Integrated Computational Materials Engineering: A New Paradigm for the Global Materials Profession

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Integrated computational materials engineering (ICME) is a new field of study that is evolving within the global materials profession. It promises to revolutionize the way the engineering community deals with materials and the way the materials community provides input to the engineering and scientific communities. In fully mature form, ICME entails integration of information across length and time scales for all relevant materials phenomena and enables concurrent analysis of manufacturing, design, and materials within a holistic system. The ICME approach involves systems engineering analysis (e.g., multi-attribute optimization and uncertainty analysis) to solve complex design and materials problems. Integrated computational materials engineering offers a solution to the industrial need to quickly develop durable components at the lowest cost. It has important potential for accelerating the development of new materials.

At its core, ICME involves the development of materials models that quantitatively describe processing-structure-property relationships for use by the engineering community. The development of these relationships, as depicted in Figure 1, has been a unifying paradigm in the field of materials science and engineering since its inception. However, this important paradigm has not yet produced an effective computational engineering tool comparable to those used by mechanical engineers to analyze heat transfer, fluid flow, and structural mechanics. In no small part, this is due to the profound complexity and breadth of issues that must be addressed in the engineering of materials. We postulate, however, that the lack of a computational tool for materials engineering has been largely due to a culture within the materials profession that has focused on digging deeply to understand isolated phenomena such as solidification or fatigue behavior (so-called knowledge "nodes") at the expense of the linkages between the knowledge nodes. The focus of ICME is on developing these linkages, building quantitative models and databases that populate the knowledge base, and using the resulting system to solve materials development and application problems.

Modern computing, in many instances, enables the prediction of microstructures and properties from fundamental principles. These tools are diverse and range from the atomic level to the continuum level and from thermodynamic models to physics-based property models. While the models provide important insights, there is no widespread organized effort to link them and provide them within an integrated suite of engineering tools. This is the vision for ICME: a comprehensive, integrated suite of validated computational materials models linked to analysis systems for manufacturing processes and engineering design. Such a suite of tools in a robust, user-friendly computational environment would enable simultaneous optimization of manufacturing process and component design, materials selection, or rapid materials development with calculation of uncertainty metrics.

Optimal development of any engineering component requires equal and ready knowledge of the performance require-

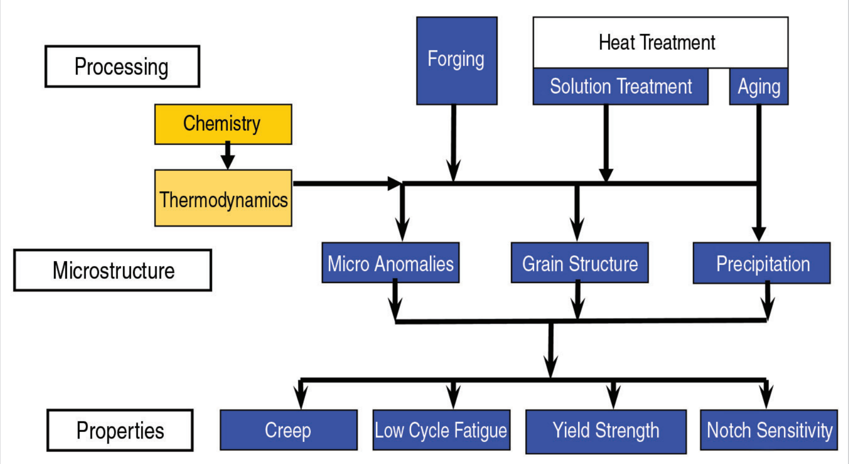

Figure 1. An example of key processing-structure-property linkages for forged nickel-based superalloys.

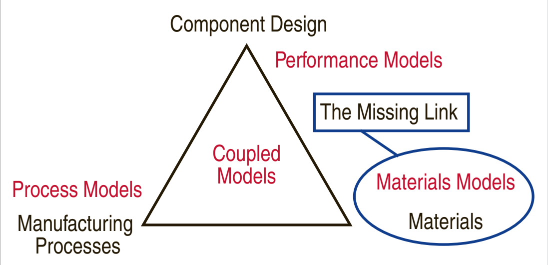

Figure 2. Integrated computational materials engineering (ICME) enables the integration of manufacturing and design via advanced materials models.

ments of the component, the manufacturing process used, and the materials from which it is fabricated (Figure 2). Due to the complexity of the constraints and the need to optimize for multiple properties, this optimization process can be most effectively achieved by using models. Closely coupling computational models for manufacturing processes and engineering design has many important benefits, including reducing the time and cost required to develop new products, reducing manufacturing costs, and enhancing performance. The missing link, however, has always been the absence of the materials models to bridge these disciplines, or more specifically, materials models that robustly capture the dependence of material properties on manufacturing history.

The lack of such materials models in an integrated modeling framework that includes manufacturing and design has also limited the development of new materials. Because of its complexity and broad scope, materials engineering is a decade or more behind other engineering disciplines in developing a core set of computational tools available to practicing engineers. Finite-element analysis and computational fluid dynamics are central to mechanical engineering curricula and are routinely used by practicing engineers in manufacturing and engineering design. There is no analogous computational tool available to materials engineers despite many significant accomplishments in computational materials science. Thus, development of new materials has required the slow and costly experimental approach.

Although there is currently no widespread effort to create ICME tools, proof-of-concept of the ICME approach has been demonstrated in programs such as the U.S. Defense Advanced Research Projects Agency's Accelerated Insertion of Materials program, the U.S. Air Force Office of Scientific Research's Materials Engineering for Affordable New Systems, and in limited cases within industry.[1,2] These developments have been for metallic materials such as nickel-based superalloys for forged aeroengine turbine disk development and aluminum alloys for cast automotive powertrain components. Although they have only recently been developed and are thus not yet fully mature, these tools are currently in use within industry and have demonstrated significant economic benefits. Two of the articles in this issue are illustrative of applications of ICME tools within Ford Motor Company and General Electric. Some of the capabilities demonstrated by these proof-of-concept studies include the ability to reduce the number of materials development iterations and thereby reduce the cost and duration of materials development by up to 50%; the simultaneous optimization of product and manufacturing processes, with multiple property constraints; a substantial decrease in the time and cost required to develop a new engineering component; and the earlier assessment of material variability.

These programs have also revealed lessons learned that highlight ICME development needs that must be met and success factors that must be considered, including the importance of deciding which high-priority problems should be solved by ICME and identification of the specific system outputs required by design and manufacturing engineers/systems; database-driven empirical models are acceptable when physically based models are not ready; development of ICME material models by a geographically distributed work team is feasible; the acceptance of ICME results can be improved by diligently characterizing the range of applicability of specific models, including their uncertainty and the propagation of this uncertainty in linked models; for the foreseeable future, the pragmatic designer and manufacturing engineer will require the validation of ICME-derived solutions; and to use these tools in an effective manner within industry, thoughtful attention to how ICME-based models fit efficiently into engineering methodologies is required. Culture changes may also be required within industrial organizations.

The future development of ICME as a new paradigm for the materials profession is enabled by a number of factors. Arguably the most important enabler may be the growing recognition within academic institutes, industry, national laboratories, and professional societies that ICME is feasible and important. We believe that this represents an important culture change within the materials profession. With the increased attention and efforts this engenders, it is conceivable that ICME will begin to self-propagate. Another important factor is that a well-developed, fundamental, and quantitative knowledge base exists for many mature materials, metallic materials, in particular. Integrated computational materials engineering is also enabled by the availability of the open framework of some commercial software products. By allowing user-defined subroutines that describe material behaviors, these commercial codes allow customization without the need for extensive programming. Computational efficiency is especially important for large components with complex geometries, complex manufacturing processes, and where capturing complex non-linear physics is required. The widespread availability of high-performance, multi-processor computing hardware and software has provided a means to at least partially resolve this issue.

TMS ICME TECHNICAL COORDINATION GROUP

Over a five-month period in 2005, an 18-person ad hoc advisory group, consisting of representatives from key TMS technical committees and specialists from industry, academia, and government collected information on current efforts in integrated computational materials engineering (ICME), provided their own insights on problems and challenges, and developed a set of recommendations and associated action items for consideration by the TMS Board of Directors. At the 2006 TMS Annual Meeting, the Board of Directors commissioned the current ICME Technical Coordination Group (TCG). In particular, the group has been charged to:

- Develop an integrated three year plan for information dissemination on ICME
- Become the professional home for the ICME community
- Facilitate educational development in ICME
- Facilitate technical development of ICME

The TMS Board approved special project funds to enable this activity. Many of the implementation actions will be via existing TMS technical committees with the TCG acting in an advisory and catalyzing capacity. By taking an integrated approach and building on the TMS web infrastructure, the group seeks to provide mechanisms to accelerate the development and linkage of models and databases, leading to the broader application of computational methods in materials science and engineering.

The realization of the full potential of ICME is a grand and worthy challenge for the global materials profession. A central requirement to meet this challenge will be the development of a global infrastructure or protocol for information exchange and interfacing of models. This will include interfaces for different manufacturing simulation software with materials models and, in turn, with design analysis tools. Protocols must be developed to integrate hierarchical modeling approaches and to link microstructural evolution models with property models. To effectively harness the global knowledge base, these infrastructures must enable geographically distributed modeling activities and allow networks to develop naturally and effortlessly while protecting proprietary and security interests. This will also require a cultural shift within the materials community to concentrate equal attention on fundamental insights and the linkages between the knowledge nodes.

Other important requirements for ICME are the identification of gaps in our knowledge base and the development of models and theory to fill these gaps; increased development of materials informatics systems, which fuse high-fidelity experimental databases with models of physical processes (an article on this topic rounds out this special group of papers on ICME); continual emphasis on computational efficiency; and experimental validation of models.

Finally, there is a growing awareness of the importance of coordinating efforts and funding for ICME. The benefits of ICME are substantial; however, due to the enormity and complexity of the task, no single institution or firm can accomplish the ultimate goal alone. It truly represents a grand challenge that will require coordinated efforts of many organizations. There are important roles to play for governments, professional societies, funding agencies, and consortia. In this regard, three recent activities bode well for the future of ICME. First, the National Materials Advisory Board has initiated a major study sponsored by the U.S. Department of Defense and Department of Energy to develop a more complete understanding of ICME and to roadmap this technology. Second, TMS has established an ICME Technical Coordination Group to foster awareness and activities in this field (see the sidebar for details on this group). Finally, the U.S. Automotive Materials Partnership is initiating an ICME pilot project on magnesium alloys and processes. The initial goal of this project is to develop a global infrastructure and the required knowledge base and linkages to allow optimization of magnesium alloys and manufacturing processes for future automotive applications.

CONCLUSION

Integrated computational materials engineering is a field of study whose time has come. It promises to link manufacturing and design via advanced materials models in a seamless, integrated computational environment. The feasibility of ICME and its benefits have been demonstrated by several projects that have developed methods which are in use in the aerospace and automotive industries. To fully realize the potential of ICME, a number of technical, cultural, and organizational challenges have been identified and must be overcome.

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