Liu and McDowell *Integrating Materials and Manufacturing Innovation* (2014) 3:28
DOI 10.1186/s40192-014-0028-2

Integrating Materials and Manufacturing Innovation
a SpringerOpen Journal

CASE STUDY Open Access

The Penn State-Georgia Tech CCMD: ushering in the ICME Era

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Abstract

This case study paper presents the origins, philosophy, organization, development, and contributions of the joint Penn State-Georgia Tech Center for Computational Materials Design (CCMD), a NSF Industry/University Cooperative Research Center (I/UCRC) founded in 2005. As a predecessor of and catalyst for Integrated Computational Materials Engineering (ICME), the CCMD served as a basis for coupling industry, academia, and government in advancing the state of computational materials science and mechanics across a portfolio of process-structure-property-performance relations, with emphasis on education and training of the future workforce in computational materials design.

Keywords: ICME; MGI; CCMD; NSF I/UCRC; Materials design; Computational materials science

Background

The past decade has witnessed the emergence of *Integrated Computational Materials Engineering* (ICME) as an early twenty-first century joint industry, academic, and government initiative for integration of modeling and simulation with materials development and product improvement. ICME is concerned with multiple levels of structure hierarchy, as is typical of materials, and aims to reduce the time to market of innovative products by exploiting concurrent design and development of materials, products, and process/manufacturing paths. As described in the National Materials Advisory Board committee [1] report from the National Research Council, ICME is 'an approach to design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales'. ICME embraces the engineering perspective of a top-down, goal-means strategy discussed cogently by Olson [2] and is fully cognizant of the important role of microstructure in tailoring materials properties/responses in most engineering applications, well beyond the atomic or molecular scale. Many materials properties/responses not only depend on atomic bonding and atomic/molecular structure but are also strongly influenced by the existence, spatial arrangement, and morphology of multiple phases and resulting phase interface/interphase strengthening effects.

This perspective was embraced and refined for the academic, industry, and government research communities at a 1998 National Science Foundation (NSF)-sponsored workshop hosted by Georgia Tech and Morehouse College [3] entitled 'New Directions in Materials

Design Science and Engineering (MDS&E)'. As stated in the workshop report, 'The field of materials design is entrepreneurial in nature, similar to such areas as microelectronic devices or software. MDS&E may very well spawn a "cottage industry" specializing in tailoring materials for function, depending on how responsive large supplier industries can be to this demand. In fact, this is already underway'. That workshop report 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 materials and products. It also forecasted that the twenty-first century global economy would usher in a revolution of the materials supply/development industry and realization of true virtual manufacturing capabilities, not only geometric modeling but also consideration of realistic material behavior. It was recommended to establish 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.

Inspired by the 1998 NSF MDS&E workshop report and the educational effort at Northwestern University led by Olson, Zi-Kui Liu, Long-Qing Chen, and Karl Spear at Penn State spearheaded development of a fundamentally new kind of computational materials science curriculum and laboratory experience in 2001 to 2003 [4,5]. This NSF-funded effort established a computational teaching facility and addressed theoretical and computational aspects of thermodynamics and kinetics. Thermodynamic and kinetic databases in the forms of Gibbs energy functions and atomic mobility in individual phases were utilized through computer programs to predict phase stability and simulate phase transformations [6]. As shown in Figure 1, thermodynamics is at the core of this conceptual framework to establish configurations, either stable or metastable, and driving forces for microstructure evolution. Then, considering kinetics of transition states for defects and crystallography, properties and performance (structure-property relations) can be modeled. Experiments play a vital role in motivating, calibrating, and validating models at various time and length scales.

This educational activity further inspired them to develop the Materials Computation and Simulation Environment (MatCASE) program [4,5] in 2002, and in the same year, the name MaterialsGenome® was coined by Professor Liu in establishing the

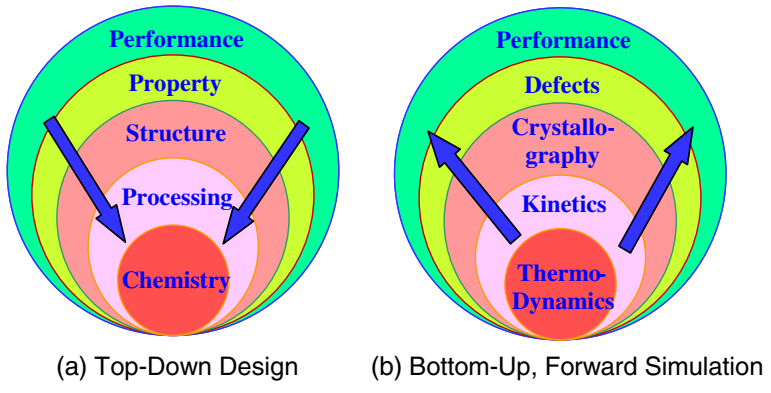

Figure 1 Relationship of key components in materials design. These components affect combined **(b)** bottom-up and **(a)** top-down materials design [5,6].

MaterialsGenome, Inc. in Pennsylvania and later trademarked (cited by the MGI web site at http://www.whitehouse.gov/mgi). In the MatCASE program, the Penn State team developed unique strengths in conducting multilevel modeling by passing information from first-principles calculations and computer coupling of phase diagrams and thermochemistry (calculation of phase diagrams (CALPHAD)) modeling to phase-field simulations and structure-property relations, which was later leveraged into the Center for Computational Materials Design (CCMD). It was realized that first-principles calculations based on density functional theory (DFT) were becoming a critical component in not only providing insights to physics of phenomena but also quantitatively predicting thermodynamic, kinetic, and mechanical properties of individual phases, thus significantly enhancing the predictability of CALPHAD modeling of individual phases in multicomponent materials [6,7]. The properties of individual phases and phase interfaces thus obtained are used as input parameters for phase-field simulations of microstructure evolutions. The microstructures resulting from phase-field simulations, along with properties of phases and phase interfaces, enter into the finite element analysis of materials responses to external stimuli. Thus, in the hierarchy of material structure [8-10], individual phases can be considered as the building blocks of materials in designing microstructures that meet desired performance requirements.

Prior to forming the CCMD, the 2001 to 2003 Defense Advanced Research Projects Agency (DARPA)-funded *Accelerated Insertion of Materials* (AIM) program [11-13] sought to build systems approaches to accelerate the insertion of new and/or improved materials into products. The AIM program demonstrated that legacy materials development (both polymer composites and aircraft gas turbine materials) could be significantly accelerated by integrating process-structure and structure-property modeling with processing and experiments using a designer knowledge database in collaborative teams involving the materials supply chain, original equipment manufacturers (OEMs), and university research laboratories.

Case description

Forming the CCMD

This historical setting formed the basis for initial discussions starting in 2003 between Zi-Kui Liu and David McDowell in framing a computational materials design initiative within the context of a NSF Industry/University Cooperative Research Center (I/UCRC). At that time, there was no I/UCRC in existence or other federally funded center that dealt with the materials process-structure-property-performance paradigm shown in Figure 1. The Penn State-Georgia Tech collaboration was conceived to take advantage of the pioneering work in computational thermodynamics and phase-field modeling at Penn State, complementing recognized leadership in experimental and computational microstructure-property relations and systems-based materials design methods at Georgia Tech.

The initial conceptualization of the CCMD considered materials design objectives, with a primary goal to characterize sensitivity of properties to microstructure and process route and to capture essential dominant mechanisms and their transitions with applied loading and environment in applications. A related challenge is addressing the uncertainty associated with forms of models, model parameters, microstructure stochasticity, and

microstructure hierarchy, in addition to the transfer of information from fine grain, high-resolution models to coarse grain models with reduced degrees of freedom at higher scales. Given these sources of uncertainty, the notion of design *optimization* using hierarchical or concurrent multiscale models is not particularly useful in many cases. Instead, extension of concepts of systems-based *robust* design to multilevel integrated design of materials and products [8-10] is more practical, with sensitivity of various responses to microstructure variation playing a central role. A combined top-down and bottom-up strategy that served to inspire the CCMD is shown in Figure 2, with application to Ni-base superalloys for aircraft gas turbine engines.

This conceptual basis for a center that would develop novel predictive algorithms and methods to support materials design and development led to engagement of a set of initial industry and government stakeholders in fall 2003 to write a letter expressing support for the concept of the CCMD, including Air Products, Inc., ALCOA, Allegheny Ludlum, Boeing Company, Caterpillar Inc., ExxonMobil Upstream Research Company, Ford Motor Company, GE Global Research Center, GE Power Systems, General Motors, Honeywell-Aerospace, Intel, KennaMetal, Inc., Marlow Industries, Inc., Nippon Steel Corporation (Japan), Pratt & Whitney, Questek LLC, RTI International, Special Metals Company, ThermoCalc Software, AB (Sweden), Timken, Los Alamos National Laboratory, Lawrence Livermore National Lab, NASA, Natural Resources Canada (Canada), NIST, Oak Ridge National Lab, Sandia National Labs, SRI International, Exponent, GE Aircraft Engines, DuPont, Argonne National Laboratories, Synaps, Inc., Dana Technology Development Group, U.S. Air Force Research Laboratory (AFMC), and SI Flooring Systems. This led to submission of a planning proposal to the NSF I/UCRC program to establish the CCMD in 2004, followed by a 21 January 2005 planning workshop held at Penn State. The strategy to form the CCMD rested on the complementary nature of strengths. Penn State's world class capabilities in computational thermodynamics and phase-field theory were

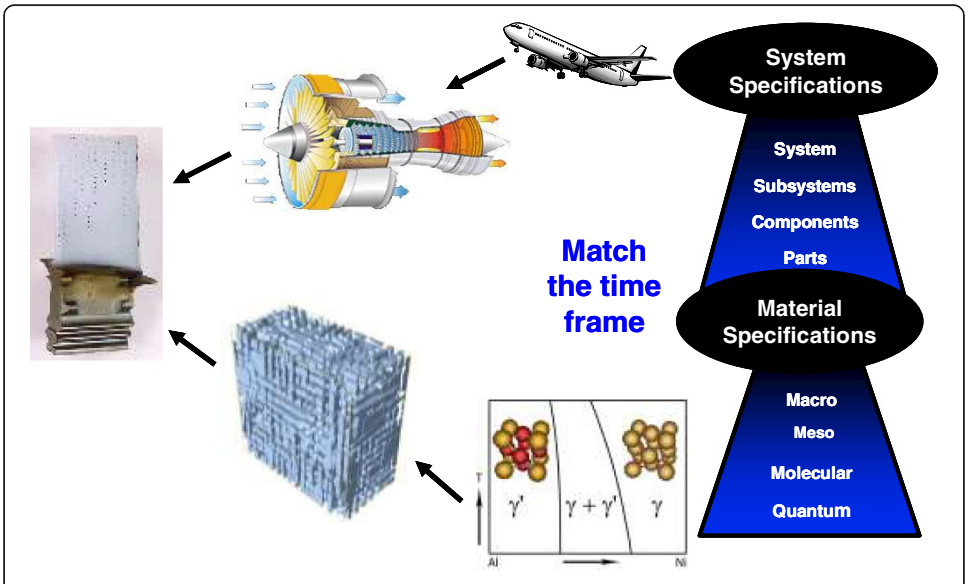

Figure 2 Combined bottom-up and top-down strategy for concurrent design of materials and systems. Engineering systems design should be extended to the material as a sub-system, with hierarchy of atomistic, mesoscopic, and macroscopic scales, in this case applicable to gamma-prime precipitate strengthened Ni-base superalloys used in the hot section of aircraft gas turbine engines.

combined with Georgia Tech's widely recognized expertise in microstructure-property relations and systems-based materials design. Based on the discussion and feedback from the industry and government labs, a full proposal was submitted to the NSF in June 2005. The proposal for phase I CCMD was funded, with the 1.5-day kickoff meeting held on 3 to 4 November 2005 at Penn State, with 13 initial members. Phase I was in effect from 2005 to 2010. A follow-on phase II was funded by the NSF from 2010 to 2013. This time frame spans the era preceding and leading up to the National Materials Advisory Board report on ICME, as well as the 2011 launch of the U.S. Materials Genome Initiative (MGI) [14].

CCMD vision, mission, structure, and operations

The mission and vision of the CCMD remained consistent over its entire duration of NSF funding:

> Mission: Educate the next generation of scientists and engineers with a broad, industrially relevant perspective on engineering research and practice.
>
> Vision: To be recognized as the premier entity for collaborative activities in computational materials design among universities, industries and government laboratories.

The intellectual merit of the CCMD was based on the integration of multiscale, interdisciplinary computational expertise at Penn State and Georgia Tech, ranging from atomistic calculations to continuum phase-field, finite element, and statistical continuum microstructure-property modeling with interfaces between engineering systems design, information technology, and physics-based simulation of process-structure and structure-property relations of materials. Details of membership and research projects are herein protected from disclosure owing to the terms of the Memorandum of Agreement (MOA). Suffice it to say that the CCMD provided leadership in articulating the importance of integrated design of materials and products to industry and the broad profession of materials engineering and developed a significant body of new methods for estimating structure and corresponding properties/responses based on first-principles, atomistic, phase-field, and finite element strategies. Moreover, a component of phase I contributions added value to algorithms for concurrent design of components and materials and decision-based design methods. Tools and methods explored by the CCMD included first-principles calculations, CALPHAD, phase-field, crystal plasticity, molecular dynamics, cohesive finite element methods, homogenization, and systems integration and design tools. Materials systems addressed include Al, Ni, Ti, Mg, and Nb alloys, as well as steels.

Professor Zi-Kui Liu at Penn State served as CCMD Director and was responsible for center activities. He managed membership dues contributions and allocations to funded projects at both Penn State and Georgia Tech, based on input from the Member Advisory Board (MAB) management team, and tracked status of dues collections and new member recruiting, assisted by Center Manager at Penn State, Sandy Watson. In addition to communication among PIs at both universities, students, members, and potential members, Penn State maintained the CCMD website (http://www.ccmd.psu.edu/).

Professor Dave McDowell served as Co-Director of the CCMD and directed the Georgia Tech site. He collaborated closely with Professor Liu in all aspects of assessing progress on projects, developing and pursuing the vision for the CCMD, member recruiting, retention, planning meetings, interactions, and monitoring mentoring relationships that members offer to CCMD-supported students and was assisted at Georgia Tech by Cecelia Jones in organizing annual CCMD meetings in Atlanta.

The management structure of the CCMD is shown in Figure 3. The CCMD had a MAB, in lieu of the Industry Advisory Board (IAB) label used by many I/UCRCs, comprised of one representative per member organization, with different numbers of votes for full and associate members. The CCMD management team was comprised of the CCMD Director, Co-Director, MAB Chair and Vice-Chair, and members for the respective University Policy Committees (Penn State and Georgia Tech administrative representatives). The independent Center Evaluator applied online assessment tools ('Level of Interest and Feedback Evaluation' forms) at every CCMD meeting for each project presented, attended closed MAB meetings, provided liaison with members to discuss any concerns with CCMD management or policies, and administered annual member and faculty surveys to acquire feedback regarding the overall progress of the Center. Faculty, students, and postdocs at both universities interfaced with the MAB, Center Evaluator, and CCMD Management Team, as shown in Figure 3.

The CCMD represented a ground-breaking effort to instill the culture shift associated with ICME, viewing materials design as an integral part of multidisciplinary engineering systems design. Both Professors Liu and McDowell maintained heavy involvement in external workshops and conference presentations, often presented jointly, to publicize the ICME-oriented perspective of the CCMD and the field of computational materials design to the external community [15-28]. With The Minerals, Metals, and Materials Society (TMS) as a partner organization, CCMD management was intimately involved with offering presentations and workshops at TMS meetings.

Development of partnerships among industry, academia, and government laboratories was emphasized through:

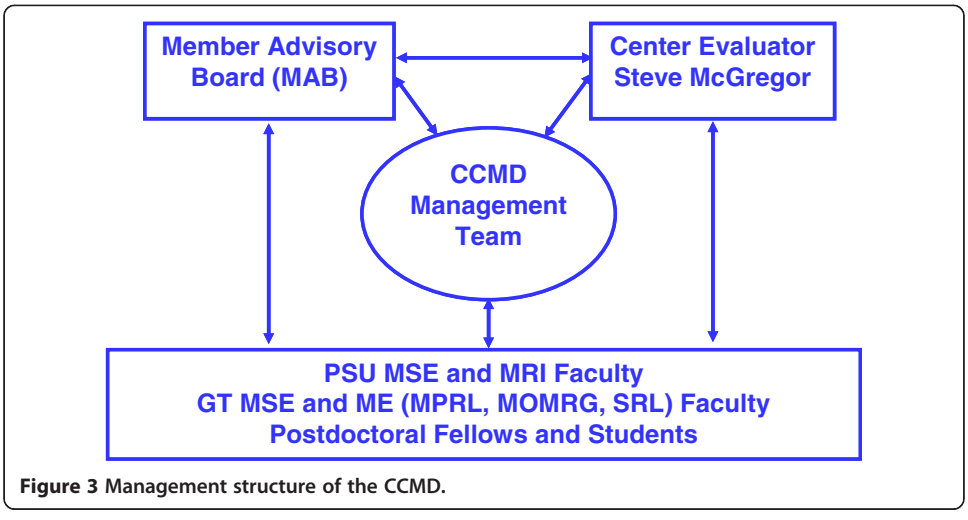

Figure 3 Management structure of the CCMD.

- Educating future generations of scientists and engineers in ICME/MGI pertinent research themes;
- Improving the intellectual capacity of the workforce through industrial participation, high-quality research projects in computational materials science and materials design;
- Promoting research programs of interest to both industry and academia;
- Enhancing the infrastructure of computational materials research in the nation; and
- Exploring and extending physics-based simulations of process-structure and structure-property relations of materials.

Working with CCMD membership, final forms of its MOA and Bylaws were established during the early years of the CCMD. The MOA addressed center objectives, member advisory board, reports including invention disclosures and patent protection and patent rights, royalties derived from licensing, rights in software, data, and publications, confidential communications, publicity, supersedure, representation, termination, indemnity, satellite sites, and warranty disclaimer. The CCMD Bylaws governed the operation of the Center, including membership qualification, privilege, benefits, revocation, and costs, and procedures for proposal voting, project funding, and project reporting.

The CCMD established policies in its MOA for sharing intellectual property developed by funded projects among center members and has successfully implemented such sharing via license agreements. These policies have served the CCMD well in terms of intellectual property policies in accordance with the Bayh-Dole Act, as policies for distribution of software and codes developed in the CCMD are clearly set forth that permit non-exclusive, royalty-free licenses for center members and the possibility of exclusive, royalty-bearing licenses. Although provision for patents was made available as part of the MOA to membership, no such patents were pursued, as is typical for I/UCRCs, and the CCMD effectively operated as a pre-competitive research consortium.

Industry and national laboratory member dues provided the primary financial resources for the CCMD. The CCMD maintained a two-tiered membership structure, $40 K (phase I)/$48 K (phase II) per year for full members and $15 K (phase I)/$18 K (phase II) per year for associate (SBIR eligible small company) members. A very strong incentive for members to join the CCMD was provided by the NSF stipulation that the universities should charge only 10% F&A (overhead) on research projects funded by member dues (Penn State provided further cost sharing with additional overhead reductions). Annual NSF funding of the CCMD was used to partially offset administrative operations (Penn State MRI provided additional support annually). A significant fraction of NSF funding was used to support the Independent NSF Center Evaluator, who served a role as liaison between center membership, leadership, and the NSF, particularly during phase II in which the full cost for such compensation was covered by Penn State, consisting of more than half of the NSF support provided.

Clearly, the level of per project funding was sufficient to support the primary objective of preparing the future workforce in computational materials design, creating an interface between students and postdocs and stakeholder companies and laboratories interested in ICME. During this period, the CCMD was arguably well ahead of the curve in producing such students relative to other academic programs, with 41

graduate students and postdoctoral fellows fully or partially supported. One student was supported by a DoD laboratory internship through completion of his doctoral degree in summer 2010, more than 2 years beyond the end of the formal CCMD funding. A number of students obtained summer internships at member organizations over the years. Important goals for student development were set as follows:

Leadership experience:

- Introduction to industry applications
- Participation and presentations at bi-annual reviews and meetings
- Competition among students for R&D funding and communicating ideas
- Group/team work - collaborate on and between projects

Networking:

- Networking and contacts with industry, academic, and government members
- Guidance and direction via interaction with industry, university, and government
- Lab tours and workshops - communicate with visitors/members

Industry experience:

- Exposure to industry applications and culture - budgets, timelines, competitors, IP
- Research proposals - how to develop 'fundable' ideas
- Feedback from industry sponsors - learn what is important to industry
- Mentoring - project and career guidance
- Internship and employment opportunities

CCMD meetings, available for participation only by members and potential members as per NSF I/UCRC guidelines, were held twice per year for 1.5 days each, including a mid-February meeting at Georgia Tech and a mid-August meeting at Penn State. Prior to each August meeting, project ideas were solicited from members, with sufficient lead time for faculty to prepare proposals. These proposals were distributed to members approximately 2 to 4 weeks before the meeting and were presented by faculty at the meeting. Thereafter, the projects were discussed at length and ranked by members. Based on this input, new projects were then finalized in the following 1 to 2 months by the Chair and Vice-Chair of the Member Advisory Board and CCMD Director and Co-Director, taking into account balance of the portfolio shown in Figure 4, as well as distribution between Penn State and Georgia Tech sites in accordance with attribution of membership dues recruiting. In addition, several industry members hosted the CCMD meetings. The typical agenda for the August meetings consisted of presenting proposals for the next round of funded projects in response to member-developed initiatives offered in late spring or early summer of each year. The February meetings at Georgia Tech focused on student presentations of progress on active CCMD projects, receiving guidance and feedback for the next 6 months. Poster sessions and workshops were commonly held 1 day in advance of each meeting, affording members an opportunity to delve into greater detail and learn modeling principles, interface with CCMD software and algorithms, and explore applicability to their organizations.

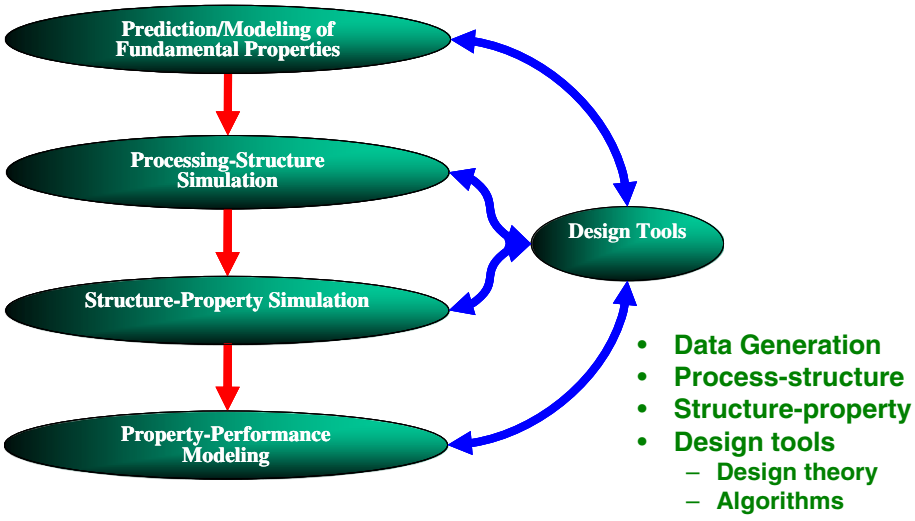

Figure 4 Four foundational areas of projects to support the CCMD vision. Integrating the design of materials and products, the basis of ICME.

At any point in time, given the membership levels, approximately ten projects were underway simultaneously. Projects were configured for a 2-year period, with an option to apply for renewal that was encouraged only for projects receiving strong support and feedback from membership. Projects in phase I focused on filling out a balanced portfolio of research and development in the four foundational elements shown in Figure 4. Materials of focus in phase I included FCC Al and Ni-base alloys, HCP Mg and Ti-alloys, steels, ceramics/oxides, and polymers.

Based on feedback from the Member Advisory Board in 2008, monthly web meetings were organized with presentations for projects led by supported graduate students and postdocs. In addition to monthly web-based presentations by students, mentor-led meetings were organized by supported students. Project mentors from the CCMD membership offered guidance through the year and in some cases provided additional support for on-site student internships. During phases I and II, a total of 38 CCMD projects were executed. In addition to the associated tools and methods, member benefits from CCMD projects included:

- Active interactions with many faculty members with different expertise
- Influence on pre-competitive CCMD projects
- Contributions to education through mentoring projects
- Networking with other CCMD members

The business model for flow of value from CCMD efforts in developing novel modeling and simulation tools to enable computational materials design is shown in Figure 5. It served as the approach for transition from basic cross-cutting research in the CCMD to applications involving specific alloy systems or other materials of proprietary interest to members. CCMD projects supported innovative, publishable basic research that fostered development of graduate students, while the transition to industry-specific applications was funneled downstream into internships, active mentoring roles, and additional research contracts between CCMD members and Penn State or Georgia Tech faculty.

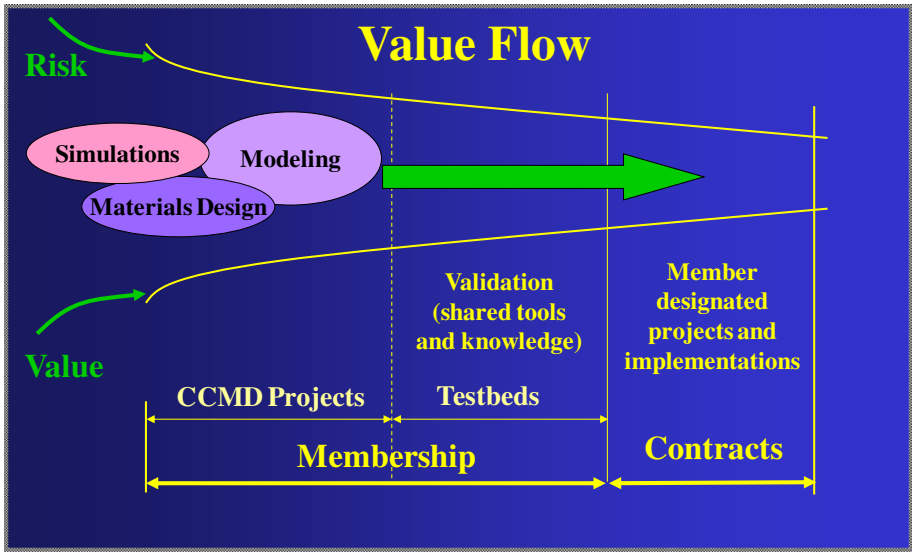

Figure 5 Flow of value offered by CCMD projects. Risk is reduced over time by virtue of enhanced modeling and simulation tools and methods.

The primary research findings were summarized in the project deliverables report submitted with each annual report. The members-only portion of the CCMD website (http://www.ccmd.psu.edu/) posted project quarterly reports and presentations, papers, the project final report, project deliverables, and associated documentation, providing ease of access for members. Moreover, updated quad charts were provided for each project to assist members in communicating relevance of CCMD accomplishments and deliverables within their organizations.

In addition to Center memberships, TMS joined as a partner organization of the CCMD in 2006, with an agreement to publicize the CCMD and host workshops. The CCMD co-organized the annual ASM-TMS Symposium on Computational Materials Design in 2007, held at GE Global Research Center. A workshop, 'Center for Computational Materials Design: Experiences & Perspectives Workshop', was held in 2009 at the Materials Science and Technology (MS&T) conference with partial support from Office of International Business Development, Department of Community & Economic Development, Pennsylvania's Center for Trade Development. The CCMD contributed significantly to establishing the annual symposium at the MS&T conference: Phase Stability, Diffusion Kinetics, and Their Applications (PSDK), which was initiated in 2006.

In May 2007, the CCMD teamed with the Center for Dielectric Study (CDS) at Penn State to submit a successful proposal on 'Computational Modeling of Defects and Minor Chemical Additives in Functional Materials' to the TIE program at NSF, which sought to link efforts of multiple I/UCRCs. This work focused on the thermodynamics and defects formation in perovskites, starting from the prediction of properties of constituent pure element and binary systems such as Ti, TiO_2, and $PbTiO_3$. A 2-year NSF supplement funding project IIP-0823907, *Fundamental Supplement Proposal: Bridging First-principles and Molecular Dynamics Methods to Support Alloy Design in the CCMD*, was funded from 2008 to 2010. Investigators included D.L. McDowell, T. Zhu, and K. Jacob from Georgia Tech and Z.-K. Liu and V. Crespi from Penn State. By definition, simulation-based materials design requires computational exploration of new

materials that have not previously been envisioned or developed. This necessitates the use of first-principles and atomistic simulations to estimate fundamental properties of crystals and phases, thereby facilitating consideration in design.

From 2010 to 2013 in phase II, the CCMD focused more on interfaces between phases in addition to fundamental phase properties, congruent with the phase II vision shown in Figure 6 outlined in the renewal proposal. Specific additional gaps addressed in phase II of the CCMD are outlined in the vision shown in Figure 6:

- Linkage of first-principles calculations to higher scales of hierarchy in structure-property simulations, e.g., linking Penn State models, codes, and expertise in the former to Georgia Tech models, codes, and expertise in the latter.
- Mapping modeling, simulation, and design tools developed within the CCMD to various material classes and application domains.
- Materials processing experiments and simulations.

The CCMD made key advances in setting the tone for collaboration and future workforce training that addressed the academic-industry-government cultural paradigm shift towards computationally assisted materials design and development associated with ICME [1] and the more recently framed MGI [14]. In addition to research, outreach was an important element of CCMD operations. In 2007, the CCMD participated in the Women in Science and Engineering Research (WISER) program at Penn State. In this program, female freshmen start their research activities in their second semester at Penn State. The CCMD also explored various NSF supplementary support including Research Experience for Undergraduates (REU), Research Experience for Teachers (RET), and Research Experience for Veterans (REV). In one exemplary success story from the RET program, a math teacher and a group of students from local high school near Penn State worked with faculty and graduate students of the CCMD for several

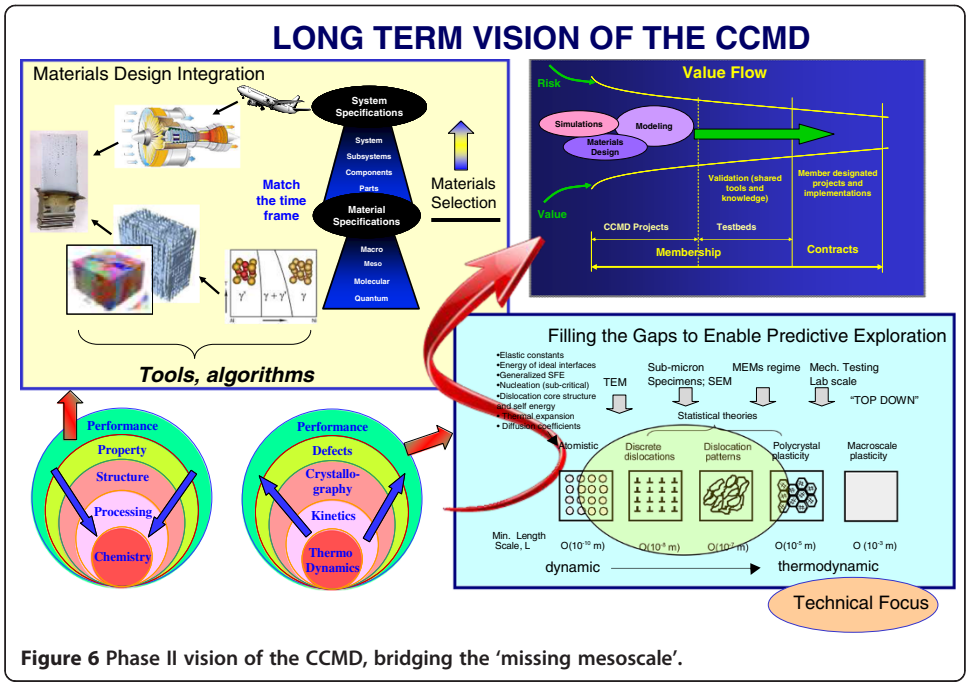

Figure 6 Phase II vision of the CCMD, bridging the 'missing mesoscale'.

years on several projects related to data analysis and geometry. The math teacher and his students participated and presented their posters at CCMD meetings. The REU/RET/REV and WISER programs at Penn State were complemented with programs at Georgia Tech, including the NSF-funded Summer Undergraduate Research Fellowship (SURF) program and the Georgia Industrial Fellowship for Teachers (GIFT) program, which coordinates recruitment of high school STEM teachers for summer positions in research laboratories.

CCMD accomplishments and impact

The CCMD spawned fundamentally new science and technology developments in support of ICME. CCMD projects pioneered the following revolutionary new scientific and engineering in terms of methods and tools to support systems-based computational materials design:

- First-principles prediction methods for elastic constants, thermal expansion coefficient, and antiphase boundary energies (Liu, PSU).
- Framework for automation of CALPHAD thermodynamic modeling (Liu, PSU).
- Software-engineered phase-field codes and libraries to facilitate parametric studies of grain growth and coarsening phenomena (Chen, PSU).
- Methodology for complete treatment of nucleation phenomena using diffuse interface phase-field models (Du and Chen, PSU).
- Quantitative prediction of plane strain fracture toughness of realistic microstructures using cohesive zone models (Zhou, GT).
- Extreme value statistics approaches for high-cycle fatigue strength informed by multiple computational realizations of polycrystals (McDowell, GT).
- Computational methods for effects of inclusions on fatigue strength/life of high-strength bearing steels in rolling and sliding contact (Neu, GT).
- Linkage of phase-field model predictions for polycrystalline structures with continuum polycrystal plasticity simulations to close the loop on process-structure-property relations (Chen, PSU, in collaboration with Garmestani and McDowell, GT).
- Comprehensive approach for robust design of materials based on hierarchical computational modeling and simulation, with a monograph published in 2009 by Elsevier (McDowell, Mistree, and Allen, GT).

A range of codes and tools were developed and made available to members as listed on the CCMD web page accessible by members. For example, Professor Zi-Kui Liu and Drs. ShunLi Shang and Huazhi Fang developed a web-based tool to calculate fundamental properties of Ni and Mg alloys. Graduate student Yan Li, advised by Professor Min Zhou, developed a GUI for microstructure characterization, image processing, and mesh generation of microstructures, as well as automated cohesive element assignment. In addition to these fundamental science and technology advances, the CCMD substantially impacted the national discussion regarding ICME, through the aforementioned presentations at major conferences of materials societies (e.g., [15-28]) as well as book chapters, conference proceedings, and archival journal articles related directly to ICME challenges (e.g., [29]).

CCMD members have provided input regarding the impact of the CCMD and the vision of Integrated Computational Materials Engineering within their organizations. For example, Figures 7 and 8 present CCMD member testimonials of impact on their organizations that were presented and submitted to the NSF. The U.S. Army Research Laboratory reported that their organization 'is actively pursuing the materials-by-design approach to accelerate/shorten the materials development time line. As such, independent of the CCMD, but essentially with the same philosophy, we have been hiring more modelers along all of the appropriate skill set being able to deal with different modeling length scales'.

CCMD faculty members were successful in developing grant proposals beyond internal CCMD projects, written in collaboration with CCMD members or in part due to their affiliation with the Center, or written as an outcome of faculty liaison with previous or current members. Some of these projects were in the form of direct funding from current or previous CCMD members, and others were subcontracts from current or previous CCMD members as flow through on federal prime funding to the members. Over $3 M total awarded proposal budgets were reported for 'CCMD-spinoff' research, representing additional funding arising from relationships with the CCMD members.

ICME relevant contributions to education

Two new courses were approved in 2007 and are now part of regular courses in the materials science major and the computational science minor at Penn State. Both courses have been further updated with results from CCMD research activities. The two courses are taught in alternative years:

- MatSE580: Computational Materials Science I: Computational Thermodynamics
- MatSE581: Computational Materials Science II: Continuum, Mesoscale Simulations

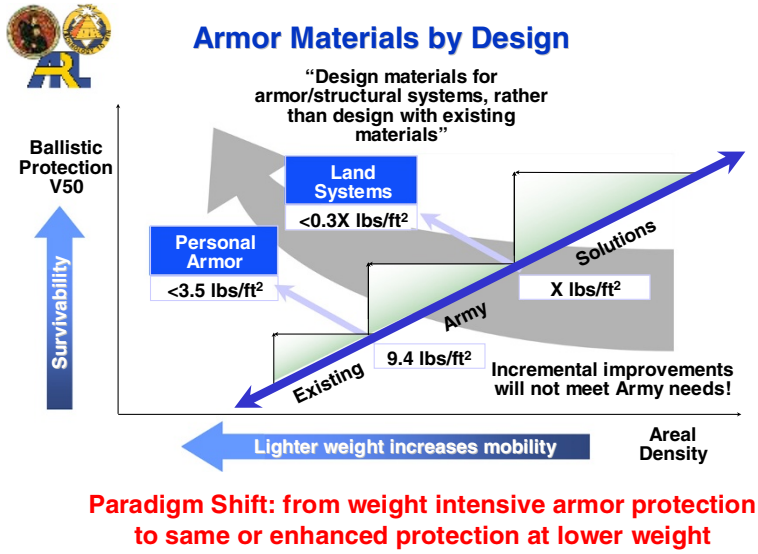

Figure 7 CCMD highlight from ARL on Mg-Alloys. Presented by Suveen Mathaudhu and Jim McCauley at TMS Computational Materials Design Roundtable Luncheon organized by the CCMD, 27 October 2009.

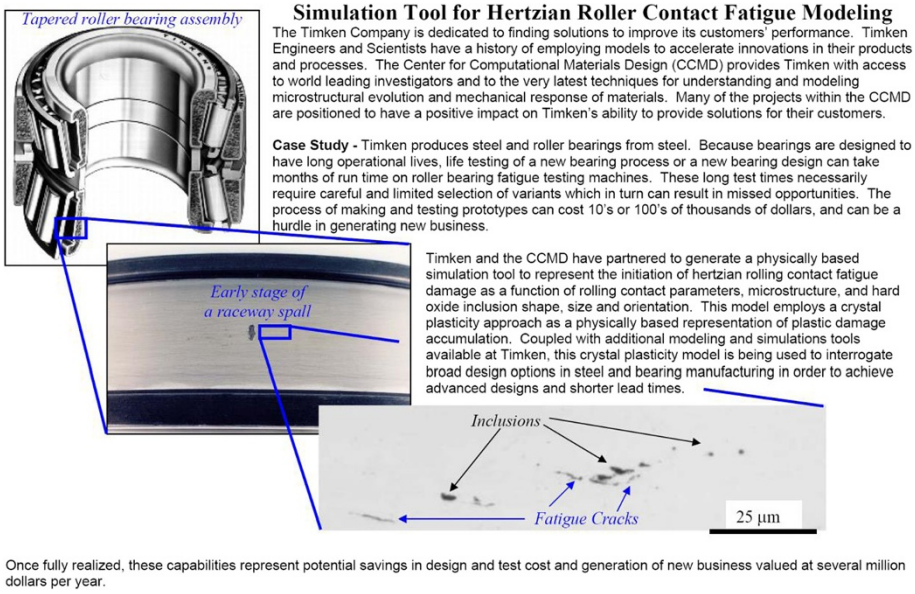

Figure 8 CCMD highlight from Timken Company on rolling contact fatigue.

Professors Liu and Chen at Penn State have integrated computational components in their respective undergraduate and graduate courses: Thermodynamics of Materials (401), Phase Relations (410), Thermodynamics of Materials (501), and Kinetics of Materials Processing (503).

Professsor McDowell developed a new advanced graduate course at Georgia Tech ME/BME 7205 entitled 'Mechanics and Applications of Nanostructured Materials and Devices.' The course is team-taught and covers quantum mechanics, molecular modeling and applications in mechanical and thermal properties and responses of interest. Elements of materials design were added to ME4213, Materials Selection & Failure Analysis, a technical elective primarily aimed at seniors at Georgia Tech and led by Professor R.W. Neu. McDowell also introduced a new junior level required core course in Materials Science and Engineering (MSE 3025, *Statistics and Numerical Methods in Materials Science and Engineering*) that is consistent with trends in Integrated Computational Materials Design and the CCMD vision of greater awareness and capability of undergraduate students in materials science and engineering in the areas of statistical methods and numerical methods/computational materials science. Several graduate level courses in a materials design sequence at Georgia Tech have been positively influenced by the CCMD, including:

- MSE 6795 Mathematical, Statistical and Computational Techniques in Materials Science;
- MSE 6796 Structure-Properties Relationships in Materials; and
- MSE 6797 Thermodynamics and Kinetics of Microstructural Evolution

McDowell served as lead-author on one of the first ICME-relevant textbooks [10] entitled 'Integrated Design of Multiscale, Multifunctional Materials and Products', a collaborative effort that had its roots in the CCMD and other ICME-relevant research

programs. The layout of chapters in this book shown in Table 1 reflects the multidisciplinary nature of ICME; it is broader than just a computational materials science-centered activity, showing that materials design and development is an integrated activity involving designers, materials suppliers, OEMs, characterization and testing labs, and manufacturers. The linkage to products is clear from the title as well, reflecting the top-down, requirements driven nature of materials development for economic and societal benefits. This is also a clear underlying theme of the Materials Genome Initiative [14].

Clearly, such a book could not be written from the singular perspective of a materials scientist, chemist, or physicist, nor by a designer, nor by a manufacturing specialist, etc. ICME textbooks that aim to prepare the future workforce will need to enrich the linkages and bring fields together. We have learned from our CCMD experience that ICME requires large-scale integration of stakeholders in an innovation ecosystem.

Discussion and evaluation

The CCMD was originally envisioned to embrace the intersection of materials modeling and simulation at various length and time scales with systems design. One may consider such a goal as pertaining to integrated materials design and development problems with a focus on a given material class and under constraint of limited resources. In reality, the diversity of member interests in various distinct materials classes in the CCMD consortium made it difficult to focus on a specific material system or design/development application. It became apparent that limited available resources from member dues within such a consortium drove projects towards addressing specific gaps in modeling and simulation, rather than overall frameworks for integrating process-structure-property-performance relations.

Some lessons learned related to the capability of the structure of the NSF I/UCRC program to support ICME-related research. The prospect of leveraging core NSF funding was helpful in attracting industry membership in the CCMD. In particular, the NSF I/UCRC program requirement of a limitation to 10% indirect costs associated with projects funded by member dues served as a significant incentive to join the CCMD rather than fund university research independently at much higher rates. However, as ICME

Table 1 Chapter titles for 'Integrated Design of Multiscale, Multifunctional Materials and Products' [10]

Chapter numbers	Chapter titles
1	Integrated Material, Product and Process Design - A New Frontier in Engineering Systems Design
2	Critical Path Issues in Materials Design
3	Overview of the Framework for Integrated Design of Materials, Products and Design Processes
4	Decision-Making in Engineering Design
5	Mathematical Tools for Decision-Making in Design
6	Robust Design of Materials - Design Under Uncertainty
7	Integrated Design of Materials and Products: Robust Topology Design of a Cellular Material
8	Integrated Design of Materials and Products: Robust Design Methods for Multilevel Systems
9	Concurrent Design of Materials and Products: Managing Design Complexity
10	Distributed Collaborative Design Frameworks
11	Closure: Advancing the Vision of Integrated Design of Materials and Products

developed, industry appeared to be interested in leveraging higher levels of federal investment provided by other sources (e.g., DoD, DoE) than the NSF I/UCRC program. The NSF funding level in the I/UCRC ($50 K per year to Georgia Tech and $60 K to lead institution Penn State during phase I, reduced in phase II) was too low to justify pursuit of cohesive foundational engineering problems or to entice member companies to explore extensions of their in-house proprietary materials design and development protocols. Moreover, a significant fraction of the NSF budget supported the Independent NSF Evaluator and I/UCRC mechanisms for running meetings (e.g., real-time web-based feedback from members during presentations); it was not clear that these expenditures and modes for evaluations/discussion provided higher utility in providing assessment and guidance in improving projects or team building than more conventional open discussion at meetings, combined with periodic teleconferences and student presentations.

Experience within the CCMD indicated that something like the ambitious, integrative DARPA AIM program or other Foundational Engineering Problems [8,11-13] could not be effectively addressed in the context of the NSF funding level for an I/UCRC consortia. It takes major focused investment. Nonetheless, the fundamental contributions to methods and tools within the CCMD served to substantially advance ICME capabilities, as did the education of the next generation of graduate students and postdocs working in the context of the ICME paradigm. We see the need for companies to place higher priority on current and future workforce development relative to an emphasis on software tools. We also see the need to hire students educated and trained with the ICME 'mindset' and/or to engage universities in extended working relationships and student exchanges. Several CCMD stakeholders pursued such opportunities with excellent results, particularly those who engaged students as interns and/or committed engineering personnel to collaboration with the CCMD research programs to transfer technology and implement codes and methods in their organizations.

It became very clear to industry and government participants, as well as faculty and students involved in the CCMD, that ICME involves a change of culture and is not just an algorithmic addition to existing organizational processes and methods. Implementation of ICME within an organization requires buy-in and investment and a change of operations to incorporate modeling and simulation in a systematic way to accelerate decision-making in materials development. Moreover, materials development must integrate with manufacturing, quality control and automation, verification and validation, materials synthesis, processing, characterization, and property measurement. A computational materials design research center is therefore inherently limited in its breadth in addressing ICME. Nonetheless, bridging the fundamental gaps identified in the CCMD vision shown in Figure 6 is critical to facilitating the role of computation.

Along these same lines, the overarching goals of the CCMD align closely with those of the MGI announced by the White House in June 2011 [14]. Additionally, the fundamental concept underlying CCMD research reflects the essence of the opening statement 'A genome is a set of information encoded in the language of DNA that serves as a blueprint for an organism's growth and development. The word genome, when applied in non-biological contexts, connotes a fundamental building block towards a larger purpose'; the fundamental building block of materials is the individual phase. The CCMD has focused on developing approaches to model the properties and responses of individual phases as a function of process variables and to simulate their contributions to the

properties and responses of microstructures consisting of polycrystalline/polyphase aggregates and their interfaces.

Conclusions

The vision of ICME is compelling in terms of value-added technology that reduces time to market for new products that exploit advanced, tailored materials. This case study considers the foundation, operation, and contributions of the joint Penn State-Georgia Tech CCMD, a NSF I/UCRC funded from 2005 to 2013. In spite of limitations on per project funding and constraints on mounting systematic, large-scale integrated materials design and development for specific materials systems, several key aspects of the current ICME and MGI emphases were established by the CCMD in this earlier time frame:

- Systematic development of the ICME workforce of the future;
- Building a culture of materials design and development, with increasing emphasis on computation; and
- New advances in computational tools to deal with diffusion, microstructure evolution, fracture and extreme value fatigue problems.

In advancing methodologies and tools to address ICME, it is essential to maintain a consistent long-term vision among industry, academia, and government. The required change of culture in academia towards materials research and development, as well as evolution of the curriculum, is an essential aspect with a relatively long time scale (perhaps a decade or more). Moreover, there is a critical need for industry to embrace this culture shift as well, which can be greatly facilitated by hiring students exposed to research initiatives such as the CCMD. Such students will employ modeling and simulation in industry practice. Furthermore, although engagement of materials suppliers within the CCMD was rather limited compared to involvement of OEMs, we view the materials supply chain as critical to the future of increasing the pace of materials discovery and development to meet ICME and MGI objectives. The materials supply chain might very well establish strong entrepreneurial leadership in the future of ICME, which will be advanced through innovative new business models and incentives.

A closing comment pertains to the broad multidisciplinary nature of ICME and materials innovation. Too often the discussions seem to revolve around the discipline of Materials Science & Engineering in the context of computational materials science, particularly in professional society and government planning venues. The materials innovation ecosystem is much broader. For example, the CCMD embraced from its inception the coupling of computational materials science, computational solid mechanics, and systems-based engineering design. These are rather disparate fields that typically do not strongly overlap in professional societies and archival journals. Students involved in the CCMD were witness to broad discussions across these disciplines to appreciate how scales and organizations can be bridged to achieve ICME goals by incorporating essential contributing elements of these different perspectives.

Following the CCMD vision in Figure 6, Penn State has engaged in expanding the concept of MaterialsGenome® and developing infrastructure for phase-based property data [30,31]. It is articulated that new data repository infrastructure is necessary so that

when new models are developed or new experimental and computational information becomes available, the hierarchically structured materials property databases can be re-assessed efficiently to develop the new multicomponent descriptions. The ongoing effort of ESPEI (Extensible Self-optimizing Phase Equilibrium Infrastructure) serves as one example [32].

Georgia Tech has followed up on lessons learned with the CCMD experience in ICME to invest in developing a materials innovation infrastructure that broadly addresses the ICME vision and that of the MGI [14] as a highly multidisciplinary enterprise, with various expanded elements shown in Figure 9. The Institute for Materials (IMat) was founded in 2012 at Georgia Tech by CCMD Co-Director Dave McDowell (www.materials.gatech.edu). Reporting to the office of the Executive Vice President for Research, IMat is framing Georgia Tech's materials innovation ecosystem involving over 200 faculty members engaged in materials research to provide an institutional framework for collaboration in materials research. Connecting expertise, infrastructure, and resources that underpin the science and engineering of materials, the Institute serves as a hub for materials education and research across Georgia Tech and within the broader materials community. In addition to coordination of access and utilization of shared facilities within Georgia Tech, IMat is building a model for materials innovation that:

- Pursues a 'Materials + X' strategy in forming approaches that address grand challenges, with materials as an enabler of advances in energy, mobility, security, health, etc.;
- Promotes development of novel approaches to materials data sciences and informatics as part of a materials information infrastructure; and
- Fosters collaborative concepts for accelerating materials discovery, design, and development via high throughput computational and experimental strategies.

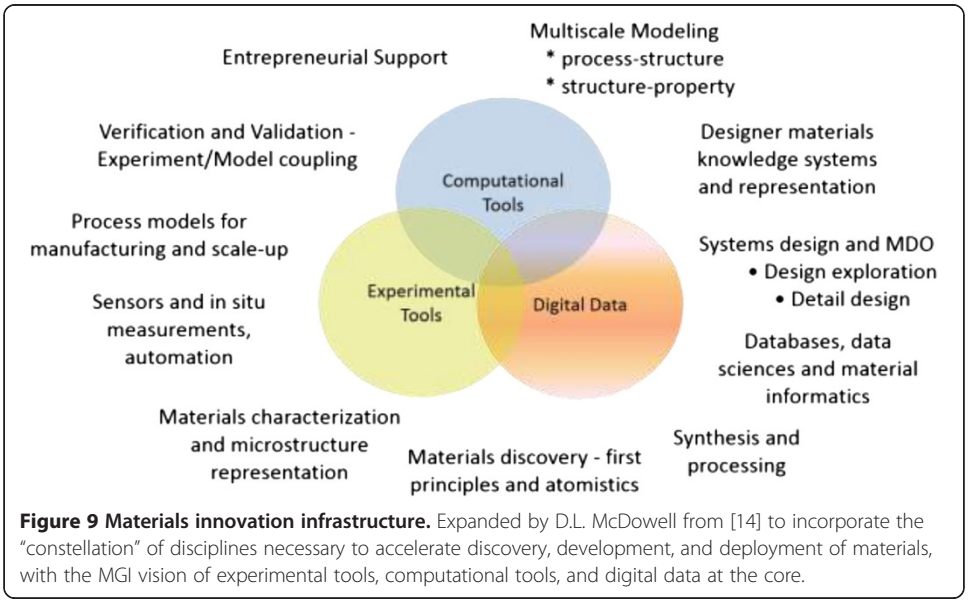

Figure 9 Materials innovation infrastructure. Expanded by D.L. McDowell from [14] to incorporate the "constellation" of disciplines necessary to accelerate discovery, development, and deployment of materials, with the MGI vision of experimental tools, computational tools, and digital data at the core.

In addition to hosting a 28 March 2014 Southeastern U.S. regional workshop for the MGI, IMat collaborated with the University of Wisconsin-Madison and the University of Michigan to co-organize the workshop '*Building an Integrated MGI Accelerator Network*', held at Georgia Tech 5 to 6 June 2014. An initiative that arose through discussions with the White House Office of Science and Technology Policy, the purpose of the Accelerator Network is to launch a nationwide dialogue to connect centers, institutes, and future efforts to fulfill the MGI (http://acceleratornetwork.org/).

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
ZKL and DLM co-directed the CCMD with NSF support from 2005 to 2013, and both contributed substantially to this case study. DLM drafted this manuscript with significant additional input from ZKL, with a number of iterations between them to reach final form. Both authors read and approved the final manuscript.

Acknowledgements
The authors are grateful for the long-term support of the NSF Industry/University Cooperative Research Center for Computational Materials Design (CCMD), including dues contributions of CCMD members, through grants IIP-0433033 (Penn State), IIP-0541674 (Penn State) and IIP-541678 (Georgia Tech) from 2005–2010, and IIP-1034965 (Penn State) and IIP-1034968 (Georgia Tech) from 2010 to 2013. The authors would like to thank our collaborators at Penn State and Georgia Tech for their enthusiastic and innovative contributions to CCMD projects and meetings over the years, including Co-PIs of the CCMD planning, phase I, and phase II proposals (Long-Qing Chen, Qiang Du, James Kubicki, Evangelos Manias, Padma Raghavan, and Jorge Sofo at Penn State, and Hamid Garmestani, Farrokh Mistree, Richard Neu, and Min Zhou at Georgia Tech), various additional Penn State and Georgia Tech faculty involved in CCMD proposals and projects, and students who conducted research with CCMD support. ZKL also acknowledges Penn State for further reduced overhead rate and Penn State MRI (Materials Research Institute) that provided partial support of the CCMD administrative staff. DLM also acknowledges the support of the Carter N. Paden, Jr. Distinguished Chair in Metals Processing. Any opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect the views of the NSF, Penn State, or Georgia Tech.

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Received: 18 September 2014 Accepted: 14 November 2014
Published online: 17 December 2014

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