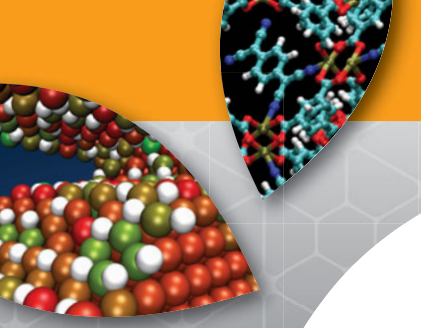

Integrated computational materials design for high-performance alloys

Wei Xiong and Gregory B. Olson

Major advances have been made over the past 30 years in the development of an integrated computational materials design (ICMD) technology. The hierarchical structure of its methods, tools, and supporting fundamental materials databases is reviewed here, with an emphasis on successful applications of CALPHAD (calculation of phase diagrams)-based tools as an example of ICMD, expressing mechanistic understanding in quantitative form to support science-based materials engineering. Opportunities are identified for rapid expansion of CALPHAD databases, as well as a major restructuring of materials education.

Introduction

In the past 25 years, many different programs have been launched to promote research in materials design, and several reports have been published regarding related activities in relevant research communities. An early report by the US National Research Council (NRC) in 1989[1] placed great emphasis on the role of the universal relationship among processing, structure, properties, and performance (see **Figure 1**[2]) for modern materials engineering and its impact on industrial applications. A 1999 NRC report[3] presented a strong industry perspective with an emphasis on the materials needs of clients. Such an emphasis required innovations based on design in materials and mechanical engineering. The report highlighted the importance of performance during both manufacturing and service, as well as its connection to user needs and constraints, and explored the importance of potential approaches to the acceleration of the materials development cycle.

It should be especially noted that a 2004 report on accelerating technology transition released by the NRC[4] prioritized a materials fundamental database initiative in support of accelerated insertion of materials (AIM) technology. This report stated, "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 report recommended that "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."[4]

In 2011, materials scientists were privileged to witness the unveiling of the Materials Genome Initiative (MGI) proposed by the US Office of Science and Technology Policy, further leveraging resources and capabilities of integrated computational materials engineering (ICME),[5] which is a landmark for advancing computational materials modeling in practical engineering applications. The AIM technology is considered to be a major component of ICME techniques.[5] As a result of the MGI, a complete integrated computational materials design (ICMD) hierarchical infrastructure for advanced materials development based on ICME and the materials genome is under construction as a global enterprise.[6–11] One of the goals of this article is to review and clarify the different levels of this infrastructure.

Through a review of historical milestones and a discussion of promising research directions, this article takes a close look at state-of-the-art ICMD driven by engineering applications. The article starts with a history of alloy design. The framework of ICMD is then illustrated by reviewing representative

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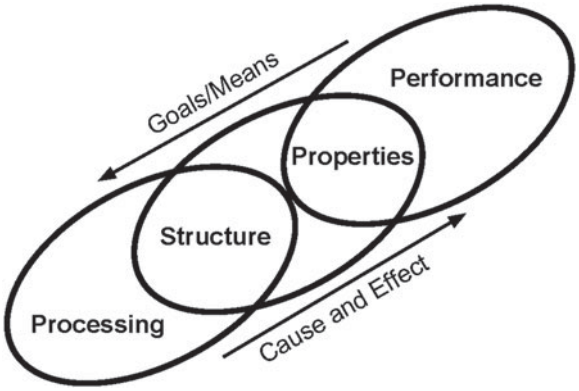

Figure 1. Three-link chain model of the central paradigm of materials science and engineering. Reproduced with permission from Reference 2. © 1997 American Association for the Advancement of Science.

integration efforts made through collaboration between research communities and industry. Finally, future research focuses for addressing remaining opportunities are recommended. It should be noted that, although the cases elucidated in this work are for metals and alloys, the thermodynamics-based methods of the ICMD infrastructure and the associated design philosophy should be applicable to polymers, ceramics, and biomaterials as well. Therefore, ICMD can be considered to be representative of the broader effort in computational materials science for engineering applications.

Milestones in alloy design

To be efficient, quantitative materials design needs informative databases from experiments or modeling. Without computational modeling, numerical solutions for theoretical equations are difficult to obtain, limiting the integration of theories for different phenomena. Therefore, design attempts made before the emergence of computational materials science were mainly based on trial-and-error experiments, which are time consuming and costly.

The earliest documented materials composition development was performed for the copper–tin-based alloy system in ancient China, generally known as the Bronze Age of China.[12,13] In "Six Alloys" (or "Liu Qi"), optimal weight percentages of copper and tin were summarized to guide the casting of various civil and military tools (see **Table I**).[14] Certainly, this can be considered only as a purely empirical optimization of alloy compositions. It is remarkable that such an empirical development persisted for more than three millennia.

A landmark in the field of predictive alloy design is the Hume-Rothery rules,[15] which have had a significant impact on research in physical metallurgy and materials science. These rules are for solid phases in metals and alloys and can be applied to both substitutional and interstitial solutions. Atomic size, electronegativity, valence, and crystal structure are considered to be the most important factors, based on experimental studies of numerous alloys performed by Hume-Rothery and colleagues. It should be noted that the Hume-Rothery rules are still used as component selection criteria. Tsai[16] showed that the Hume-Rothery rules are valid for all discovered stable quasicrystals with icosahedral structures by considering the characteristic range of valence concentrations in the quasicrystal alloys. Moreover, studies on the formation of high-entropy alloys also invoked size effects[17] and valence-electron concentration as criteria,[18] in line with the Hume-Rothery rules.

Similarly to the Hume-Rothery rules based on single-phase attributes, another method focused on the deleterious topologically close-packed (TCP) phases, such as the σ phase,[19] in nickel superalloys. This method, called PHACOMP (from "phase computation"), was invented in 1964[20] based on the criterion of the average number of electron vacancies in the metal *d* band above the Fermi level. This method was later revised several times, and more refined models were proposed to cover more detrimental intermetallic phases in the model prediction.[21–23] One of the pronounced disadvantages of this method is the temperature independence of the phase-stability criterion, which means that the model is valid for only a certain range of processing temperatures. As a consequence, it is quite limited in application to complex alloy processing. Despite many revised versions,[21–23] PHACOMP is mainly used today for rough estimations to avoid the formation of TCP phases, rather than optimizations of composition and processing parameters. It should be mentioned that another improved method following the PHACOMP approach, called the *d*-electron method,[24] was proposed that calculates the *d*-orbital energy level of the alloying transition element and the bond order as indicators for materials element selection. However, it also fails to optimize the alloy composition because of the very limitations inherited from PHACOMP.[24,25] A principal limitation of such methods is their basis in attributes of a single phase rather than direct treatment of phase competition.

A true breakthrough in alloy design was initiated in 1956[26] and developed throughout the 1970s, when Kaufman and co-workers formulated a methodology using thermodynamic

Table I. Compositions of copper–tin alloys for tool manufacturing.

	Composition (wt%)	
Tool	**Copper**	**Tin**
Zhong ding[a]	86	14
Axe	83	17
Dagger-axe	80	20
Blade	75	25
Arrowhead	71	29
Concave mirror[b]	50	50

These are documented in ancient China in Liu Qi, which presents six recipes for bronze and is the earliest known documentation of alloy compositions.
[a]One type of music instrument in the Shang Dynasty (ca. 1600–1046 BCE).
[b]Used for lighting fires by solar power.

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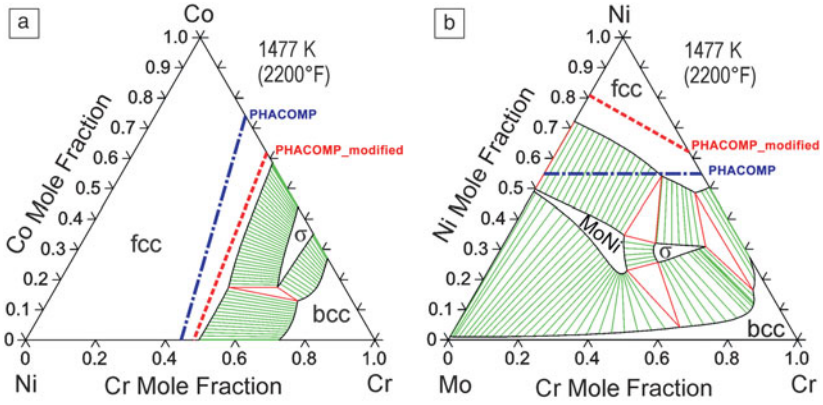

Figure 2. Comparison of σ-phase boundary prediction between CALPHAD and PHACOMP for the (a) cobalt–nickel–chromium and (b) molybdenum–nickel–chromium systems. The red dashed line is the revised model proposed by Murphy et al.[23] Note: bcc, body-centered cubic; fcc, face-centered cubic. σ is the topologically close-packed embrittling phase.

models to compute phase diagrams of alloy and oxide systems based on experimental phase diagrams and thermochemical properties. This allowed for the evaluation of multiphase competition in multicomponent systems spanning wide composition and temperature ranges.[27] This method was named CALPHAD (from "calculation of phase diagrams") and has become central to composition and process design.[28] After two decades of development since the 1970s, CALPHAD databases blossomed with the release of standard lattice stabilities by Scientific Group Thermodata Europe (SGTE)[29] in 1991.

Meanwhile, the development of software tools was correspondingly triggered to support thermodynamic database construction by the CALPHAD community. Because of the importance of diffusion phenomena in alloy design, the CALPHAD method was expanded to diffusion kinetics by researchers at the KTH Royal Institute of Technology in Stockholm, Sweden.[30] A landmark of this effort is the DICTRA (from "diffusional-controlled transformations") multicomponent diffusion software released by the spinoff company Thermo-Calc Software, which was the first software developed for the simulation of kinetic diffusion in multicomponent alloy systems. CALPHAD databases now provide both Gibbs energies of alloy phases and atomic mobilities of different components in multicomponent systems, allowing for the modeling of both phase stability and phase transformations during alloy processing.

A comparison of CALPHAD with PHACOMP is shown in **Figure 2**. In conjunction with a commercial thermodynamic database, Thermo-Calc provides a well-defined phase boundary for the face-centered cubic (fcc or γ) phase over a wide temperature range up to the melting point for each alloy composition. Because PHACOMP models for determining the σ-free phase boundary are applicable only in limited composition and temperature ranges, PHACOMP process designs address limited circumstances as compared to those obtained by the CALPHAD approach. Studies performed on nickel-based alloys* UDIMET 720 and UDIMET 720Li by Reed et al.[31] demonstrated the strength of the CALPHAD method in superalloy design. In that work, a CALPHAD thermodynamic database was used to estimate σ-phase formation from the γ matrix phase. In addition, temperature–time–transformation diagrams were constructed for design purposes using the CALPHAD thermodynamic and kinetic databases.

Over the past three decades, CALPHAD-based alloy design has been carried out in the Steel Research Group design consortium led by Northwestern University and its spin-off company QuesTek Innovations LLC, funded by government research agencies with supplemental industry support. This can be considered as the full ICMD process applied to different kinds of materials. It has directly driven materials development to the top technology readiness level (TRL),[32,33] as defined by the US National Aeronautics and Space Administration (NASA) for components in flight, and demonstrated the capability of computational materials design and accelerated qualification for brand-new alloy compositions on an industrial scale. **Figure 3** shows the achievement of a total of seven component-level TRLs corresponding to specific achievement levels of materials properties and manufacturability for two computationally designed landing-gear steels.

The development of aerospace materials by the traditional approach requires more than 15 years from concept to final manufacturing for testing under real conditions.[5] In contrast, using the ICMD technique, this development cycle can be shortened significantly. The development of ultrahigh-strength steels Ferrium S53 and M54 took only 8.5 years and 6 years, respectively, to reach materials flight qualification. Both steels are now replacing current landing-gear steels. Prototype hook-shank arresting gear components manufactured from Ferrium M54 steel are flying in US Navy T-45 aircraft, and Ferrium S53 steel landing gears have been flying on T-38 supersonic training jets since December 2010. Development of the ICMD approach approved for designing Ferrium S53 and M54 is discussed in the next section.

Development of the iCMD infrastructure

Strategy of iCMD application

The hierarchical infrastructure of the ICMD process developed by QuesTek, denoted as iCMD, is sketched in **Figure 4**.[11] It is built on two primary methods, namely, Materials by Design and AIM, which are both grounded in mechanistic models. The underlying materials genome corresponds to the fundamental databases supporting mechanistic modeling to reach a higher

*Compositions (wt%): UDIMET 720, Ni–2.49Al–0.032B–0.02C–14.8Co–18Cr–0.03Fe–3.04Mo–0.003N–4.98Ti–1.25W; UDIMET 720Li, Ni–2.57Al–0.015B–0.011C–14.7Co–16.3Cr–0.01Fe–3.00Mo–0.002N–5.02Ti–1.31W.

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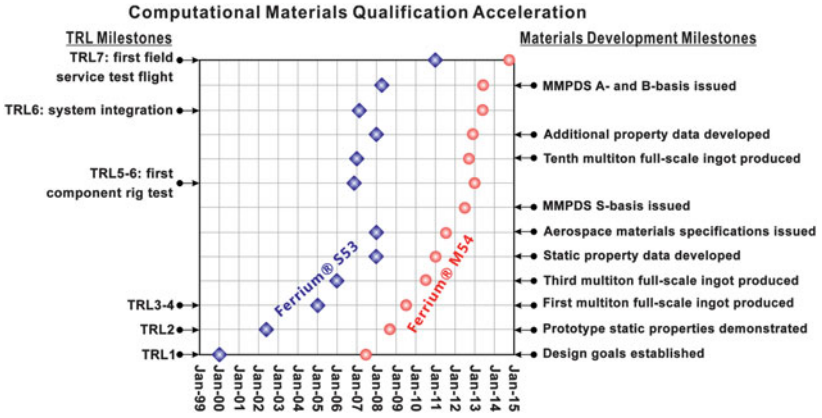

Figure 3. Time evolution of component-level technology readiness levels (TRLs) and materials development milestones for the two computationally designed landing-gear steels Ferrium S53 and M54 developed by QuesTek Innovations LLC.[11] Application of Materials by Design and accelerated insertion of materials technology greatly accelerated the development of Ferrium S53 and M54. Note: MMPDS, Metallic Materials Properties Development and Standardization. Adapted with permission from Reference 11. © 2014 Elsevier.

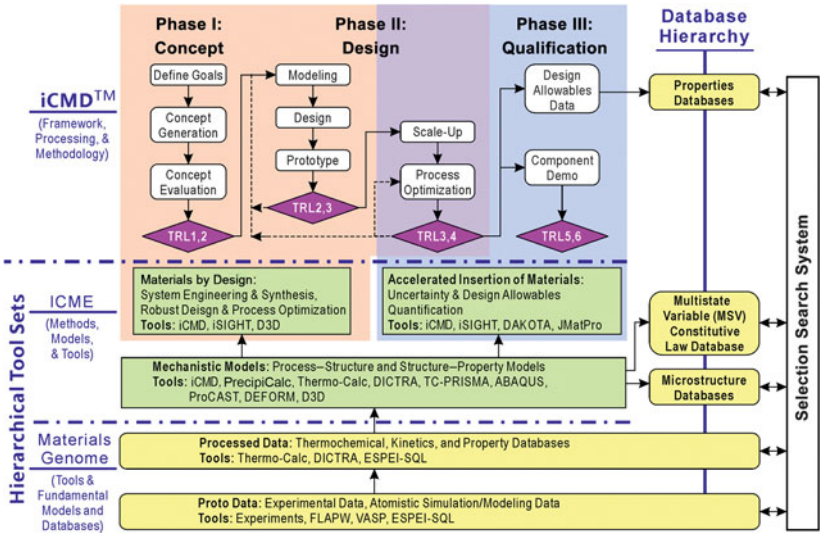

Figure 4. Overall hierarchical architecture of QuesTek's iCMD methods, tools (green), and databases (yellow) for next-generation computational materials design and accelerated qualification.[11] Note that iCMD is a toolkit used during application of ICME methods based on the materials genome. Reproduced with permission from Reference 11. © 2014 Elsevier.

level of quantitative model accuracy. The current discussion examines each structural component of the iCMD system.

In Figure 4, the top-level iCMD framework summarizes the complete materials design and development cycle, as a new material is moved through its sequence of TRLs, culminating in statistically validated minimum property "design allowables" for the materials user at the component level. Successful materials development driven by engineering applications needs to be scaled up from laboratory processing to industrial manufacturing. Technology readiness assessment[33] quantifies materials development from concept generation to practical process specification, ending with qualification, as shown in Figure 4. Development of an engineering-applicable alloy before industrial commercialization requires a minimum level of TRL6, which is a demonstration of a system/subsystem model or prototype in a relevant end-to-end environment.

Development of a completely new alloy goes through three phases, as shown in Figure 4. Phase I requires a broad understanding of materials performance and cost impacts of manufacturing and processing; product installation and use; operations, repair, and maintenance; recycling/reuse; and other factors encountered along the manufacturing and application chains. Therefore, a project kickoff meeting is conducted to discuss the initial property design goals between materials designers and clients, who can be producers, original equipment manufacturers, and sometimes end users and key stakeholders. Preliminary computations are then launched using Materials by Design. An initial TRL roadmap, such as that in Figure 3, is outlined at this stage, assisted by initial feasibility calculations. This roadmap includes defining tests to demonstrate key material properties, manufacturability from initial prototype to industrial scale, and processing requirements.

Evaluation of the concept with preliminary design ideas is the final outcome of phase I. Using iCMD, the toolkit developed for systems design (see Figure 4), materials designers can perform preliminary modeling of alternative concepts. Thus, the whole process is expedited compared to traditional concept evaluation without design tools.

After the options for a design concept have been narrowed, detailed design, modeling, and invention activities are performed iteratively in concert with prototype material evaluation. Laboratory-scale alloys are processed following the conceptual design. Preliminary results on these alloys are utilized reciprocally to calibrate iCMD models and extend databases. Two or three design iterations are typically required, with refinement not only for composition and processing of the prototype alloys, but also for design models and databases. The fidelity of the design models and databases is thus constantly improved through this feedback loop.

The cause-and-effect logic of processing–structure–property model refinement with iterative feedback is summarized in **Figure 5**. Production of the prototype material provides an important feedback mechanism for the iterative approach of Materials by Design. Through the analysis of prototypes, initial design qualities can be evaluated to further validate and refine

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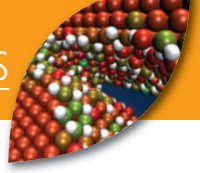

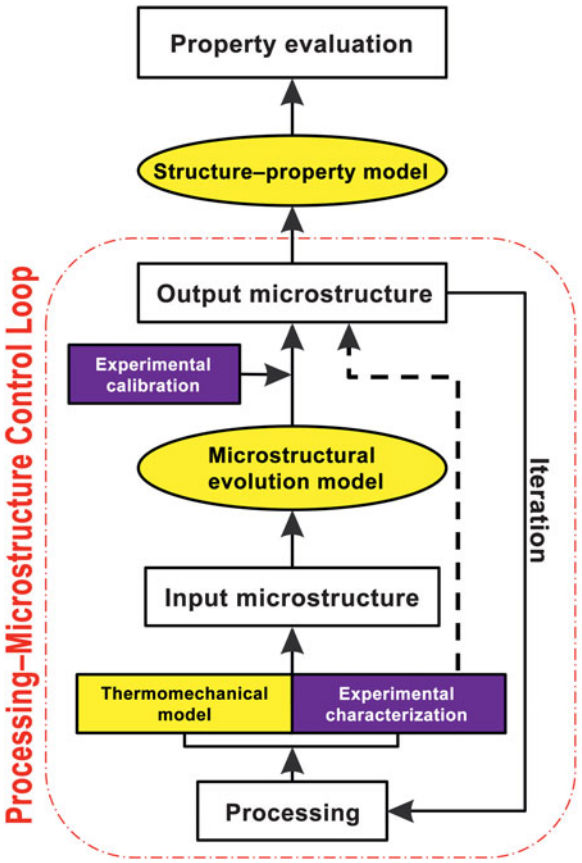

Figure 5. Working flowchart for revealing process–microstructure–property relations.

computational mechanistic models and design tools and to optimize designed composition and processing paths. Complete microstructural characterization and property analysis using combined experimental techniques is essential for full optimization.

As the next step, iCMD can be utilized to optimize alloy processing and composition specifications and thus achieve the best possible balance of microstructural features (including at the nanoscale) and properties. When optimal process conditions for a prototype alloy have been determined, the materials properties are validated according to the TRL roadmap show in Figure 3. Through processability constraints derived from macroscopic process simulations of final production-scale requirements, parametric design constraints applied during phase I ensure the scalability of material production.

Modeling efforts during phase II include the refinement and implementation of mechanistic models to address critical factors in the design of the down-selected concepts. Materials designers continue to refine key parameters in fundamental property databases and estimate database accuracy within the targeted design range. The whole process is performed by applying the iCMD toolkit, which includes an application program interface that allows extra implementation of project-specific design models. The iCMD platform allows materials designers to exploit specific microstructural features and search for design optima across length scales from atomistic to component level. This stage typically culminates in the detailed design of one or more materials for subscale prototype production and evaluation. Review meetings between materials designers and clients are helpful to update the risk map, predict values of critical design factors, and clarify design tradeoffs and materials specifications. This generates a prototyping plan that recommends suppliers or service providers for each production step, evaluates process sequences, and plans characterization and testing efforts to validate model predictions and materials properties at the prototype scale.

In robust materials design, the lowest bounds of mechanical properties need to be predicted with the highest level of confidence. Therefore, probabilistic models are implemented in iCMD. To minimize intrinsic variations in parametric design, Monte Carlo simulations are performed in which parameters are varied within the allowed tolerances of input parameters, such as alloy composition, processing time, and temperature. **Figure 6** shows an example of Monte Carlo sensitivity analysis based on a variation of alloy composition for the uncertainty analysis of the scale-up of Ferrium S53 steels.[35]

In phase III (Figure 4), AIM qualification and uncertainty management directly influence the timeline for commercializing newly designed alloys. Under the US Defense Advanced Research Projects Agency (DARPA) AIM program of

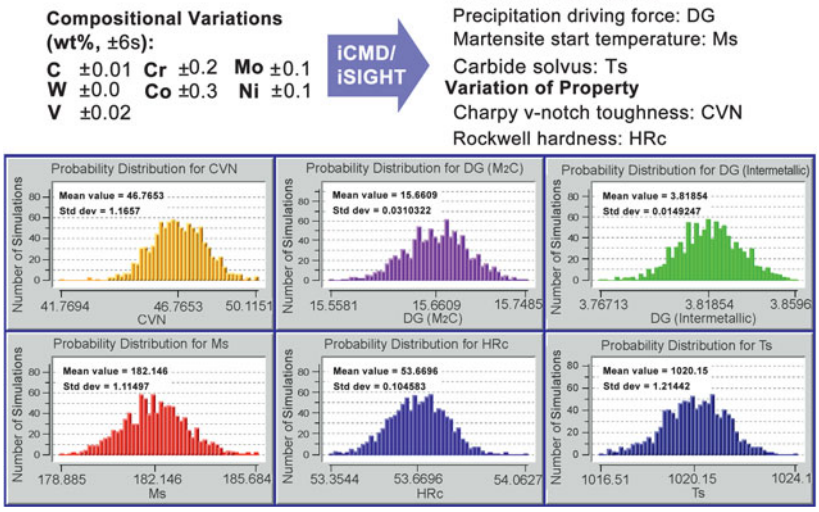

Figure 6. Sensitivity analysis with composition variations for Ferrium S53 alloys.[35] Results were generated by 1000 runs on a Pentium IV 2.2-GHz CPU for 12 min. Precipitation phases include the M_2C carbide phase and intermetallics. Reproduced with permission from Reference 35. © 2006 C. Kuehmann.

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2001–2003,[4] QuesTek's PrecipiCalc microstructural simulator was integrated with finite-element heat-transfer simulations to accelerate thermal process optimization of nickel-based superalloy aeroturbine disks. The CALPHAD-based PrecipiCalc mean-field precipitation code[36] was optimized to balance accuracy and efficiency in the prediction of the phase compositions and size distributions of trimodal γ′ precipitate populations, alloy carbides, and associated Zener-pinned grain size, for the accurate prediction of alloy strength using calibrated analytical structure–property models. Predictive process optimization of a subscale IN100 alloy disk was validated by overspin burst tests, with companion disk forgings sectioned to validate the predicted spatial distribution of microstructure and strength, the latter validated to within 1 ksi (7 MPa). A large-scale Monte Carlo simulation of manufacturing variation was then performed using recorded process-variable distributions over six stages of thermomechanical and thermal disk processing, for a legacy turbine disk application with a well-established final property distribution. Using the science-based prediction of the shape of the strength probability density function (PDF), a final data fusion strategy was devised whereby small randomly selected strength datasets were used to recalibrate the PDF by linear transformation[37] to account for additional epistemic variation. It was demonstrated that as few as 15 random data points could be fused with the calculated PDF to predict the 1% minimum strength value within 1 ksi (7 MPa), corresponding to the experimental error of the strength measurement.

The first application of the AIM method to forecast minimum strength properties during qualification of a new material was demonstrated for the aforementioned Ferrium S53 landing-gear steel. The exercise used limited data from three production-scale heats (as required for aerospace material specification S-basis allowables[38]) to forecast the final 1% minimum strength as ultimately validated by 10 full production heats (as required for Metallic Materials Properties Development and Standardization [MMPDS] A-basis allowables[38]), within 1 ksi (7 MPa).

As summarized in the time evolution of component-level TRLs and corresponding material qualification milestones shown in Figure 3,[11] recent AIM-accelerated qualification of a second aircraft landing-gear steel (Ferrium M54) compressed the full materials design and qualification cycle from a clean sheet to MMPDS materials qualification to under six years.[11] This early success attested to the feasibility of the acceleration goals of the US Materials Genome Initiative.[34]

The current frontier of AIM methodology development is uncertainty management in the prediction of microstructures and properties. A follow-up project addressed protocols for management of quantified uncertainty in all aspects of PrecipiCalc-based AIM process–structure modeling, using a series of third-generation alloys for aeroengine turbine disks, in preparation for accelerated process optimization of dual-microstructure heat treatment for enhanced hybrid-disk performance.[36] The standard error of each model prediction was characterized experimentally by standard practices. A hierarchical uncertainty-management strategy was adopted, balancing final structure–property model sensitivity against the intrinsic accuracy of the fundamental databases employed in process–structure predictions. For fixed alloy compositions, high-temperature equilibration experiments were used to assess the error in the predicted phase fraction from the CALPHAD genomic databases. Because of the dominant role of phase fraction in strength models, the phase-fraction error was efficiently reduced (to the level of experimental error) by applying rigid shifts to the second-phase free-energy functions in the thermodynamic database. With the recalibrated volume thermodynamics fixed, high-temperature diffusion couples were then run against pure nickel for each alloy and compared with DICTRA diffusion simulations combining the thermodynamic database with atomic-mobility databases for diffusivity prediction. Improved accuracy of the diffusivity predictions was then achieved by small adjustments (on the order of 20%) in the mobility prefactors of some of the alloy components.

With the thermodynamic and mobility databases thus recalibrated for the specific alloys, important surface thermodynamic quantities were then calculated. In view of the high sensitivity of nucleation to interfacial energy, the γ/γ′ coherent interfacial energy was efficiently measured using a cost-effective single-sensor differential thermal analysis technique to directly measure the critical nucleation undercooling in each alloy in rapidly quenched 3-mm-diameter pins. Using the precisely measured thermal history of each pin, the interfacial energy was calibrated in PrecipiCalc simulations to match the observed critical undercooling. Validation of the PrecipiCalc-predicted final microstructure in the pins by atom-probe microanalysis then demonstrated high accuracy in a far-from-equilibrium microstructure. The high precision of microstructural predictions employed in AIM process optimization motivated the Office of Naval Research/DARPA "D3D" (digital three-dimensional) structure consortium program from 2005 to 2010 to assemble a suite of 3D tomographic characterization tools addressing phase distributions at multiple length scales, to bring experimental microstructural characterization to a new level of fidelity to support this technology.[11]

Materials genome: The database foundation

As the foundation of ICME, materials genome fundamental databases are the cornerstone of the iCMD infrastructure. Developing reliable protodata and processed data in repositories with sustainable maintenance is a prior requirement. As indicated in Figure 4, ICME models of multiphase dynamic microstructural evolution are structured to be quantitative by the materials genome foundation, consisting of fundamental genomic databases describing thermochemical, physical, and kinetic attributes as functions of the chemical composition and temperature at the phase level. In addition, application of iCMD is aided by an effective selection search system,

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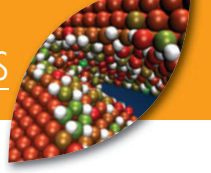

allowing for exhaustive research to assist decision making during phase and component selection in early stages of materials design.

Figure 4 shows research activities that contribute to accelerated genomic database development. In alloy design, atomistic modeling based on density functional theory (DFT) provides helpful fundamental values to many other modeling techniques. CALPHAD database development based on DFT digital input has already made significant progress. Related studies have further extended the integrated DFT and CALPHAD methodology from thermodynamics to diffusion. The CALPHAD approach also necessitates experimental data as primary input. Hence, further development of efficient experimental techniques to support integration of DFT atomistic modeling and CALPHAD is one of the major focuses in the Materials Genome Initiative.[34] Important contributions have been made in the field of high-throughput experimental techniques.[39–43]

Opportunities and outlook

Opportunities for further enhancement of the ICMD approach can be found in four areas: (1) performance of fundamental genomic research, (2) enhancement of databases and repositories, (3) development of linkage models for ICME research, and (4) teaching of ICME approaches in materials science and engineering programs.

On the foundational level of the materials genome, substantial improvement of its methods could have a broad impact. For example, evaluating magnetic effects on phase stability using quantum mechanical DFT models, such as for fcc iron, is still a challenge.[44–47] The current physical model is not sufficient for magnetic substances with itinerant spin orbitals, such as iron and chromium. In fact, similar issues limit the CALPHAD approach as well.[46,48,49]

A recent workshop on phase transformations highlighted several future directions for atomistic modeling and the CALPHAD approach in alloy development. The reports from this workshop[50–54] cover thermodynamic modeling of crystalline and liquid-amorphous phases, high-pressure systems, magnetic transitions, and defects and provide guidance for the next generation of database development for the materials genome. As a consequence, more effort is needed to transfer these models into materials genomic tools, such as Thermo-Calc and DICTRA, that can facilitate the development of more accurate databases. It is noteworthy that, as one of the components in the materials innovation infrastructure,[34] improvement of experimental tools for high-throughput purposes is also valuable. A convincing example is the high-throughput experimental diffusion multiple for large-scale determinations of diffusivities and thermophysical quantities for database construction.[39,43]

Secondly, model predictions using ICMD rely heavily on the quality of genomic databases. Therefore, database development should be the highest-priority research topic to support ICMD. Database sharing and development also demand standards. Taking CALPHAD as an example, if lattice stability had not been standardized by SGTE,[29] CALPHAD would not have been broadly adopted in practical materials design. Fortunately, the US National Institute of Standards and Technology is creating data repositories and setting up standards for materials genomic databases.[8] Such efforts call for greater involvement of different scientific communities across different disciplines.

Regarding enhancement of the ICME framework, systems design can benefit from further advances in linkage models of process–structure and structure–property relations. Here, advances in continuum modeling methods have more to contribute. It should be noted that precipitation modeling based on classical theory, such as the Kampmann–Wagner numerical model,[55] has been used in industrial process optimization, fostering several revised models.[56–58] Similarly, structure–property linkage models for mechanical behavior are rapidly advancing through new methods of micromechanical simulation

Table II. Computational materials modeling methods and tools.[a]

Category	Representative Software	Employer (%)	Faculty[b] (%)	Index[c]
Mechanics (mostly finite element)	DEFORM, ABAQUS	80	14	0.175
Thermodynamics (CALPHAD)	Thermo-Calc, Pandat	53	7	0.132
Density functional theory	VASP, ABNIT	47	21	0.447
Programming language/integration	MatLab, Fortran, iSIGHT	40	43	1.075
Casting	proCAST, MAGMAsoft	40	0	0
Molecular dynamics/Monte Carlo	LAMMPS	27	14	0.519
Fluid flow/heat transfer	COMSOL, Fluent	20	7	0.35
Diffusion/microstructural evolution	DICTRA, PrecipiCalc, JMatPro	20	0	0
Statistics	Informatics	13	7	0.538
Materials modeling suite	Materials Studio	13	0	0
General visualization	Mathematica, Tecplot	7	29	4.143
General data processing	Spreadsheet	7	21	3
Special purpose	K-Flow, WARP 3D	7	0	0
Materials selection	CES Materials Selector	0	36	–
Crystallography	CaRIne	0	7	–

These are cited by employers, categorized and ranked by the normalized frequency of citations, along with corresponding results from a survey of computational faculty.[a]
[a]Adapted with permission from Reference 60. © 2009 Springer.
[b]Some of the responses did not provide software or categories, and, therefore, one expects some degree of undercounting in these data.
[c]Index = Faculty/Employer.

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and, in particular, are being investigated to provide empirical correlations prior to mechanistic understanding, such as the neural network method.[59] We note that, although significant research has been performed using these techniques separately, limited work has been reported so far that integrates mechanistic models and materials genomic databases using neural network modeling and data-mining techniques.

Because the ICMD infrastructure is a hierarchical architecture integrating different engineering approaches of materials and mechanical engineering, educational program design becomes more challenging, requiring engineering design courses at different levels in a multiyear curriculum. However, a survey on computational materials science and engineering education summarized in **Table II**[60] found that the present education in materials genomic methods and ICME tools is generally lacking. The results are based on responses from 43 survey participants, including 29 US universities, one Canadian university, nine materials-related industrial companies, and four materials research laboratories.[60] The index column in Table II indicates the adequacy of education programs and faculty numbers in related teaching fields, where lower values reflect insufficient programs. Surprisingly, although CALPHAD appears to be one of the most useful computational techniques in industry (see the employer column in Table II), the importance of teaching CALPHAD and computational diffusion knowledge is underestimated in academic institutions. Therefore, related curricula should be considered in the course design for materials and processing education. A leading example of multiyear design education at Northwestern University is described in the recent Materials Genome Institute Strategic Plan.[61]

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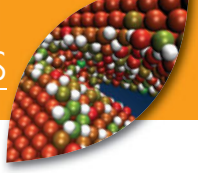

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