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ACCELERATING TECHNOLOGY TRANSITION

Bridging the Valley of Death for Materials and Processes in Defense Systems

Committee on Accelerating Technology Transition
National Materials Advisory Board
Board on Manufacturing and Engineering Design
Division on Engineering and Physical Sciences

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Enabling Tools and Databases

The well-established success of computational engineering in various disciplines has fostered a rapid adaptation of computation-based methods to materials development in the commercial sector in recent years. Several examples are shown in Table 3.1. Early successes in computational materials engineering provide a clear vision of the way forward to enhance capabilities across the academic, industrial, and government technology developers and users. The importance of this opportunity is well recognized in recent national studies. For example:

- Acknowledging materials as one of the five critical technologies for U.S. competitiveness in the new century, the President's Office of Science and Technology Policy identified computational materials design as a principal opportunity.[1]
- In addition to emphasizing the primary importance of accelerating materials technology transition, recent studies of the National Research Council on materials and manufacturing research needs of the Department of Defense (DoD) have made computational materials design based on mechanistic models a principal recommendation for research investment.[2,3]

ESTABLISHED COMMERCIAL PRACTICE: ACCELERATED DEVELOPMENT

The aerospace original equipment manufacturer (OEM) community in particular has established a viable track record in the computation-assisted, accelerated development of materials and processes. In the environment of a modern integrated product team (IPT), the risks of materials development have been identified early in the process, and empirical materials models have been integrated with other computational tools (e.g., finite-element method) for early risk reduction and for the accelerated attainment of specific technology readiness levels (TRLs). Two specific examples presented at the workshop by Jack Schirra of Pratt & Whitney were the rapid (in 4 months) resourcing of a fan hub bonding process using available process and property models, and the rapid introduction of a new, high-temperature, high-strength shaft alloy through the integration of empirical microstructure and property models into finite-element processing models, demonstrating a three to four times reduction in time and

[1] S.W. Popper, C.S. Wagner, and E.V. Larson. 1998. New Forces at Work: Industry Views Critical Technologies. Washington, D.C.:The Science and Technology Policy Institute of the RAND Corporation, MR-1008-OSTP.

[2] National Research Council. 2003. Materials Research to Meet 21st Century Defense Needs. Washington, D.C.: The National Academies Press, pp. 3-4.

[3] National Research Council. 2004. Retooling Manufacturing: Bridging Design, Materials, and Production. Washington, D.C.: The National Academies Press.

TABLE 3.1 Some Computational Materials Engineering Tools

Type	Tool	Company	Function
Design integration	iSIGHT	Engineous Software (Salt Lake City, Utah)	Multidisciplinary design optimization (MDO)
	CMD	QuesTek Innovations LLC (Evanston, Illinois)	Parametric materials design
Macroscopic process modeling	ProCAST	ESI Group (Paris, France)	Solidification processing
	DEFORM-HT	Scientific Forming Technologies Corporation (Columbus, Ohio)	Deformation processing and heat transfer (finite-element method)
Microstructural simulation	PrecipiCalc	QuesTek Innovations LLC (Evanston, Illinois)	High-fidelity precipitation simulation
	DICTRA	ThermoCalc AB (Stockholm, Sweden)	Multicomponent diffusion
	J MatPro	Thermotech Ltd. (Surrey, United Kingdom)	Phase relations and basic microstructural modeling
Thermodynamics	ThermoCalc	ThermoCalc AB (Stockholm, Sweden)	Multicomponent thermodynamics and phase diagrams
	Pandat	CompuTherm LLC (Madison, Wisconsin)	Multicomponent thermodynamics and phase diagrams
	FactSage	Thermfact CRCT (Montreal, Canada)	Multicomponent thermodynamics and phase diagrams

an 80 percent reduction in cost. These examples use statistically derived deterministic models to accelerate process optimization based on the behavior of mean property values.

At the workshop, Joel Clark of the International Motor Vehicle Program of the Massachusetts Institute of Technology (MIT) discussed practices that are well established for the application of technical cost modeling tools throughout the development cycle. Based in a process cycle context, these tools allow the quantitative consideration of the economic consequences of choices regarding material, process, and design, with the goal of anticipating opportunities and tactical choices at very early stages while the costs of change are still small. The tools integrate quantitative materials kinetic models to assess temperature and time trade-offs in materials process cost analysis. Such tools are broadly applied across diverse manufacturing sectors, including the automotive and optoelectronics sectors.[4]

[4] J.P. Clark, F.R. Field III, and R. Roth. 1997. Techno-economic issues in materials selection. ASM Handbook, Vol. 20, Materials Selection and Design. Materials Park, Ohio: ASM International, pp. 225-265.

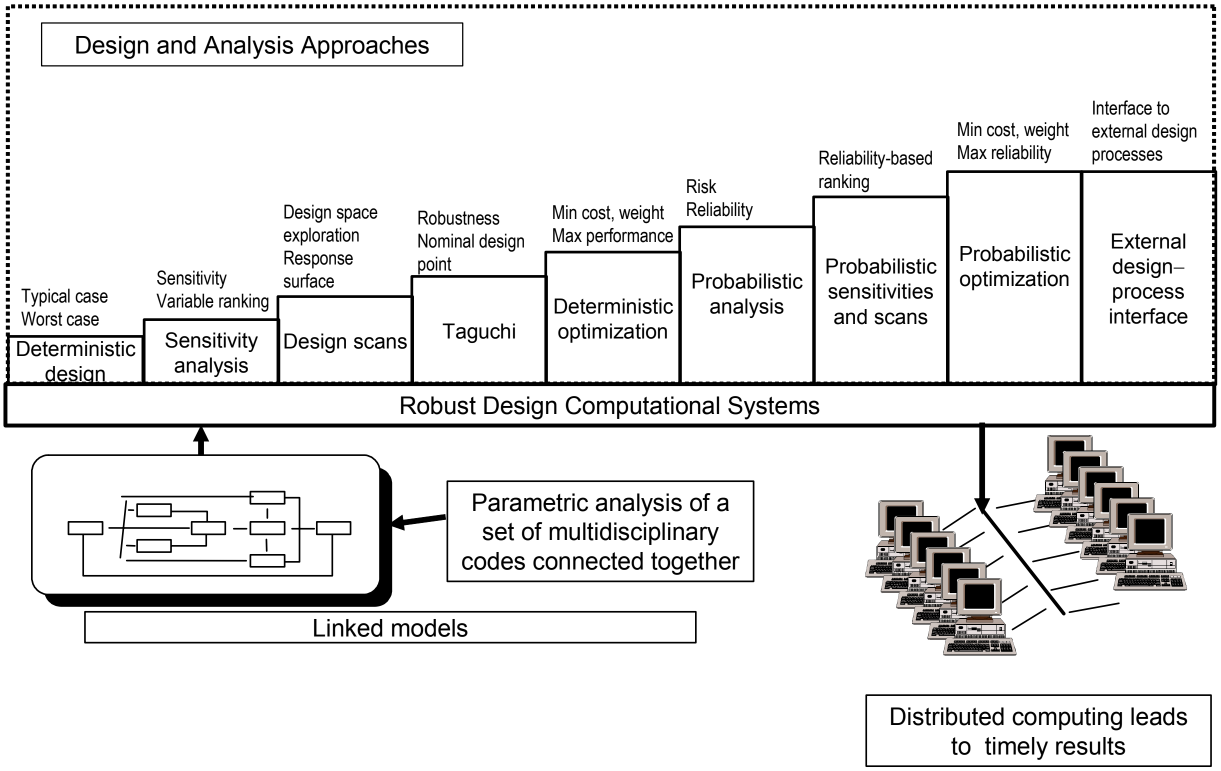


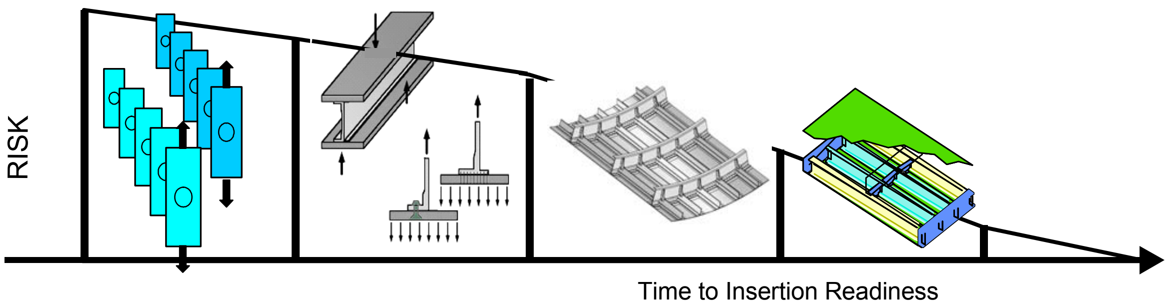
FIGURE 3.1 Range of design and analysis tools employed under the Robust Design Computational System (RDCS)—the design integration system used in the Accelerated Insertion of Materials–Composites (AIM-C) effort for the accelerated development of polymer-matrix composites. SOURCE: Copyright 2003, The Boeing Company. Used with permission.

EMERGING COMMERCIAL PRACTICE: DARPA'S ACCELERATED INSERTION OF MATERIALS PROGRAM

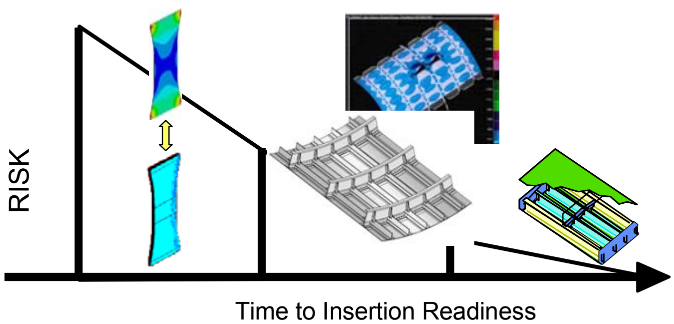
A new level of capability has very recently been demonstrated in the highly successful 2.5-year Phase I effort of the national Defense Advanced Research Projects Agency (DARPA)-AIM (Accelerated Insertion of Materials) initiative. Several presenters at the workshop described various aspects of this effort. A metals team led by Pratt & Whitney and GE Aircraft Engines and a polymer matrix composites team led by Boeing were involved in this initiative. The teams have integrated OEM, small company, university, and government laboratory activities in an IPT approach, to establish a new framework and methodology for the integration of available tools in the accelerated development and qualification of new materials and processes. The Phase I effort successfully demonstrated the ability of the methods to efficiently reconstruct both optimal processing conditions at the component level and observed property variation as established by legacy databases of existing materials; it also provided preliminary demonstrations of effective prediction of improved processing conditions for these materials.

The collaborative framework adopted by both AIM teams has employed the existing multidisciplinary design optimization (MDO) software broadly employed in systems engineering design to link diverse computational tools spanning multiple platforms and locations, efficiently integrating them with modern optimization strategies. One AIM metals team (Pratt & Whitney and GE Aircraft Engines) has employed the commercial iSIGHT design integration system, while the Boeing Accelerated Insertion of Materials-Composites (AIM-C) team has employed the Robust Design Computational System (RDCS) software. Figure 3.1 summarizes the range of capabilities of the computational systems employed in the AIM-C effort, spanning deterministic and probabilistic methods of analysis and design.

Efficient and effective integration of existing models has demonstrated a significant qualitative



(a) Traditional test supported by analysis approach.



(b) AIM provides an analysis approach supported by experience, test and demonstration.

FIGURE 3.2 Examples of materials and process development acceleration using computational tools demonstrated under the Accelerated Insertion of Materials–Composites (AIM-C) effort. SOURCE: Copyright 2003 The Boeing Company. Used with permission.

shift from an analysis-supported testing-based approach to a testing-supported analysis-based approach with an emphasis on efficient, model-driven focused testing. Figure 3.2 summarizes AIM-C demonstrations of successful model integration replacing traditional 6-month experimental efforts with 2- to 3-day modeling-based activities.

The original AIM Phase I goal was to accelerate the process of producing a traditional design knowledge base (DKB) specifying materials properties for fixed processes. A natural consequence of the new linked concurrent materials modeling capability, however, has been to create a new, active form of DKB in which the system designer can assess process and property trade-offs on the basis of estimated properties as an active part of the system design process. An example presented by Schirra at the workshop from the AIM metals program indicates that active linking of materials models to the integrated design of a subscale disk and its thermal processing accurately predicted improved performance and failure modes validated in actual disk burst tests. The timescale of the demonstration was 4 months from concept to validation.

The AIM metals effort has also demonstrated the potential predictive power of fundamentally based mechanistic models as an alternative to the more expedient statistically based empirical models commonly employed in earlier industrial efforts. This capability was achieved by the rapid concurrent development of a numerical precipitation code (PrecipiCalc) grounded in fundamental alloy thermodynamics and multicomponent diffusion. After small extensions of both a commercial thermodynamic database, Thermotech NiDATA, and a National Institute of Standards and Technology mobility database to include one additional alloying component, the mechanistic precipitation model gave highly accurate predictions of trimodal precipitate size distributions and phase compositions as functions of complex industrial thermal processing cycles in both IN100 and Rene88DT disk superalloys.

Coupled to finite-element simulations of disk heat transfer via the iSIGHT integration system, the model has given quite accurate predictions of the measured macroscopic spatial variation of precipitate

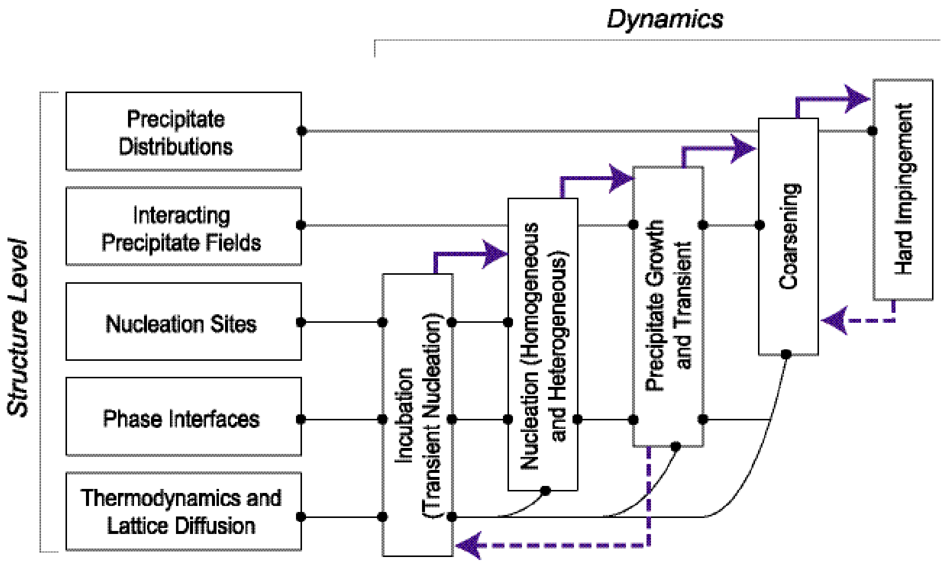


FIGURE 3.3 Schematic representation of mechanistic numerical precipitation code (PrecipiCalc) employed in Accelerated Insertion of Materials (AIM) metals demonstrations. SOURCE: C. Kuehmann, QuesTek, Tools for Design, Development and Qualification of New Materials, briefing presented at the Workshop on Accelerating Technology Transition, National Research Council, Washington, D.C., November 24, 2003.

distributions in actual turbine disks. Linking the microstructural predictions to a structure and property model accurately predicts measured spatial variation of yield strength. The essential physical behaviors incorporated in the general-purpose precipitation code are summarized schematically in Figure 3.3. Examples of output shown include the time evolution of average precipitate size and the final size distribution. For efficiency, the numerical model is designed to compute only the microstructural parameters needed to support existing structure/property relations.

The deterministic modeling of mean behaviors has proved quite effective in the demonstration of accelerated process optimization at the component level. A major thrust of AIM research in accelerated materials qualification, however, has been the development of probabilistic modeling approaches for the reliable early prediction of DKB minimum properties, with greatly reduced reliance on test data. Adopting a mechanistic approach in which property variation is tied back to process and composition variation through predictable microstructural variation, the numerical precipitation code has served as the central transfer function allowing extensive supply-chain legacy process data to be transformed into predicted property variation under the AIM metals program. The exercise demonstrated multisite computation under the iSIGHT integration system linking distributed software capabilities in Connecticut, Utah, and Illinois; the exercise combined heat transfer, microstructure, and property calculations under a Monte Carlo simulation, incorporating known process variation as well as quantified variation in model parameters such as surface heat transfer coefficients. Computed probability distributions of yield strength at room and elevated temperatures resulted in predictions of minimum properties employing limited test data for model calibration, in good agreement with extensive legacy property data. In addition to early prediction of conventional DKB property minimums, accurate prediction of the full property probability distribution supports improved probabilistic design methods.

The industry-led DARPA-AIM team projects have provided a new clarity to the needs for computational materials engineering capability from an industrial perspective. This knowledge has already had a positive impact on allied academic research initiatives under DoD support. These notably include the Air Force Office of Scientific Research's (AFOSR's) Materials Engineering for Affordable New Systems (MEANS) initiative and the Office of Naval Research's (ONR's) Grand Challenge initiative in Naval Materials by Design. Together these foster a significant realignment of academic materials research activity to meet the computational engineering needs of a changing industry.

SMALL BUSINESS ROLE: MATERIALS BY DESIGN

Small businesses remain a vital source of technological innovation, as is evident from their supporting role in the DARPA-AIM program. The AIM program has drawn on traditional software companies serving broad industry markets, such as Engineous Software, Inc. (Salt Lake City, Utah) providing the iSIGHT design integration system and Scientific Forming Technologies Corporation (Columbus, Ohio) providing the DEFORM-HT finite-element analysis software applied in the turbine disk heat transfer simulations. In addition, the AIM effort has drawn on more recently emerging materials-centric businesses providing software products and services specific to computational materials engineering. These include QuesTek Innovations LLC (Evanston, Illinois), developers of the PrecipiCalc precipitation code; and several suppliers of materials thermodynamic software and databases including Thermotech Ltd. (Surrey, United Kingdom), CompuTherm LLC (Madison, Wisconsin), and ThermoCalc AB (TCAB) (Stockholm, Sweden).

Software products include a range of thermodynamics, multicomponent diffusion, and microstructural evolution codes supplemented by structure/property models. In addition to the PrecipiCalc code, specific software tools include the ThermoCalc (TCAB) and Pandat (CompuTherm) computational thermodynamics codes, the DICTRA (TCAB) multicomponent diffusion code, the JMatPro (Thermotech) suite of thermodynamics and simplified microstructural evolution models, and the CMD (QuesTek) materials design integration system. Available commercial services range from custom fundamental databases to full computational materials design and development on a proprietary contract basis. Commercial fundamental databases are supplemented by freeware databases distributed by NIST, representing an important new role of government laboratories in supporting this new industry.

As discussed by Charles Kuehmann of QuesTek at the workshop, small businesses may be able to support new cultures and can enable more visionary approaches than are typically possible in larger OEMs. He observed that while the DARPA-AIM initiative has focused on the later stages of development and the qualification of a material after it has been devised by traditional methods, QuesTek has implemented a broader approach for materials-by-design that builds on long-term research[5] to address the full design, development, and qualification cycle depicted in Figure 3.4.

In this approach, a broad set of tools and methods based on fundamentals are used for the rapid parametric computational design of complete materials and processes prior to making even the first laboratory prototypes. Parametric design models share a common foundation in fundamental databases and computational software to model thermodynamic and diffusion processes. These models use diffusion distance, time, and temperature constraints to provide efficient convergence to composition and process combinations. This is highly efficient compared to the more computationally intensive, explicit simulations of path-dependent time evolution of microstructure inherent in process optimization at the component level and probabilistic property modeling required in the later development and qualification stages of the materials cycle.

The incorporation of sensitivity analysis in parametric materials design allows design strategies that limit the potential for downstream property variation. The incorporation of scale effects in process models supports an approach to design for ease in processing that also reduces the risk of unanticipated scale-up problems inherent in the traditional materials-by-discovery approach. In contrast to the intensive characterization effort that was essential for the DARPA-AIM capability demonstrations on existing turbine disk alloys, the inherent predictability of materials designed this way makes them suited for more efficient accelerated development and qualification, applying the same models and validation results that created them in the first place.

As a specific example, the efficacy of computational materials design has been demonstrated with a family of high-performance gear and bearing steels designed to exploit capabilities of high-

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[5] G.B. Olson. 1997. Computational Design of Hierarchically Structured Materials. Science 277 (August):1237.

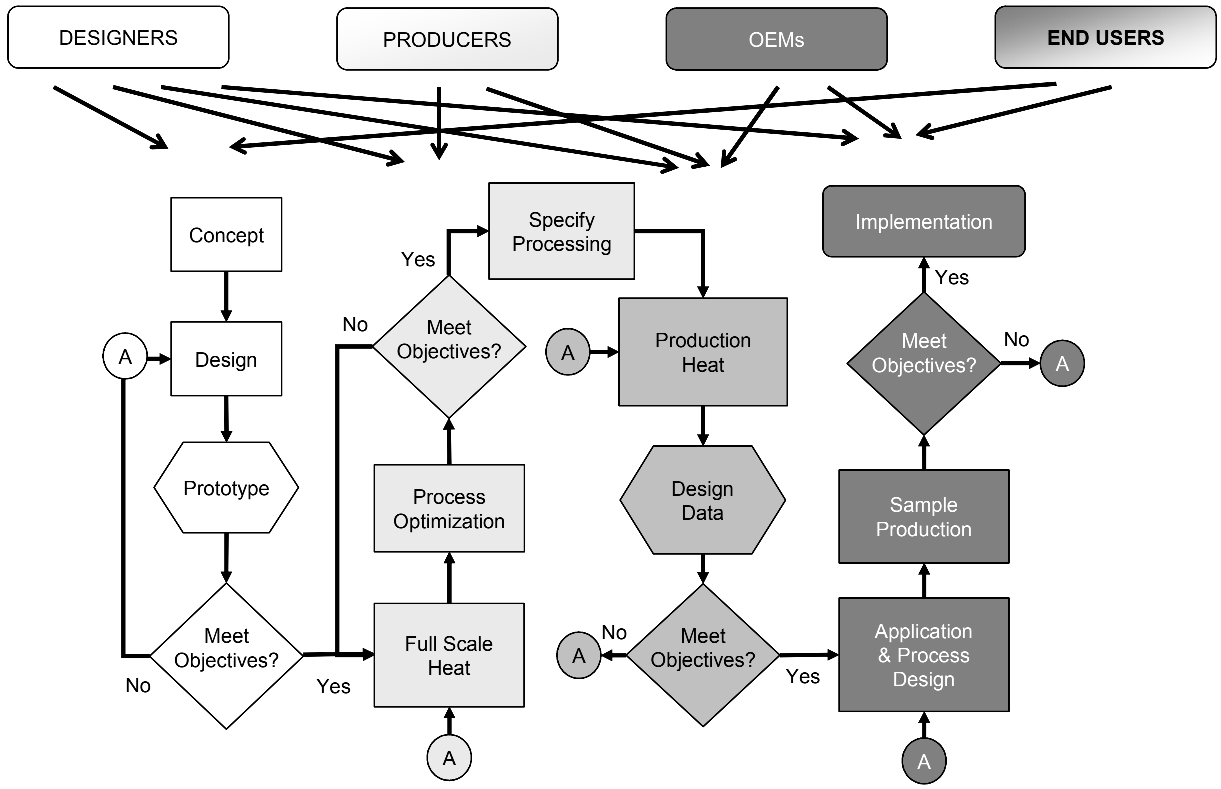

FIGURE 3.4 Flow chart of a full materials-development cycle, including initial materials design, process optimization/scale-up, and qualification testing. SOURCE: C. Kuehmann, QuesTek, Tools for Design, Development and Qualification of New Materials, briefing presented at the Workshop on Accelerating Technology Transition, National Research Council, Washington, D.C., November 24, 2003.

temperature carburizing processes.[6] Aided by process modeling based on the DICTRA multicomponent diffusion code, control of the new processing has enabled consistent achievement of new performance levels in automotive gearing, providing winning results on the racetrack, in parallel with certification testing for critical aerospace applications. These designs have spanned a range of materials, including high-performance shape memory alloys, metallic glasses, and ceramic systems.

The improved ability to predict the behavior of designed materials may also enable the expansion of the cycle to encompass the full material life cycle. Such phenomena as microstructural evolution in service may be modeled as a basis for structural health monitoring and forecasting. The inherent efficiency of design versus the traditional materials discovery approach also provides a system for affordable change in support of environmental sustainability. These methods to design materials have been used to achieve the goal of a stainless landing-gear steel, which can eliminate the need for cadmium plating. This new steel is undergoing accelerated certification testing. The project responsible for this development represents the first application of the AIM methodology to a new alloy, exploiting the full set of computational tools that created it.

In general, the AIM program has been successful at suggesting how to assemble the tools necessary to accelerate materials insertion. However, AIM methodology still needs to be transitioned into

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[6] C.E. Campbell and G.B. Olson. 2001. Systems Design of High Performance Stainless Steels: I. Conceptual Design; II. Prototype Characterization. Journal of Computer-Aided Materials Design 7:145-194; and C.J. Kuehmann and G.B. Olson. 1998. Gear Steels Designed by Computer. Advanced Materials and Processes 153(5): 40-43.

common practice, and the technology transition roadblocks identified in this report apply to it as well.

Another notable contribution of small business to the acceleration of materials technology implementation is the novel materials- and process-selection systems and supporting databases developed by firms such as Granta Design (Cambridge, United Kingdom) and Material ConneXion (New York, New York). These systems aid materials adoption by efficiently providing the information set for selection decisions from the perspective of a materials user. While Granta's Cambridge Engineering Selector system focuses on the technical needs of structural engineers, the Materials ConneXion system integrates aesthetic factors to support the broader needs of industrial designers and architects. This system also provides a natural architecture for the efficient integration of technical cost modeling in early design decisions, with the potential to support technical value analysis from a total performance perspective.

DISSEMINATION AND INFRASTRUCTURE

As an echo of the computational engineering revolution that has passed rapidly through other disciplines, the relatively recent appearance of computational materials engineering in high-tech ventures represents a new capability that is largely unknown to the majority of the materials community. An important first step in enhancing capabilities is simply that of spreading the word with respect to the tools, methods, capabilities, and achievements that already exist. An appropriate mechanism may be through ASM International—possibly in collaboration with NIST, modeled after their previous joint effort in phase diagrams. Regarding materials property data, a formal collaboration has already been established between ASM International and Granta Design to employ their selection system in the broad dissemination of new materials information.

The issues surrounding bringing modern engineering practices to such academic institutions as research universities and national laboratories has been a much-discussed issue in recent years. From the perspective of education, a series of workshops at Harvey Mudd College[7] has broadly addressed the challenges and opportunities for embedding a new design culture across all engineering disciplines including materials.[8] Under the current academic system, substantial investment in computational materials science has produced a wide array of computational tools. The majority of these, however, have so far proved to be of very limited engineering utility because they were never intended to support specific engineering needs.

Very significant exceptions are found in some materials-centered small businesses that are university spin-offs, typically founded by faculty forsaking the standard academic reward system to pursue commercially viable tools and methods meeting real needs of a new industry. In each case a productive synergy has been maintained with the parent university, which in turn enhances educational programs. A notable benchmark is the recent addition to the undergraduate materials science and engineering program at the Royal Institute of Technology in Stockholm, Sweden (originators of the widely used ThermoCalc thermodynamic software) of a degree in materials design and engineering.[9]

Wider development of technological competence in our academic institutions will require a higher level of vision from mission-oriented funding agencies. This could build on the examples of the focused

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[7] C.L. Dym, ed. 1999. Designing Design Education for the 21st Century. Proceedings, Mudd Design Workshop II, Harvey Mudd College, Claremont, Calif., May 19-21, 1999; Special Issue of International Journal of Engineering Education 17(4,5), 2001; C.L. Dym, ed. 2001. Social Dimensions of Engineering Design. Proceedings, Mudd Design Workshop III, Harvey Mudd College, Claremont, Calif., May 17-19, 2001; Special Issue of International Journal of Engineering Education 19(1), 2003; and C.L. Dym, ed. 2003. Designing Engineering Education. Proceedings, Mudd Design Workshop IV, Harvey Mudd College, Claremont, Calif., July 10-12, 2003; Special Issue of International Journal of Engineering Education 21(3), May/June 2004.

[8] G.B. Olson. 2000. Designing a New Material World. Science 288 (May): 993-998.

[9] Royal Institute of Technology in Stockholm. 2004. Curriculum in Materials Design and Engineering. Available at *http://www.kth.se/student/studiehandbok/04/lot_lista.asp?lang=1&program=BD&id=418*. Accessed July 2004.

AFOSR MEANS program, ONR Grand Challenge initiatives, and National Science Foundation centers.

A productive model may be the health-driven research system operated by the National Institutes of Health, spanning the full range from molecular biology to medicine. While the academic value system of the physical sciences has generally suppressed the creation of engineering databases, the life sciences have forged ahead with the Human Genome project representing the greatest engineering database in history. A parallel fundamental database initiative in support of computational materials engineering could build a physical science/engineering link as effective as the productive life science/medicine model. The highly successful DARPA-AIM initiative, which exposed academic participants to a well-managed IPT experience with clearly defined engineering objectives, can serve as a model for the new form of collaborative research activity enabling this needed transformation.

CONCLUSIONS AND RECOMMENDATIONS

Building on the success of computational engineering in various disciplines, rapid advances have occurred in recent decades in the adaptation of these methods to accelerated materials development in the commercial sector. While the first demonstrations have integrated empirical materials models, a new level of capability has been demonstrated very recently in the development and application of more predictive mechanistic numerical models under federally funded initiatives such as the DARPA-AIM program. Demonstrated capabilities include the following: accelerated process optimization at the component level, reducing scale-up risk; efficient, accurate forecasting of property variation to support qualification, with reduced testing for early adoption; and the active linking of materials models (exploring broader process and property trade-offs) in the higher-level system design process for the optimal exploitation of new material capabilities. Follow-on projects are actively applying the new tools and approach in the accelerated implementation of materials and processes in both polymer-matrix composites and metallic alloys for aerospace applications. Small businesses have played a vital role in these collaborative efforts. They have provided databases, tools, and methods and have expanded their capabilities to include initial parametric design of new materials, offering a unique level of predictability ideally suited to the accelerated development and qualification process.

The principal challenges and opportunities for the advancement of these capabilities concern (1) the wider dissemination of information on current capabilities and achievements, (2) the rapid transformation of the current array of academic computational materials science capabilities into useful engineering tools, (3) the broader development of necessary fundamental databases, and (4) a major infusion of modern design culture into our academic institutions to provide a pertinent research and education environment.

Recommendation 3. The Office of Science and Technology Policy should lead a national, multiagency initiative in computational materials engineering to address three broad areas: methods and tools, databases, and dissemination and infrastructure.

- *Methods and tools.* A collaboration between academia and industry built on such models as the Accelerated Insertion of Materials (AIM) program of the Defense Advanced Research Projects Agency should focus on the rapid transformation of existing, fundamental materials numerical modeling capabilities into purposeful engineering tools on a pre-competitive basis. The scope of the effort should encompass all classes of materials and the full range of materials design, development, qualification, and life cycle, while integrating economic analysis with materials- and process-selection systems.
- *Databases.* An initiative should focus on building the broad, fundamental databases necessary to support mechanistic numerical modeling of materials processing, structure, and properties. Such databases should span all classes of materials and should present the data in a standardized format. New, fundamental database assessment protocols should explore

optimal combinations of efficient experimentation and reliable first-principles calculations.

- *Dissemination and infrastructure.* A dissemination initiative should provide ready access to a Web-based source of pre-competitive databases and freeware tools as well as accurate information on the range of existing, commercial software products and services. Integrated product team-based research collaborations should be deliberately structured so as to firmly establish a modern design culture in academic institutions to provide the necessary, pertinent, research and education environment.