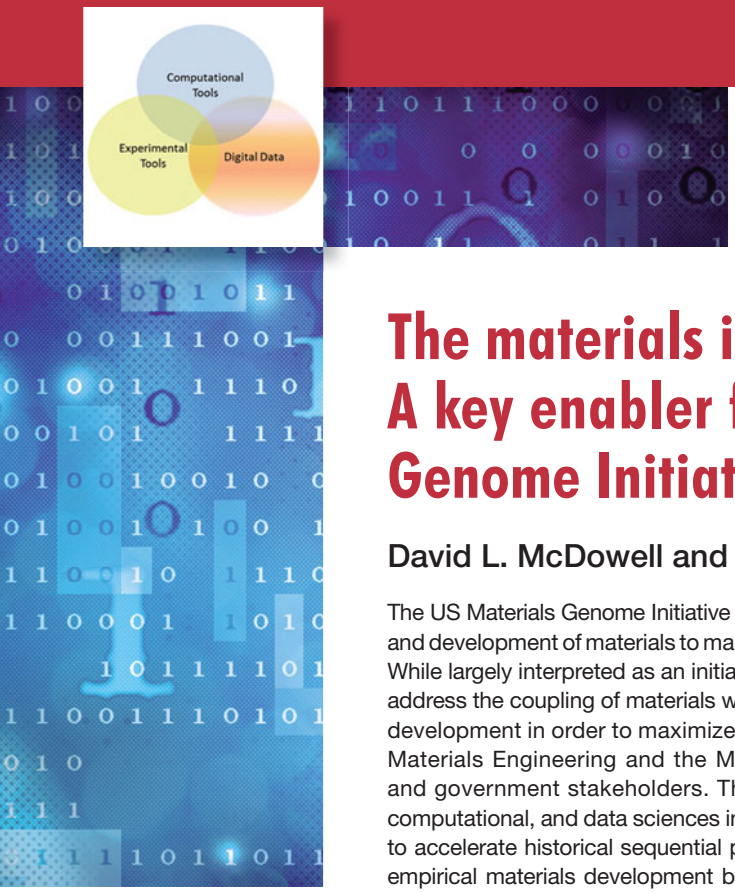

The materials innovation ecosystem: A key enabler for the Materials Genome Initiative

David L. McDowell and Surya R. Kalidindi

The US Materials Genome Initiative (MGI) has emphasized the need to accelerate the discovery and development of materials to maintain industry competitiveness in new and existing markets. While largely interpreted as an initiative arising from the materials community, it is important to address the coupling of materials with manufacturing and all other relevant aspects of product development in order to maximize its impact. The dual thrusts of Integrated Computational Materials Engineering and the MGI represent a long-term vision of industry, academic, and government stakeholders. The goal is to build a new kind of coupled experimental, computational, and data sciences infrastructure. The emphasis is on high-throughput methods to accelerate historical sequential processes of serendipitous materials discovery and largely empirical materials development by leveraging computation and modern data sciences and analytics. The notion of a materials innovation ecosystem is introduced as the framework in which to pursue acceleration of discovery and development of materials consisting of various elements of data sciences, design optimization, manufacturing scale-up and automation, multiscale modeling, and uncertainty quantification with verification and validation.

A vision for the materials innovation ecosystem

The primary goal of the US Materials Genome Initiative (MGI) is to accelerate the discovery and development of new and improved materials.[1,2] There has been historical emphasis on empirical routes for materials development, with computational modeling and simulation playing an increasing role over the past few decades. The predictive character of modeling and simulation has steadily improved, but it principally remains a means of providing decision support for materials development, particularly for metastable materials and nonequilibrium structures. At the same time, the use of first-principles methods to parametrically explore stable compounds for potential functional applications such as batteries has taken on great importance in opening up new venues for materials discovery, greatly reducing empiricism.[3] A basic tenet of MGI is that the efficiency, throughput, and connectivity of distributed materials discovery and development efforts can be greatly enhanced by modern data sciences and informatics implemented within the context of big data and high-performance computing.

Early manifestations of the data component of MGI focused on database structures and protocols for archiving digital data of various types. This is perhaps understandable given the historical lack of attention to archiving and open publication of materials data from research and development.[1,2] In our view, this phase of development is only a first step, with the more pressing issues defined by how data sciences can enrich the value of data to individual researchers and team collaborations. In the modern era, materials are rarely developed without anticipating a need, nor by the materials R&D community in isolation. Hence we embrace a vision for a broader materials innovation ecosystem shown in **Figure 1**.[1,4] Clearly, materials synthesis, processing, characterization, property measurement, and modeling and simulation at various length and time scales are foundational elements of materials discovery and development. This vision for the materials innovation ecosystem in Figure 1 does not correspond to the organization of a typical research university's materials research or education programs.

Much of the focus of the scientific community with regard to MGI has been toward combinatorial first-principles methods and high-throughput synthesis strategies to facilitate materials discovery, whereas the broader stream of materials development involves manufacturing and product realization. This latter

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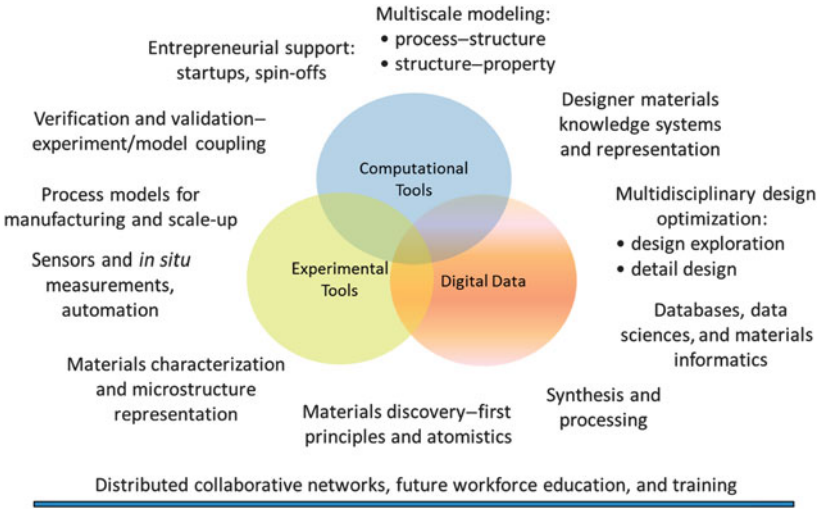

Figure 1. Our view of the materials innovation ecosystem, comprised of various sub-disciplines. The inner overlapping Venn diagrams form the basis for the Materials Genome Initiative,[1,2] surrounded by the necessary disciplines that affect materials discovery and development.[4]

stream has been clearly articulated in terms of the difficulty in moving new and improved material concepts from basic research into scale-up manufacture of products, the so-called "valley of death" for materials development and deployment as outlined in a 2008 National Academy of Engineering National Materials Advisory Board report on the Integrated Computational Materials Engineering (ICME) initiative.[5] Materials discovery and development pursuits have been historically decomposed along a sequence of stages,[1,2] typically consuming 15–20 years from discovery to deployment. ICME represents an approach to the design and development of materials that considers product requirements, and chiefly focuses on integration of modeling and simulation at various length and time scales with materials synthesis, processing, characterization, and property measurements to provide enhanced and more rapid decision support. The ICME study[5] featured Ford Motor Company's next-generation cast Al-Si alloy engine block as an example of integration enabled by modeling and simulation of process–structure and structure–property relations.

The goal of accelerated materials discovery, development, and deployment requires full accordance with the overlapping objectives of MGI and ICME. Regardless of how individual stakeholder communities distinguish goals of MGI and ICME, the fact remains that they are fused into compliance with the long-term vision of accelerating all stages of materials research, development, and deployment. Although programmatic incarnations of MGI have largely emphasized materials discovery and coupling of modeling and simulation with synthesis, processing, characterization, and property measurement, it is to be noted that the MGI strategic plan, issued in December 2014[2] by the subcommittee on the MGI tasked by the National Science and Technology Council, encompasses both discovery and development aspects, and requires joint investment by the science and engineering communities.

A key to unleashing the power of such a materials innovation ecosystem is the ability to represent hierarchical material structure (including chemical composition) at multiple levels in digital format along with simulation results, experiments, and various other sources of information and associated metadata (important additional information about the data) in a way that provides an objective lexicon with which to communicate. It should also provide an incentive to collaborate by adding value in each transaction. This latter aspect is very important, as broad discussions of MGI have focused on digital data structures and formats. In other words, such an ecosystem, as is the case for any naturally occurring ecosystem, can only be sustained by adding value to the capabilities of all participants to incentivize collaboration.[6]

Materials discovery and development are highly competitive enterprises, both within academic and government research and development, as well as product-driven industrial operations. Incentivized participation can increase the rate of interactions, serving the purposes of accelerating science, engineering, and technology translation beyond the "early-adopter" stage. Some examples of value-added scenarios include:

- Incorporation of material process–structure–property (PSP) correlations into computer-aided design and design for manufacture, enhancing concurrency to support design for manufacture;
- Linking downstream materials certification requirements to screening protocols in the materials discovery stage;
- Coupling multiscale modeling of materials with uncertainty quantification and associated decision support in multiobjective systems design;
- Coupling experimental observations at multiple length and time scales with modeling and simulation through data science in mutually beneficial ways, serving to objectively identify how and where future efforts should be directed;
- Providing new capabilities to quantify outcomes of materials synthesis and processing by quantifying spatial statistics of microstructures using n-point spatial correlations, forming a natural data linkage to modeling and simulation; and
- New high-throughput materials synthesis routes, as well as structure and performance characterization protocols that provide the critical information needed for simulation of manufacturing processes.

Data analytics can catalyze sharing of data by offering new insights. Traditional "build it and they will come" strategies focus on data structures, formats, and data storage/retrieval

in centralized repositories; although part of the necessary infrastructure, these strategies have not proven compelling in their own right to engage academic, government, and industry stakeholders. Otherwise, these strategies would have already witnessed explosive development and adoption. Much more attention should be devoted to collaborative web-based platforms (hereafter referred as e-collaborations) that support all phases from basic research in materials discovery through applied materials development.

As an example, the Institute for Materials at the Georgia Institute of Technology (Georgia Tech) has been fostering the vision of the materials innovation ecosystem shown in Figure 1 as an academic "test bed" for ICME and MGI.[7] The inner Venn diagram of experiments, computation, and data from the MGI plan[1,2] is at the core of this constellation of disciplines. Note also that the supporting technologies and workforce elements of various stages of materials discovery and development are incorporated as part of this innovation ecosystem to promote their concurrent linkage to the greatest extent possible.

This article focuses on critical gaps regarding elements of this materials innovation ecosystem. Web-based collaboration of distributed experts addressing generation and management of data, high-throughput methods, and infrastructure for obtaining information from experiments and computational modeling to support materials development decisions, approximate inverse methods that consider PSP relations in reverse order, materials information infrastructure, and future workforce development are discussed.

Key underdeveloped elements of the materials innovation ecosystem

Materials have hierarchical structure, ranging from nanostructures through various levels of microstructure. Experimental routes have long served the purposes of empirical materials discovery and development. The past few decades have witnessed an accelerating role for high-performance computing in materials modeling and simulation to support the vision of the MGI, yet significant gaps remain.

e-Collaboration

It is vital to recognize that a single research group or organization is unlikely to harness the diverse resources, cross-disciplinary expertise, and the investment capability needed to establish the envisioned materials innovation ecosystem shown in Figure 1. Indeed, even assembling and organizing all of the core materials science and engineering knowledge (i.e., the PSP linkages covering all of the salient hierarchical length and time scales) and the associated tool sets is by itself a daunting task. Such an endeavor is made particularly difficult by the fact that legacy data sets and tools, in their existing forms, exhibit a high level of variety (in formats, protocols used, etc.) and are broadly distributed geographically and organizationally. The current fragmented state of materials data, knowledge, tool sets, and expertise presents a strong case for the tremendous benefits that could readily accrue from a synergistic aggregation to incentivize collaborations. It should be recognized that aggregation of data and knowledge pursued as an essential component of collaborations (as opposed to the aggregation efforts aimed primarily at sharing data) is likely to identify/discover results of high value to the broader materials community, as the collaborations are themselves most often sharply focused on imminent problems of high value/interest.

Data is the dominant currency of collaborative transactions. Here, we adopt a very broad definition of the word "data." The definition includes any information present in any form (e.g., numeric, image, text, metadata, workflows, communications). Clearly, a major challenge lies in its vast size, distribution, and highly heterogeneous character, as well as the inconsistency of associated metadata that provide additional insight and description. The absence or shortage of important annotations and metadata for existing data is a tremendous challenge, as is the opportunity to more completely incorporate metadata arising from modification and transaction of existing data sets. Moreover, materials discovery and development workflows are commonly of anecdotal nature, detached from their associated data. Tools for effectively recording workflows are lacking, resulting in difficulties in identifying and transferring best practices to other teams and other projects. This substantially impedes development of standards and automation. Moreover, such workflows are necessary to quantify cost and time reduction in assessing the extent of acceleration in materials development; one must have comparative baselines in this regard.

The challenge of establishing collaborations is familiar to most stakeholders in the materials-development enterprise. It can be difficult, time consuming, and expensive to find the right expertise at the right time. One of the challenges in building the ecosystem in Figure 1 lies in the difficulty of communicating and achieving proper understanding of relative roles across disciplines. For example, an engineering systems analyst involved in optimization does not become a materials scientist by learning the nomenclature and file structures. A materials synthesis expert does not adopt the state of the art in uncertainty quantification by having short-term discussions with the uncertainty quantification, verification, and validation community. However, each can comprehend the added value of their complementary expertise if the interactions are configured to run more deeply than brief introductions and periodic team meetings.

What is the missing link? We believe that it lies in the use of e-collaborative tools, methods, and protocols that are yet to be fully established and realized. The materials community can benefit tremendously from adoption of emerging concepts and tools in data and information sciences. For example, it is now widely accepted that the use of hierarchical data formats (such as the Hierarchical Data Format [HDF] data model, library, and file format for storing and managing data [e.g., HDF5][8]) enhance our capability to keep connected data together. As another example, much more attention is now being devoted

to the form of metadata associated with a given data set. It is becoming fairly obvious that it is impossible to centralize and manage all materials data in one location, therefore, data will likely continue to be federated for the foreseeable future. The large file sizes make it difficult to store and move data, and the large variety of data requires adaptive, flexible, and distributed strategies. Federated data are very difficult to find and are generally not searchable based on content. On the other hand, it is much easier to centralize metadata in a single location (because of its much smaller size) and create metadata databases that can be easily searched.

As mentioned earlier, sharing of data and tools is an important aspect in establishing highly productive collaborations, but is inadequate by itself. Human beings must derive a sense of leveraging into new, extended capabilities at the individual level in the interpretation, knowledge extraction, and decision support derived from data. This is the power offered by advanced Internet search tools, for example. Successful e-collaborations are contingent on the availability of tools that allow rich annotations of data, community development of codes, data analytics tools for extraction of high-value information (insight and interpretation that guide decisions), searchable data and metadata databases, meaningful visualizations, and intimate discussions of results. Web-based e-collaboration platforms, broadly deployed and adopted, can enable the necessary accelerative transformations envisioned within the materials innovation ecosystem.

High-throughput decision support and inverse methods for materials design exploration

Much initial emphasis in MGI has been placed on screening strategies to support materials discovery.[3,9,10] However, many of the challenges in materials development reside in control of processes of mesoscopic material structure evolution and ways to more rapidly and efficiently provide decision support at various stages of the materials development process.[11–15] High-throughput decision support is critical in all stages. Particular scientific and engineering gaps include high-throughput synthesis and processing in materials discovery, consideration of both thermodynamics and kinetics in screening potential new materials based on first-principles approaches, parallel modeling and simulation protocols for design exploration, and inverse methods of approximate character for process–structure and structure–property relations. Uncertainty quantification, verification, and validation are foundational to progress on each of these gaps. This is a hallmark of multidisciplinary design optimization (MDO), namely consideration of uncertainty in various aspects of the "system" (experiments, computation, data, and their coupling) set in place to support materials development. A caveat is that MDO has been typically applied in situations where models and information are complete. Moreover, MDO employs reduced-order metamodels or surrogate models that may not be accurate enough to model real materials in all cases. New advanced high-performance computing algorithms are necessary in this regard.[16]

The Inductive Design Exploration Method (IDEM)[11,17,18] is an example of a practical strategy that provides robust decision support for top-down, inverse methods for process–structure–property relations while employing parallelized bottom-up simulations and experiments. Starting with a ranged set of product performance specifications or requirements, the goal is to identify candidate ranged solution sets that satisfy these requirements in a top-down manner (given performance, along with resulting properties, structure, and process route) consistent with bottom-up (experimental- or model-based) mappings of the material process–structure–property performance relations. In other words, materials development and product development are inextricably linked.[11] Bottom-up information flow is combined with top-down guidance from applications and associated performance requirements. As discussed elsewhere in detail,[11] solutions to design problems in the presence of uncertainty are not unique. The designer can express preference among a set of possible solutions to maximize a multiobjective function or to express insensitivity with regard to changes of process or microstructure design variables. In making this choice, the designer can exercise principles of robust design as laid out by Taguchi for process control.[19]

IDEM provides a step-by-step strategy to facilitate the combined bottom-up modeling and simulation or experiments, leading to consideration of top-down mappings that satisfy high-level performance requirements and manage uncertainty propagation in model chains. As illustrated in **Figure 2**, IDEM requires initial configuration of the design process. Implementation of IDEM necessitates identifying

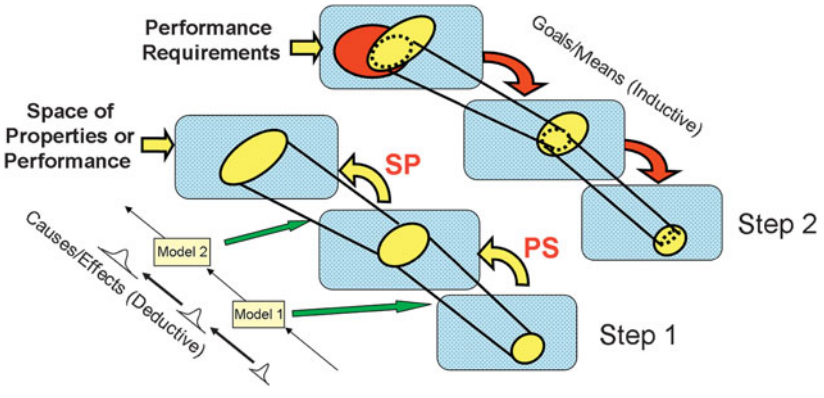

Figure 2. Schematic of Steps 1 and 2 in the Inductive Design Exploration Method.[11] Step 1 involves bottom-up simulations or experiments for process–structure (PS) and structure–property (SP) relations, typically conducted in parallel fashion, to map composition into structure and then into properties, with regions in yellow showing the feasible ranged sets of points from these mappings. Step 2 involves top-down (inductive, goals/means) evaluation of points from the ranged set of specified performance requirements that overlap feasible regions established by bottom-up (deductive, causes/effects) simulations in Step 1.

the connections of inputs and outputs of models, simulations, experiments, and databases, and decision points such that a complete graph of information flow is achieved. If certain models have greater certainty, they can be more heavily weighted. Quality experimental information can be factored in as desired. It is essentially an instantiation of the balanced decision-making process that has been employed in design for many years, biased towards quality information and insights.[14]

Applications of these robust design methods to the design of extruded prismatic metals for multifunctional structural and thermal applications[20–22] and design of multiphase thermite metal-oxide mixtures for target reaction initiation probability under shock compression have been described elsewhere,[23] and have been further summarized by McDowell et al.[11]

A key enabling capability needed to support the practical implementation of this approach to multilevel materials design and development lies in the successful formulation of surrogate models[11] (also referred to as metamodels, response surface models, or reduced-order models). It is often impractical to directly employ physics-based models to provide decision support in materials development. A much more practical approach entails the use of low computational cost surrogate models of sufficient (and quantifiable) accuracy in multilevel design exploration and development. In this regard, recent advances in materials data sciences have paved the way for objective (data-driven) formulation of surrogate PSP linkages that exhibit a remarkable combination of high accuracy and low computational cost.[24,25] These data-driven surrogate models for hierarchical PSP linkages are central to successful implementation of high-throughput strategies in multilevel, multiscale materials design and development.

The key to successful extraction of high-value, low-dimensional PSP linkages lies in the identification of the salient descriptors of the material hierarchical structure, including chemical composition. Descriptors are employed both in combinatorial materials discovery[26,27] and in the design and development of hierarchical microstructures. While it is abundantly clear that the rich hierarchical structures of most advanced materials demand an unimaginably high-dimensional description, it is also evident from past experience that only a few salient features may dominate the material response of importance in any selected application. An example is the simple Hall–Petch inverse relation between strength and mean spacing of slip obstacles in metals.[28,29] In most cases, these salient structure descriptors are not known *a priori*, and experts conduct numerous time- and effort-intensive trials (employing both measurements and models) for each application. Since this process is often nonstandard and leads to a highly customized set of structure descriptors for each application, the knowledge gained in the process exhibits only limited transferability to other applications.

In order to dramatically improve the efficacy of the above process and attain the disruptive acceleration envisioned in MGI and ICME, it is imperative to formulate and adopt a consistent framework for the description of the hierarchical material structure. Kalidindi and co-workers[30–36] recently developed one such framework, and it has been demonstrated on a variety of material structures at vastly different length scales. The examples explored in these studies include experimentally measured and numerically simulated multiphase and polycrystalline microstructures of α–β Ti alloys at the mesoscale and atomistic/molecular structures[37,38] predicted by molecular dynamics simulations for Al as well as semicrystalline polyethylene. This specific framework employs digital representations, n-point spatial correlations, and principal component analyses to arrive at data-driven (objective) measures of the salient material structure descriptors. It is also noted that the n-point spatial correlations (or n-point statistics) provide the most complete set of measures that are naturally organized by increasing amounts of structure information.

For example, the most basic of the n-point statistics are the one-point statistics, and they reflect the probability of finding a specific local state of interest at any randomly selected single point (or voxel) in the material structure. In other words, they essentially capture the information on volume fractions of the various distinct local states present in the material system. The next higher level of structure information is contained in the two-point statistics that capture the probability of finding specified local states h and h' at the tail and head, respectively, of a prescribed vector r randomly placed into the material structure. Higher-order correlations (three-point and higher) are defined in a completely analogous manner. Once the salient structure descriptors are established, they can be utilized to establish low computational cost, surrogate, hierarchical PSP linkages in both homogenization[33–35] (i.e., information flowing from the lower scales to higher scales) and localization[39–46] (i.e., information flowing from higher scales to lower scales) problems of interest in materials development efforts. A distinctive feature of this framework is that it aims to harmoniously combine well-established micromechanical theories for heterogeneous materials[47,48] with established concepts in systems theories[49–54] and emerging concepts in data sciences[55] in ways that take full advantage of their respective strengths.

Infrastructure for high-throughput synthesis/processing–structure–property relations

Nearly 20 years of progress has been made in the US National Nanotechnology Initiative.[56] Investigators in Europe and Asia have also broadly pursued research in nanosciences and nanotechnology. Experimental and computational methods and tools that support the nanosciences are ubiquitous across academic science and engineering disciplines. In many respects, we are now in a postmodern era of nanotechnology in which we are exploring its impact on emergent solutions to grand-challenge problems. However, the nanotechnology initiative has not translated into an accelerated pace of materials development, whether nanomaterials or any other class, nor has it addressed the need to tailor materials to applications in a rapid manner that meets the timeframe of product development

University curricula for educating the future workforce

University curricula and instructional tools require integration and further development of various elements of the materials innovation infrastructure, providing education and training for the future workforce to capitalize on the competitive advantage offered by high-throughput, simulation-assisted materials discovery and development. This reformation must extend beyond traditional materials education to bridge across engineering and science academic disciplines that naturally foster various supporting elements. There is a significant gap in curricula at universities in terms of uncertainty quantification and protocols for decision support. This generally falls under the categories of systems design, data sciences, and optimization under uncertainty. More specifically, combining uncertainty quantification and management with systems approaches can dramatically accelerate materials innovation efforts.

There are already a number of distributed educational efforts on which to build. Examples include the master's program in Materials Science and Simulation at Ruhr-Universität Bochum,[1] ICME courses at Mississippi State University,[2] the ICME Masters certificate focused on design at Northwestern University,[3] the Georgia Tech program From Learning, Analytics, and Materials to Entrepreneurship and Leadership (FLAMEL) (funded through an NSF IGERT [Integrative Graduate Education and Research Traineeship]),[4] the Texas A&M IIMEC Summer School on Computational Materials Science Across Scales,[5] the University of Michigan Summer School on Integrated Computational Materials Education,[6] the Lawrence Livermore National Laboratory Computational Chemistry and Materials Science Summer Institute,[7] and the summer workshop from the University of Florida Cyberinfrastructure for Atomistic Materials Science Center.[8]

There is a need to develop and offer cross-cutting curricula and short courses in engineering and the sciences that address computational materials science, high-throughput experimental methods, advanced materials characterization and property measurements, inverse methods and metamodeling, uncertainty quantification, verification and validation, and integration with manufacturing, data sciences, and systems engineering.

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cycles—these are intrinsically related to the ICME and MGI initiatives. In this regard, high-throughput protocols are of premium importance, especially protocols that couple synthesis, processing, characterization, and property measurement with modeling and simulation at various length and time scales as appropriate to accelerate process control and achievement of desired properties and address essential aspects of the desired service environment. For example, purely computational first-principles methods for screening candidate material systems for energy storage in batteries do not typically address kinetics and mesoscale defects that limit performance under many charge-discharge cycles and under dynamic temperature and loading environments. Strategies for mesoscale modeling, data analytics, and high-throughput experimental protocols are necessary to address these issues.

A key indicator of our imbalance in investment is a severe shortage of linked cyber and physical infrastructure to advance the cause of accelerated materials discovery and development. This was identified by experts as a common theme over a wide range of materials classes as part of a recent MGI workshop.[57] The workshop report[58] listed high-priority cross-cutting recommendations as follows:

- Focus on education and training of the future MGI workforce;
- Compile a knowledge base of existing federally funded MGI-related efforts;
- Link physical and cyber infrastructure that cuts across materials classes and application domains;
- Establish working groups and networks in and across these domains;
- Define effective foundational engineering problems for each application domain to rally MGI stakeholder collaboration and networking; and
- Establish a distributed materials information infrastructure.

Below, we summarize gaps that were commonly identified across the six material domains, which map onto the previous cross-cutting recommendations:

(1) Establish a materials information infrastructure. More than just a database, a web-based environment for e-collaboration serves to glue together the materials innovation ecosystem in Figure 1. Gaps to be closed include provision of reliable reference data, standard test methods across laboratories, standardization of tools for data mining and data-driven descriptors, federated databases and access tools, and

Future workforce development

Georgia Tech was recently awarded an NSF IGERT program From Learning, Analytics, and Materials to Entrepreneurship and Leadership FLAMEL[1] that addresses some of the key educational gaps related to materials data sciences and informatics. The students in this program are required to take a certain combination of core courses that cover fundamentals of materials science and engineering, mechanical and manufacturing sciences, and computer science (including data analytics). They are also required to take two courses aimed at synthesis and integration of these different disciplines. These integration courses are focused on materials informatics and are jointly taught by faculty from engineering sciences and computer sciences.

The rich diversity of student backgrounds in the materials informatics classes present a perfect opportunity to convey the importance of cross-disciplinary e-collaborations, and to expose students to the challenges involved. With the support of the Institute for Materials at Georgia Tech, we have created and launched an open science, e-collaboration network among the students in the class. Called MATIN, this e-collaboration platform was designed to promote a healthy peer-learning environment among students. Our initial effort was focused on designing and deploying features that allow tracking (i.e., version control and provenance) and curation of all the data, codes, and discussions with connected (i.e., graphed) persistent identifiers. This was largely accomplished by provisioning existing web services. Examples of web services explored to date have included GitHub[2] for versioning and archival of codes, Dropbox[3] for storage, ShareLaTeX[4] and Authorea[5] for collaborative editing of documents, figshare[6] for citable publication of research, Plot.ly[7] for collaborative data analysis and visualization, Jekyll[8] blog posts with Disqus[9] for discussions, and Google+[10] and LinkedIn[11] for e-teaming and networking.

Nine cross-disciplinary student teams participated in the fall 2014 offering of this class,[12] and they investigated a range of diverse, highly cross-disciplinary materials research problems. A number of new research collaborations were seeded through this platform for the first time and several of these are now being converted into archival journal articles; this attests to the remarkable pace at which the e-collaborations can be established and become productive. The research projects centered around topics such as permeability of packed soils, x-ray scattering in polymers, mechanical behavior of reinforced polymer composites, growth of a tungsten trioxide hydrate layer on a tungsten nanowire surface, microstructure in chips of titanium produced during machining, process–structure–property linkages in 6061 Al, structure–property linkages in poly-3-hexylthiophene (P3HT) thin-film transistors, crystal plasticity of hexagonal metals, and process–structure linkages from molecular dynamics simulations on semicrystalline polyethylene.

One of the main lessons learned from this exercise is that it is indeed possible to design, build, and deploy a set of broadly applicable materials data analytic tools that could be applied on vastly diverse material data sets (with different materials classes and length scales) to extract new insights in a highly automated and accelerated set of protocols.

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improved coordination and access to physical infrastructure. Research infrastructure should support genuine collaboration between theory and experiments, making use of cloud resources, virtual collaboration, high-throughput synthesis and processing, tools for interrogating and analyzing data, and more relevant and predictive computational models that incorporate uncertainty quantification.

(2) Address gaps in the fundamental understanding of the relations between structure at different length scales and properties/performance. Consider long-term stability under service conditions, environmental stability, degradation, and performance lifetime at early stages of discovery and development. High-throughput screening should include environmental and service condition stability. Advanced diagnostic methods, particularly *in situ*/*in operando*, should be employed.

(3) Improve measurement science and modeling and simulation of synthesis and processing. Better understanding and development of the principles of kinetic and thermodynamic control of process route/structure relations are needed. Exert reliable control of structure over various length scales (ranging from nano to macro) during processing, including up to large scales. Employ *in situ* characterization and sensing during synthesis and processing, with data mining and analytics. Predict structure morphology (new models to predict the morphology at different length scales) and link to processing

strategies to achieve desired morphologies. Draw on elements of process control from chemical engineering and manufacturing.

(4) Establish high-throughput strategies for screening that consider capabilities and constraints on available synthesis and processing routes, including fast-acting modeling tools to assess probability of meeting structure–property requirements, including four-dimensional (space and time) data sets for evolving material microstructure. Extend first principles and atomistic simulations to incorporate predictive simulation of metastable states and nonequilibrium trajectories of evolution under service conditions for applications, enabling parametric exploration of candidate material systems for product applications. Develop length- and time-scale bridging strategies that incorporate elements of data sciences with experiments and modeling and simulation to inform decisions in materials exploration, discovery, and design.

It was generally acknowledged that accessible user facilities that link computational resources with materials synthesis, characterization, and property measurements are lacking, and that uncertainty quantification is typically not systematic or uniformly prioritized.

There are key educational and infrastructure gaps in the materials innovation ecosystem that require attention to address high-throughput demands of the MGI. These gaps span both science and engineering disciplines. There is a lack of networked integration of federated high-throughput facilities to support materials discovery and development. Parallel efforts are also underway in Europe to address similar gaps.[59–61]

Materials information infrastructure

Many materials of practical interest have hierarchical structure ranging from atomic through mesoscopic levels. Historically, structure information has been documented and communicated either as representative images or through highly simplified measures (e.g., volume fractions of constituents, average size, shape, and spacing of constituents). The use of grossly simplified structure measures pose limitations in extracting and curating the core materials knowledge.

In recent years, there has been an increased adoption of digital formats for representation of the material internal structure along with automated (computerized) extraction of structure measures. However, the selection of the structure measures and the protocols to extract them are widely varied, depending on the material class and application domains. Moreover, the materials community has been tightly focused on digital materials representation and archiving of associated data sets. From our perspective, while essential, this is only the "tip of the iceberg" of the broader data sciences needs in accelerating discovery and development of materials. Too little emphasis has been placed on data analytic tools that link high-throughput modeling and simulation with experiments to provide decision support. A key element for the successful adoption of data sciences and high-throughput strategies is a generalized and extensible framework that allows a versatile digital representation of the material internal structure and the automated computation of a large number of potential hierarchical measures of the material structure.

In spite of success stories[5] in the development and deployment of high-performance materials, we do not yet have standardized (or templated) protocols for extraction of PSP linkages. Modern data sciences have a substantial role to play in this regard, as they are ideally suited for this task. One of the main hurdles in establishing standardized protocols for extracting PSP linkages from available legacy data arises from the fact that much of the legacy data has not been accessible to the broader community. Moreover, the associated metadata may be lacking or inaccessible. Modern data sciences and informatics tools are ideally suited to address this challenge through design and implementation of converters to structured hierarchical file formats, e-collaboration platforms, tracking integration workflows, among others. Hence we reframe the notion of a materials information infrastructure from that of a data repository to focus on web-based environments for materials data sciences and informatics that respect and acknowledge the rich hierarchy of length/structure scales present in most materials used in advanced technology, while simultaneously promoting and facilitating e-collaborative visualization, interpretation, and curation of core materials knowledge in easily accessed databases through the adoption of emerging data sciences and informatics tools.

The biggest drivers for the adoption of web-based environments are most likely to come from the cost and time savings realized as a consequence of their adoption in the materials innovation cycles. Given these indicators, it behooves the materials community to engage computer and data scientists as partners in a win-win scenario for both communities. This partnership should include considering and developing the following:

- Easy-to-use graphic-user interfaces that make it extremely easy for materials experts to upload their data and to leverage other data;
- An efficient online marketplace for multiscale data sets, models, and analytic tools (similar to an online App store), as well as web-agent approaches for distributed collaboration;[11]
- Customized e-collaboration platforms (including discussions, annotations, and visualizations) for specific applications or materials classes or manufacturing routes;
- Protocols to ensure proper assignment of credit to both the original data generators as well as to those that extract high-value information from the data sets, including possibly novel modes of publishing results (as opposed to the traditional journal articles) that expand access and productivity; and

- Protocols to ensure compliance with the sharing limits desired or set by the users.

Examples of "nodes" in the US materials information infrastructure that support many of the aforementioned goals in a complementary way, ranging from atomistic to continuum modeling, high-throughput methods for discovery and development, and modern data sciences approaches include, but are not limited to, the Materials Project at Lawrence Berkeley National Laboratory,[62] the OpenKIM project on interatomic potentials at the University of Minnesota,[63] the NIST (National Institute of Standards and Technology) Center for Hierarchical Materials Design (CHiMaD)[64] at Northwestern University, Argonne National Laboratory and The University of Chicago, and the Department of Energy PRISMS (PRedictive Integrated Structural Materials Science) Center at the University of Michigan.[65] Materials data and model repositories include those at NIST,[66] Citrine Informatics' system,[67] NanoHuB,[68] and the National Data Service's Materials Data Facility.[69] Similar nodes exist in Europe (e.g., NoMaD's [Novel Materials Discovery] computational materials repository)[70] and Asia (e.g., National Institute for Materials Science [NIMS]).[71] By and large, these platforms do not address distributed e-collaboration (see the sidebars on "University curricula for educating the future workforce" and "Future workforce development").

Summary

Revolutionary new trends in accelerated discovery, development, and deployment of new and improved materials call for emphasis on high-throughput computational and experimental methods, coupled with modern data sciences approaches. In this article, we provided a vision for a materials innovation ecosystem that addresses these elements. We also included an interpretive discussion of gaps and opportunities with regard to e-collaboration, high-throughput decision support and inverse methods for materials design exploration, infrastructure for high-throughput synthesis/processing–structure–property relations, materials information infrastructure, the need for networking of academic, government, and industry stakeholders, and supportive university curricula and educational offerings.

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PLASMONICS, PHOTONICS, AND METAMATERIALS RESEARCH LETTERS

Engineering the Reststrahlen band with hybrid plasmon/phonon excitations

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There has been increasing interest in so-called phononic materials, which can support surface modes known as surface phonon polaritons, consisting of electromagnetic waves coupled to lattice vibrations at the surface of a polar material. While such excitations have a variety of desirable features, they are limited to the spectral range between a material's longitudinal and transverse optical phonon frequencies. In this work we demonstrate that for materials whose free-carrier concentrations can be controlled, hybrid plasmonic/phononic modes can be supported across a range of frequencies including those generally forbidden by purely phononic materials. DOI:10.1557/mrc.2015.81

Low-Loss silicon wire-waveguides for optical integrated circuits

Tsuyoshi Horikawa, Photonics Electronics Technology Research Association (PETRA) and National Institute of Advanced Industrial Science and Technology (AIST), Japan; and **Daisuke Shimura** and **Tohru Mogami**, Photonics Electronics Technology Research Association (PETRA), Japan

Low-propagation-loss silicon wire waveguides are key components of optical integrated circuits. In this paper, we clarified, through assessment of the relationship between waveguide loss and fabrication technology that high-resolution lithography and an adjusted lithography process window are important for low-loss waveguides. The silicon wire waveguides fabricated by high-resolution lithography technology using ArF immersion lithography process showed world-record low propagation losses of 0.40 dB/cm for the C-band and 1.28 dB/cm for the O-band. Analysis with Barwicz and Haus's theory indicated that sidewall scattering is the main cause of propagation loss even in such low-loss waveguides. DOI:10.1557/mrc.2015.84

Angled physical vapor deposition techniques for non-conformal thin films and three-dimensional structures

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The field of nanophotonics has experienced a dramatic development in recent years, which requires ample candidate structures to achieve desirable functionalities. For many novel device designs in emerging field of transformation optics, optical metamaterials, and others, non-uniform and non-conformal thin films as well as three dimensional (3D) structures are necessary to achieve advanced functionalities. Here, we report several techniques utilizing angled physical vapor deposition to obtain unique and complex 3D structures such as films with tapered thickness on planar substrates, tapered or uniform films on curved surfaces, and 3D nanorods arrays. These structures could enrich the existing practical design space for applications in nanophotonics and nanoelectronics. DOI:10.1557/mrc.2016.3

Homogenization of nanowire-based composites with anisotropic unit cell and layered substructure

Brian M. Wells, University of Hartford and University of Massachusetts, Lowell, USA; and **Wei Guo** and **Viktor A. Podolskiy**, University of Massachusetts, Lowell, USA

We analyze the optical properties of composite materials that combine nanowire and nanolayer platforms. We revisit effective-medium theory (EMT) description of wire materials with high filling fraction positioned in anisotropic unit cells and present a simple numerical technique to extend Maxwell-Garnett formalism in this limit. We also demonstrate that the resulting EMT can be combined with transfer-matrix technique to adequately describe photonic band gap behavior, previously observed in epitaxially grown semiconductor multilayer nanowires. DOI:10.1557/mrc.2016.5

Silver nanoparticles supported on electrospun polyacrylonitrile nanofibrous mats for catalytic applications

Yongkun Liu, Zhejiang Sci-Tech University, China; **Guohua Jiang**, Zhejiang Sci-Tech University, National Engineering Laboratory for Textile Fiber Materials and Processing Technology and Key Laboratory of Advanced Textile Materials and Manufacturing Technology, China; and **Lei Li**, **Hua Chen**, **Qin Huang**, **Tengteng Jiang**, and **Xiangxiang Du**, Zhejiang Sci-Tech University, China

In this work, we developed a convenient way to immobilize silver nanoparticles on the aminated polyacrylonitrile (PAN) nanofibrous mats by combing the electrospinning technology from complex-containing polymer solution, amination of PAN nanofibrous and electroless plating technique. The resultant composite nanaofibrous mats had been characterized by scanning electron microscopy, energy dispersive spectrometer, transmission electron microscopy, X-ray diffraction and Fourier transform infrared spectra analysis. The catalytic activity and stability of these resultant composite nanofibrous mats for the catalytic reactions, including reduction of 4-nitrophenol to form 4-aminophenol and selective oxidation of benzyl alcohol, were investigated. The resultant nanofibrous mats exhibited high-efficiency, convenient separation, recovery, and cyclic utilization properties. DOI:10.1557/mrc.2015.85

Allamanda cathartica flower's aqueous extract-mediated green synthesis of silver nanoparticles with excellent antioxidant and antibacterial potential for biomedical application

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The present study aimed to develop an easy method to synthesis silver nanoparticles (AgNPs) using *Allamanda cathartica* flower extracts. The phytocompounds converted silver nitrate into AgNPs. UV–visible spectra show the maximum absorbance between 350 and 450 nm and x-ray powder diffraction results reveal AgNPs crystallized in cubic phase. Fourier transform infrared spectrum reveals that phytochemicals act as a reducing, stabilizing, and capping agent. Energy-dispersive spectrum, particle size distribution, and transmission electron microscopy analyses show that the nanoparticles are pure, spherical shaped with size of 39 nm. In addition, AgNPs show significantly antibacterial and antioxidant activity compared with commercial antibiotic. Hence, *A. cathartica* flower extracts mediated AgNPs which will be a new candidate for biomedical applications. DOI:10.1557/mrc.2016.2

Naphthalene Diimide-based polymeric semiconductors. Effect of Chlorine incorporation and n-channel transistors operating in water

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We demonstrate here the design, synthesis and characterization of two new chlorinated polymers, P(NDI2HD-T2Cl2) and P(NDI2OD-T2Cl2) based on *N,N'*-difunctionalized naphthalene diimide (NDI) and 3,3'-dichloro-2,2'-bithiophene (T2Cl2) moieties. Our results indicate that organic thin film transistors (OTFTs) based on these new chlorinated polymers exhibit electron mobilities approaching 0.1 $cm^2 V^{-1}s^{-1}$ (I_{on}:I_{off} ~ 10^6 -10^7), with far less ambipolarity due to their lower highest occupied molecular orbital energies, and they are more stable under deleterious high humidity conditions (RH ~60%) and upon submersion in water, compared to those fabricated with the parent nonchlorinated polymers. In addition, OTFTs fabricated with the new chlorinated polymers exhibit excellent operational stabilities with the new chlorinated polymers exhibit excellent operational stabilities with <3% degradations upon bias-stress test. DOI:10.1557/mrc.2016.4

Hierarchical nanostructures of BiOBr/AgBr on electrospun carbon nanofibers with enhanced photocatalytic activity

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In this paper, hierarchical nanostructures of BiOBr/AgBr on electrospun carbon nanofibers (CNFs) were prepared by combination of electrospinning and carbonization. Compared with the smooth surface of CNFs, the rough surface with hierarchical nanostructures of BiOBr/AgBr can be obtained by adding the certain amount of BiOBr/AgBr precursors into the spinning solution. The as-prepared composite CNFs exhibited highly photocatalytic activities for degradation of rhodamine-B and reduction of p-nitrophenol under the visible light irradiation and at room temperature. Furthermore, the as-prepared composite CNFs showed the favor separation, recovery, and cyclic utilization properties. DOI:10.1557/mrc.2016.6