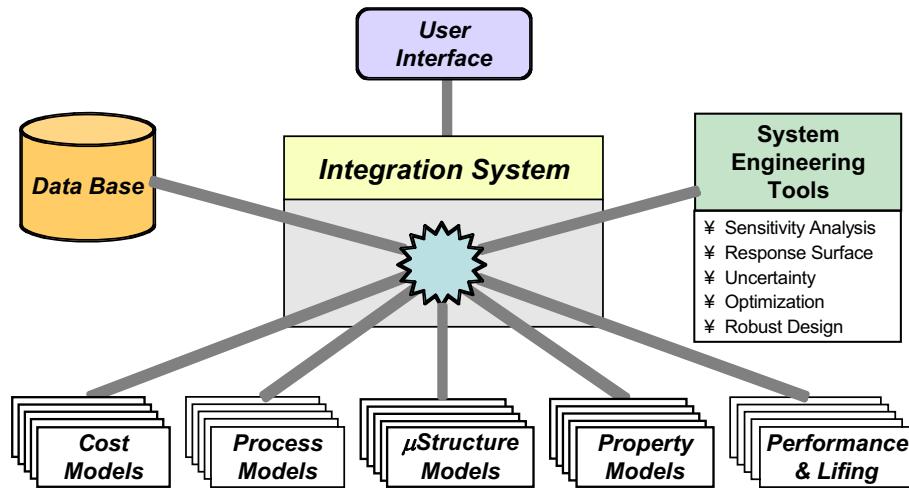


Figure 1: Pictorial representation of the typical elements of an ICME system.

Dr. Cowles et al. mentioned challenges in relation to the maturity of some of the elements shown in Figure 1. These issues of maturity (e.g., a mature validated model) will be addressed in the next section. For this section, it is important to realize that there are at least two issues beyond those of the maturity of each element. The two issues are

1. The need for databases with validated, pedigreed, data that is applicable for model development and execution.
2. Integration issues related to the protocols by which data and information is shared between the various elements

For any of the modeling tools to work, there needs to be data (at various length scales) available for those models. Conversely, the database needs to be able to capture the results from these models and store it for possible use by other models. The latter, the storage of calculated results from models at different length scales, is required in order to ensure, as argued for by Dr. Rajan, that databases become more than just a source of organized data but becomes a source of integrated information. The result is an information management system that can disseminate (both experimental and simulated data) information to other models operating at similar or different length scales.

In addition to the need for pedigreed, validated databases that contain traditional pointwise property values as well as complete response spectra; there is a need to establish standard protocol in order for each element to communicate with the other. Dr. Austin et al. proved the value in having standard-compliant format in the communication of test data from a lab to a database in his paper. Their proof of the benefits of having a standard communication protocol only further underlines the need to have a standard protocol for communication between the various elements so that the output from one element can be passed on as an input value for another element.

Not only does there need to be a standard method of communication between each element but there needs to be, as implied by Figure 1, a tool that integrates all the elements together so that a user can experience the integration of the various elements with minimal required human intervention. As explained by Dr. McDowell, this integration must go beyond the elements traditionally understood to be within the realm of material science and engineering and needs to include other engineering disciplines (e.g., uncertainty, probabilistics, multidisciplinary

optimization and engineering systems design approaches) as well as manufacturing. Dr. McDowell believes that realization of this integration is the most important gap that must be overcome for ICME to realize its full potential.

Technical and Material Science Issues

Dr. Cowles et al. find the lack of fully mature validated models as a major gap that must be overcome. The lack of these means any predictions from immature models cannot be relied upon and create doubt about the value of ICME. In Table 2 of their paper, Dr. Cowles et al. provide an overview of the various levels of maturity for various models sorted by type. While helpful, it must be recognized that the maturity level is also a function of the material in question. For example, there may be a mature finite element model for the processing of composites but not one for ceramics. As evidenced, by the success that Dr. Lacy et al. and Dr. Roy et al. had on multiscale modeling imply, modeling maturity is a function of material. This is confirmed by Dr. Gazonas et al. conclusion that model validation must take place for specific materials. This does not mean that a mature model for one material system is irrelevant to other material systems. In fact the contrary may be true. A mature model for one material system may provide us insight into developing a similar model for another material system.

Issues Related to Working Together

One of the major themes running in several papers in this book is the diverse nature of ICME. Drs. Sullivan and Arnold note that the specific field of multiscale modeling is vast because it involves various disciplines. In his argument for the involvement of four foundational groups, Dr. Spanos implies a diversity of organization. The implication of diversity is also implied in Dr. McDowell's examination of barriers unique to industry, government funding agencies and academia. ICME is diverse in the technical issues covered and diverse in the categories of organizations and disciplines involved.

Inherent in this diversity is the challenge of communication between the diverse units. Part of the communication problem can be addressed through the well thought out development of the ICME cyber-infrastructure. But the cyber-infrastructure alone, can only deal with the communication protocol between various computational tools. The question of what data/information needs to be communicated between the various computational tools, the role of each foundational group, and who needs to be involved must be addressed by other means. Dr. Spanos is on the right track in suggesting that the professional societies (e.g., ASM International and TMS) should play a role in bringing together the other three foundational groups (i.e., Academia, Government and Industry). The editors of this book feel more needs to be done in the area of working together.

CLOSING COMMENTS AND RECOMMENDATIONS

Given the above documented challenges/barriers facing ICME and the recommendations, it is the firm belief of the editors that the following three, non-mutually exclusive, items be implemented; 1) Model material concept, 2) National ICME information management system, and 3) ICME consortiums.

Model Material Concept

In an attempt to economize and streamline titanium matrix composite (TMC) material development and the associated structural design and analysis understanding, a model material concept was introduced by Arnold and Castelli [2]; wherein they defined an ideal model material

as *any material* (be it monolithic or composite) *that possesses all of the salient features* (e.g., thermal, mechanical, and chemical) *representing a class* (e.g., Metallic, Polymeric, Ceramic, and Composite (i.e., Brittle/Ductile, Brittle/Brittle, or Ductile/Ductile)) *of materials and yet can be acquired relatively inexpensively, easily and with sufficient manufacturing consistency as to be considered "high quality" material.* To assess the legitimacy of this model material concept, it was supposed that one must examine the relevance of a variety of materials contained within the defined class from three interrelated viewpoints, namely a mechanistic (e.g., atomic bond, structure (crystalline, monomers, etc.), anisotropy, crystal defect, to name a few) phenomenological, and analytical/modeling point of view. If results indicate that qualitative behavior from material to material, within the class, was the same (i.e., that the material behavior can be scaled) then the model material concept for that class of materials has been validated and only one material need be selected to represent that class of materials. Thus, given a complete mechanistic, phenomenological and analytical/modeling understanding of the model material, it could be argued that a new, relatively unassessed and untested material, that falls within the defined class, can be utilized rapidly by industry and at a significantly reduced level of testing and characterization cost. Arnold and Castelli [2] defined a material class to encompass all titanium alloy matrices reinforced with unidirectional, continuous, brittle (silicon carbide, i.e. SCS-6) fibers that are weakly bonded to the matrix material. Potential material systems that fall within this class, included titanium matrices such as Timetal 21S, Ti 15-3, Alloy-C, Ti-6-4, Ti-6-2-4-2, Ti-24-11, alpha₂, alpha+alpha₂, and orthorhombic. The validity of this concept was examined relative to the three viewpoints describe above and was found to be viable.

Clearly, for composite materials this concept has worked well and it is believed that utilization of such a concept in a broader context of both monolithic and composite materials would greatly facilitate the development of ICME. Since a model material could be the unifying element between materials scientists (those who design “the material”) and engineers (those who design “with the material”) and those in between; in that it would provide an opportunity to create a database of experimental observation at every scale (process, structure, property and response). Such a strategy would enable identification of salient features, physic-based mechanisms, accurate constitutive models at each length scale and thus the development of a multiscale modeling framework that would span all length scales for a given model material class. Further, experts from each discipline area could clearly define their requirements to complete their research on said model material system, thus stimulating synergism between disciplines and enabling maximum leveraging of evermore constrained resources. Clearly, to make this necessary interchange between disciplines a reality requires easy access to all available data (i.e., mechanistic, experimental, analytical) both planned and completed through a single information conduit (i.e. National ICME database). Another advantage of utilizing the model material concept lies in the fact that various models, MM strategies and techniques developed could be easily compared and contrasted to one another since identical data (both exploratory, characterization and validation) would be available to all modelers. Furthermore it would provide funding agencies (both government and industry alike) the opportunity to take advantage of prior work, continue to enhance understanding and model refinement on a model system, while still examining/developing a specific material of interest within the class needed for their application. Such leveraging is only possible by use of the model material concept and recognition that it enables noncompetitive model and tool development/enhancement/verification while still preserving the ability for an organization to use these tools for competitive advantage.

National ICME Information Management System

Informatics has been defined as the science concerned with gathering, manipulating, storing, retrieving, and classifying recorded information. A key aspect of informatics is its focus on understanding problems with which the information is associated and then applying information

technology as needed to address those problems. The need to build an information infrastructure that can not only capture, analyze and disseminate explicit knowledge, but also one that enables contextual linkage and association (probably through the use of metadata) so as to enable the discovery of new knowledge as well is recognized (cf. 2008 ICME report by National Material Advisory Board [1]). The existence of such a system, tailored for the ICME community, would then maximize the impact on both material and structural discipline practitioner and/or researcher. At the core of such a system is the ability to capture the fundamental response data (with its full pedigree, chemistry, processing, heat treatment, testing information, etc.) at a given length and time scale and application potential of a given material system (be it monolithic, composite, multifunctional, etc.) and not just specific predefined (generally accepted) values. So that as knowledge evolves these and other yet unmined data can be processed and linked thereby becoming information and ultimately knowledge¹.

This general data, information, knowledge pyramid is at the core of the material data lifecycle (see Figure 2) proposed by the Material Data Management Consortium (MDMC)², wherein data is captured and consolidated from external sources, legacy databases as well as internal (possibly proprietary) testing programs. Next data is analyzed and integrated to create/discover useful information and then deployed (disseminated) to the people who need and use it. With the continual maintenance of the whole system (the data and information generated as well as the relationships, or links, between them) being the last yet essential stage of the data lifecycle. Note that the middle ring of Figure 2 provides additional information regarding the type of data utilized and functions performed during each phase in the data life cycle; while the outer most ring details the individuals most likely responsible for these functions.

To support the various required activities throughout this data lifecycle requires the (preferably seamless) integration of a variety of software tools. These range from data input, reduction/analysis, visualization, reporting tools; material parameter estimation tools; process/microstructure/property/performance models (in the case of ICME); product life management tools (PLM); to structural analysis codes that utilize a central database. These tools



Figure 2 : Four Aspects of Material Data Lifecycle

¹ Knowledge begins with data, yet data in and of itself has no meaning. Data only describes what is or what was. Information is data with meaning as it puts the data in context relative to other data. Knowledge is then information with intrinsic value, implications or connections [3].

² A group of aerospace and energy sector organizations (both industrial and governmental) that have joined forces to develop best practices and associated software tools to integrate material and structural information technology with the realities of practical product design and advanced research. This group was established (through collaboration) with ASM International, NASA Glenn Research Center and Granta Design Limited in 2002 and is currently in its ninth year of operation, see www.mdmc.net.

should enable material and structural engineers to input, manage and utilize information in as an efficient, reliable and user-friendly way as possible. Finally, these tools should also enable enterprise-wide (even world-wide) solution or access.

The type and extent of material information routinely collected however, is not always sufficient to meet the current, much less future needs of the material modeling community, due in part to the ever increasing emphasis on nonlinear analysis as industry attempts to cut costs and extract maximum performance from their products. Consequently, we must not limit ourselves to the collection of material parameters and information which merely satisfy the input requirements for conventional design/analysis methods alone. Rather we must strive to collect (through exploratory, characterization and validation testing) and capture to the largest extent possible the complete multiaxial response history (e.g., stress, strain, time and temperature) for a given material (for more on this, see Reference [4]). Clearly a trade-off exists between the cost of data acquisition, storage, maintenance and dissemination and the current and future value of the data being collected. However, this trade is extremely difficult to make *a priori* as one often times does not comprehend the importance of the data/information until after some time has elapsed and the window of opportunity has passed. Therefore, one should collect as much information as possible at the time to avoid being in an “if only I had ...” situation.

A possible material information management database schema (not developed with ICME needs in mind) illustrating (at a very high level) a portion of the information contained and its associated linkage within this centralized database is depicted in Figure 3. Note that within each dotted area a number of lower level data tables would be grouped. For instance within the Test Data management area, one would find data tables for each category of test data (i.e., tensile, creep, relaxation, cyclic, crack growth, etc.) wherein each individual record would contain both the generally accepted point wise values and the complete response histories for each individual tests along with images of failure surfaces and microstructures. While within the statistical test data section, one would find the corresponding consolidated (statistically rolled-up) response of a given material for each test category of interest. Finally, after further consolidation and characterization of company specific algorithms and life modes, the corresponding material design allowables (e.g., stress, strain, elongation, etc.) would be stored for each material of interest. Such information storage and linkage enables full traceability of each and every data item. Clearly, with ICME in mind this schema could be altered so that the attributes within the design data table could correspond to process/microstructure/property/performance relationships thus facilitating ICME of the various materials (i.e., model materials) stored within the system.

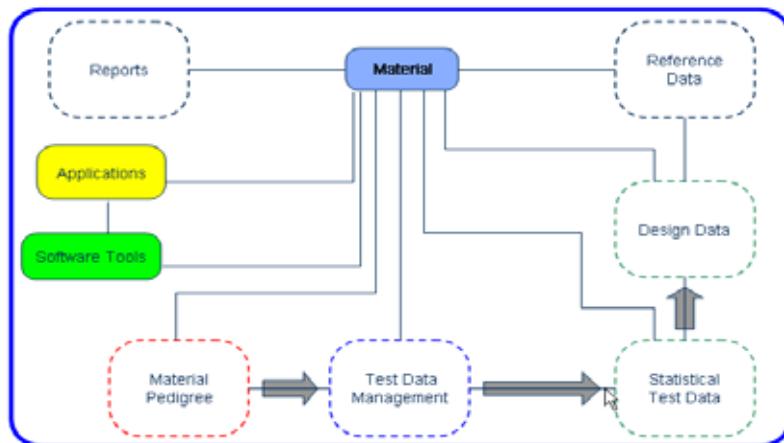


Figure 3 : Schematic illustrating a possible data schema for the material information

A robust material information management system (Granta MI[®], see [5]), specifically designed and fully equipped to handle a schema like that of Fig. 3, as well as other more complicated user-defined schemas, is currently available as a result of the MDMCs efforts.

Consequently, it is possible that a national ICME database (i.e., information management system) could be deployed without significant fundamental development work required. As an example of one type of database that will be needed for the ICME people doing atomistic work is a database of interatomic potentials. In fact one does exist. In her chapter, Dr. Chandler describes the interatomic potentials repository hosted by NIST. While it is not technically a database, the basic idea of having a repository of interatomic potentials may be crudely understood as one. The reason for bringing up this repository is not to point out that such a “database” exists but that this repository is a public one. It is public in the sense that anyone can publish their data to the website and public in the sense that it is available to anyone who desires the data. The public aspect of this “database” serves as an example of what is needed. In fact, this is not the only example. The 2008 ICME report by the NMAB [1] also make mention of the human genome project (HGP) and the database created by the U.S. Department of Energy and the National Institute of Health in order to capture and share data related to the 20,000+ genes in the human DNA and the sequences of 3 billion chemical base pairs that make up the human DNA. The 2008 ICME report laments that a similar database similar to the model developed for the HGP does not exist for ICME. But the report falls short of recommending that such a publicly funded database for ICME be actually developed.

It is the belief of the editors of this book that a public database for every aspect of ICME is needed and is achievable. A continuum of potential funding options, from fully private to fully public, can easily be envisioned. The consortium based option involving individual organizations contributing either hard cash, intellectual property (physical data or software tools) or some combination thereof to establish, populate and maintain this database is an intriguing one.

ICME Consortiums

In their chapter, Drs. Cowles, Backman, and Dutton partition the collective concept of ICME into three general focus areas:

1. **Material development:** alloy and composition, processing methods, microstructure, nominal properties.
2. **Process modeling:** thermomechanical processing of specific alloy, resultant microstructure, nominal properties, process yields, residual stresses, defect species and occurrence rate. Also, significant integration between supply chain and OEM companies would be expected here, and cost modeling of material and processes would be a critical element for that interaction.
3. **Material behavior:** microstructure, properties, service aging, residual stresses, constitutive behavior and life modeling, including variation assessments, and effects of defects. Probably limited integration here between supply chain and OEM companies would be expected; but significant interaction between OEMs and USAF and/or regulatory agencies would be likely.

The threefold division was offered to help partition the vast ICME universe into more manageable categories. They also suggested that such classification is not only helpful, but possibly even essential, to assess appropriate participants and potential sponsors, required fidelity, validation requirements, and benefits that may be achieved for specific ICME

development and implementation efforts. We would like to utilize their classifications and recommend that the ICME community establish targeted consortiums along these three focus areas in order to develop/enhance the various required ICME infrastructure thus making ICME a reality. These consortiums would ideally be comprised of and therefore necessarily engage the four “foundational groups”, i.e., 1) industry, 2) government, 3) universities, and 4) professional societies that Dr. Spanos espoused. Such a consortium helps overcome the numerous cultural and organizational barriers associated with the first three of these groups that Dr. McDowell discussed in his paper.

The establishment of either a single ICME consortium with three subcommittees (one for each focus area) or three individually focused consortiums would have the following significant advantages:

1. Provide a stable source of funding for precompetitive fundamental tool development based upon mechanistic understanding of model materials
2. Provide a forum for establishing and disseminating best practices and lessons learned, respectively.
3. Enable material scientist, physicists and mechanicians (e.g., structural engineers and constitutive modelers), both researchers and practitioners from industry, government and academia alike to interact and influence one another on a regular basis.
4. Provide a natural forum for establishing cross disciplinary/organizational teams/partnerships to respond to outside funding opportunities.

Such a consortium can be extremely successful, provided that a clear vision/purpose is established at the outset with clearly defined rules of engagement and regular (e.g., semi-annual face to face and monthly telecom) working meetings. Furthermore, it is extremely important that a steering committee be established to enable each participating organization to have an equal vote in the prioritization and allocation of internally generated development funds. In this way, each organization can get significant return on their investment, the actual multiplier depending upon the number of participating organizations. Also, we highly recommend, that the chairman of the consortium(s) be either a technically savvy government official or technically savvy person from one of the societies (provided that such a person is not connected with either industry or academia). Only such a person can maintain maximum independence, ensure a level playing field for all members, and ensure that the resulting toolsets will be most advantageous for all parties involved and for the nation. As should be clear, these consortiums are an excellent way for the four foundational groups to play a role in the development of ICME. This is exemplified by the MDMC discussed earlier in the previous section. Wherein, ASM International (a materials society) played a leading role in co-founding and sustaining the MDMC. This consortium consists of active industry and government members organizations from the aerospace, defense and energy sector and is lead by a member who is from a government agency, NASA Glenn Research Center. Together they have worked to develop a flexible material information management system (database tool – for material properties and response spectrum) that can be integrated within an ICME toolset.

Upon reflection it is apparent that the establishment and utilization of 1) the model material concept, 2) a national ICME database (ultimately information management system), and 3) ICME consortiums with particular emphasis on a) material development, b) process modeling and c) material behavior modeling focus areas should effectively break down barriers and overcome the various challenges articulated in this book. Let us therefore boldly approach this exciting and critically important new field with the full recognition of our need for interdependent collaboration, creativity and resourcefulness; but most of all a commitment to succeed - for failure is not an option.

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