The Next Production Revolution
Implications for Governments and Business

PART I

Chapter 6

Revolutionising product design and performance with materials innovation

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Increasing the rate of discovery and development of new and improved materials is key to enhancing product development and facilitating mass customisation based on emerging technologies such as 3D printing. Acceleration of materials discovery and development has been enabled by advances along multiple fronts, including capabilities of scientific instrumentation, high performance computing combined with more predictive computational methods for material structure and properties, and data analytics. Historically it has taken 15 to 20 years from laboratory discovery of new materials to their deployment in products. Systematic methods for accelerated materials discovery and development are still in early stages in the new digital era. Prospects are bright for realising a materials innovation ecosystem necessary to integrate new materials with digital manufacturing technologies to achieve new product functionality. A range of initiatives, gaps, and key policy issues to be addressed are discussed in this chapter.

Introduction

Historically, the process of discovering new materials and developing them to meet market demands has been laborious, iterative, and intuitive, driven by perception of consumer needs for new products or existing potential product improvements. The process has conventionally involved the following steps: i) generate a new or improved material concept; ii) realise this material via "Edisonian" trial and error methods in the lab; iii) measure desired property sets; and iv) repeat, improve, and refine. Unfortunately, the path to commercial viability with this schema has typically taken 15 to 20 years, with wide-scale acceptance in commercial applications requiring an additional 20 years or more, as outlined in the US Materials Genome Initiative (MGI) (Kalil and Wadia, 2011; Holdren, 2014).

In the next production revolution, engineers will concurrently design the product and its constituent materials (McDowell, 2007; Teresko, 2008), as shown in Figure 6.1. Hierarchical levels of material structure from atomic scale through interfaces of multiple phases, upward to the part level are considered, effectively treating levels of material structure and associated responses as subsystems. In Figure 6.1, the typical organisational separation of processing materials and certifying their properties in materials development is distinguished from that of materials selection in design of product systems (inset lower right). Conventionally, materials have been developed in the supply chain to meet property requirements of systems designers working with original equipment manufacturers (OEMs). Designers typically select materials that are suitable for manufacturing products. In the new world of tailoring materials for specific product applications, the linkage between the materials supply chain and OEMs/designers will become much more intimately coupled, and two-way in character, with a focus on tailoring a product-specific hierarchy of material structure as highlighted in Figure 6.1.

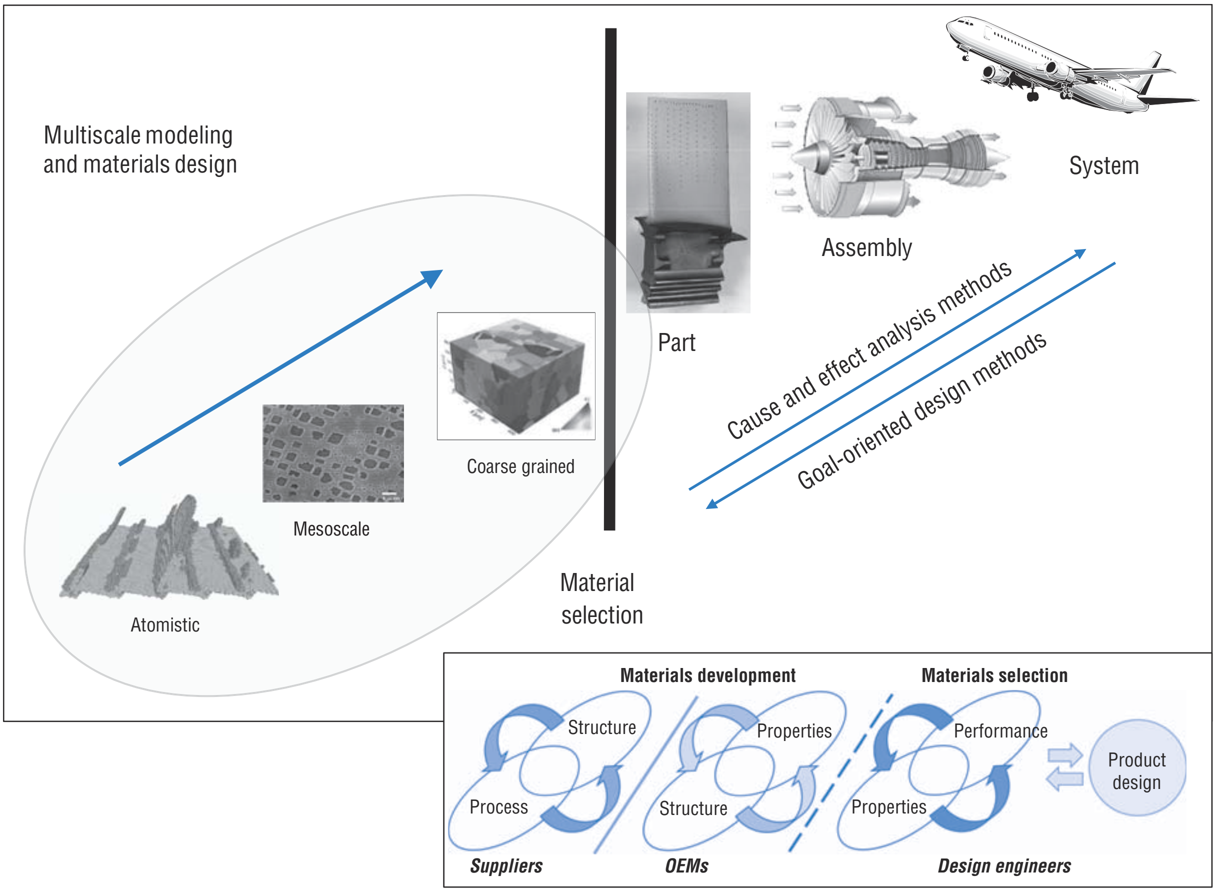
Continued 21st-century market punctuations are likely to arise at the intersection of big data and existing infrastructure and technologies, resulting in transformation of everyday means of communication, transport, and commerce. Creation and expansion of new products and even industry sectors can result**.** Accelerated materials discovery and development is about more than just anticipating, developing and addressing consumer demand and offering improved competitive products. New materials hold promise to address many grand challenge problems.

Economies that pursue development and integration of technologies to link materials development with product manufacture can realise benefits if they build a sustainable culture that supports distributed discovery, design and development of materials. Such a culture can support a robust materials innovation ecosystem that cuts across materials suppliers, OEMs, government agencies and labs, and service providers, with universities providing appropriate technical support and future workforce education.

This chapter first elaborates the promise of new materials in the digital age, trends that enable accelerated materials development, and the need for a materials innovation ecosystem to link digital materials and manufacturing. Prior to concluding by outlining new policy issues and their relation to longstanding policy concerns, the following challenges to realising the promise of cyber-enabled accelerated materials discovery, development and manufacturing can be identified and discussed:

- building the culture of the materials innovation ecosystem
- integrating a digital materials supply chain
- e-collaboration and web agent approaches to distributed materials and manufacturing
- future workforce development
- road mapping and capitalisation of the materials innovation infrastructure.

Figure 6.1. **Concept of concurrent design and bottom-up development of the material to meet top-down systems and product requirements, including manufacture and performance**



Source: Adapted from McDowell, D.L. et al. (2010), *Integrated Design of Multiscale, Multifunctional Materials and Products.*

The promise of new and improved materials

The dawn of the information age has witnessed remarkable increases in workplace efficiency and productivity. The role of automation in manufacturing of goods has increased dramatically in the past few decades, coupled with advances in digital design for manufacture that allow products and processes to be envisioned and considered in the early design stage, reducing time to market. In this new era of digital manufacturing, one can consider both solid geometries and tolerances of complex parts and assemblies prior to physical manufacture, transmitting information in digital computer-aided design (CAD) files for production. But products are manufactured from materials, and material form, structure and properties have long remained sources of great uncertainty that limit attainment of the broadest vision of digital manufacturing. Important issues persist regarding the predictive knowledge base of properties and characteristics of existing materials, including machinability, surface conditions, interplay of process route and the material structure, distortion and tolerances, residual stresses, and quality of joints between materials within sub-assemblies. The advent of new manufacturing technologies such as additive manufacturing and 3D printing have made these issues more acute and have sharpened the focus on the need for more integration between materials development and manufacturing. Furthermore, there is an important trend: advances in digital manufacturing need not rely on standard, off-the-shelf materials supply catalogues and inventories. Indeed, prospects are bright for rapid development and deployment of new and improved materials that can be integrated with the digital manufacturing workflow and offer superior new product functionality.

Progress in accelerated discovery and development of materials has been enabled by advances along multiple fronts. Advances in scientific instrumentation, such as atom probe tomography, high resolution transmission electron microscopy and x-ray synchrotron techniques allow scientists and engineers to study materials at finer scale and in more detail than ever before. Developments in computational simulation methods and tools for materials have also been critical. However, these advances must be integrated. The application of data science and high-throughput methods to explore complex data correlations and rapidly evaluate candidate materials has emerged within the last decade and is growing explosively. In conjunction with this convergence of high fidelity and high-throughput experiments, computational simulation, data science and informatics, revolutionary breakthroughs are being realised in manufacturing methods that can take advantage of materials customisation. One such breakthrough is 3D printing.

However, systematic methods for materials discovery and development are still in early stages of “catching the wave” of the new digital era. Historically it has taken 15 to 20 years from laboratory discovery of new materials to their deployment in products. This is partly due to the heavy reliance on empiricism in materials development, which has largely been undertaken in a manner that is disconnected from systems design and manufacturing. Moreover, incentives for university research productivity have emphasised quickly moving from one fundamental research advance to the next, rather than translating these findings into applications. Materials development and certification are critical steps in the “valley of death” in translating new materials concepts from the research laboratory into products (Apelian, 2004). Recent progress in the ability to create and manipulate materials will profoundly affect future production of increasingly customised goods and services. Small variations in a material’s composition or structure can lead to significant changes of response or may introduce entirely new functions. Today, materials are emerging with properties never seen before, such as ultra-low density materials with densities comparable to that of air, and metal that expands when stretched. New realities are exotic alloys and high-strength lightweight composites – materials that remember their shape, repair themselves or shape-shift to assemble themselves into components, and materials that respond to light and sound (The Economist, 2015). Manipulating microstructure makes it possible to develop materials with properties that vary from point to point in a given part or component as desired.

The era of trial and error in materials discovery and development is coming to an end

As evidenced by the categories "Stone Age", "Bronze Age", and "Iron Age", advances in civilisation have been closely connected to advances in materials. In the modern era, "ages" tend to overlap and intertwine. We have rapidly progressed from the industrial revolution (the "Machine Age"), in which a wide range of new materials enabled productivity and convenience, to the present Silicon Age, which has facilitated the emergence of ubiquitous computing. Over half of the major technology breakthroughs of the 20th century[1] were in some way enabled by advances in materials, e.g. cars; airframes and gas turbine engines for aircraft; microelectronics; spacecraft; imaging and health technologies; household appliances; laser and fibre optics; nuclear power; and high-performance, lightweight structural materials. The integration of each generation of new materials technology into consumer products such as cellular telephones, computers, appliances, sporting goods, and cars has been accompanied by a trajectory towards commoditisation as development costs are recovered and the marketplace turns to increased competition among suppliers. However, disruptive new technologies are introduced less frequently and serve to "punctuate" the equilibrium markets, providing potential for localised manufacturing that drives rapid change in consumer preferences, competition for economic viability, and eventual diversification of manufacturing necessary to sustain markets as they tend towards stasis. New and improved materials drive market flux by challenging the competitive stature of existing products.

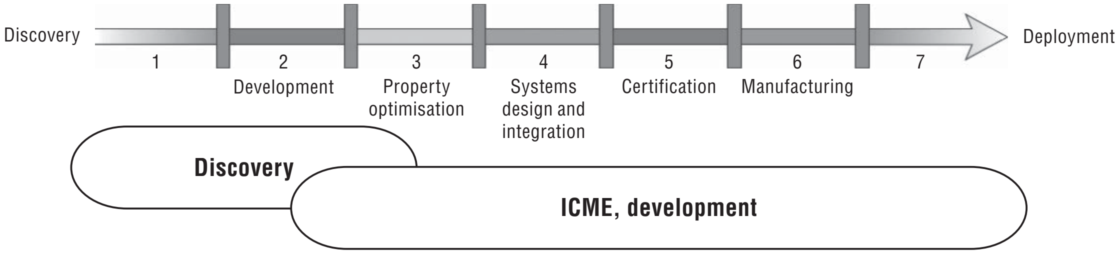
The 20th century was a golden age of invention and new technologies. Technology advancement in the 21st-century continues to accelerate. While scientists debate how long Moore's Law of scaling[2] will apply to increases in computing power based on silicon,[3] we have progressed well into the digital age that is characterised by global connectivity, on-command access to a vast array of digital information and resources, and the ability to store digital workflows that track all stages of engineering design and development, manufacturing, and commerce. Paradoxically, given the nature of global connectivity, these trends are more subtle, ubiquitous, and rapidly distributed than 20 years ago. Continued 21st century market punctuations are likely to arise at the intersection of big data and existing infrastructure and technologies, resulting in transformation of everyday means of communication, transport, and commerce. Creation and expansion of new products and even industry sectors can result. Accelerated materials discovery and development is about more than just anticipating, developing and addressing consumer demand and offering improved competitive products. New materials hold the promise to address many challenges highlighted by a US National Academy of Engineering study in 2009,[4] solutions to which are fundamentally limited by materials, such as the realisation of fusion energy, economical solar energy, carbon sequestration, managing the nitrogen cycle, access to clean water, restoration of urban infrastructure, and engineering the tools of scientific discovery. One can imagine an endless array of new modes of transportation and interpersonal communication. For example, adaptive materials can imbue environments with situational awareness and on-command flexibility via shape- and function-shifting multifunctional materials. Personalised mobile energy conversion and storage can allow people to work anywhere. One can envision that new and improved materials will enable replacements for diseased or damaged organs, sustainable food and water sources, non-toxic and recyclable replacements for consumer goods, molecular computing, and so on. The interfaces to these technologies will grow ever more subtle and less intrusive, as human-machine interfaces become more intuitive.

One of the earliest efforts aimed at designing and developing a material with targeted properties was initiated by the Steel Research Group (SRG) at Northwestern University in the 1980s (Olson, 1997; Apelian, 2004). The SRG built upon quantitative models for structure-property relations established in the physical metallurgy community to move away from "hit-or-miss" discovery of new and improved steels towards intentional design. Progress in computing power and computational materials science, physics and chemistry methods and tools over the ensuing decades has facilitated modelling and simulation of both the structure and properties of materials to inform decisions on how the material might be integrated into products. Properties such as thermal conductivity, strength, stiffness, toughness, and corrosion resistance can be intentionally designed into new structural materials, and at a a rapid pace, with assistance from materials theory and computation. Over the past decade, the integration of computational modelling and simulation with materials design and development has received considerable attention and focus through the Integrated Computational Materials Engineering (ICME) initiative in the United States (Pollock and Allison, 2008). The ICME approach aims at an increased pace of development of new and improved materials, more rapid integration of known materials into new products, development of new materials-based technologies, and the ability to improve existing products and processes. For example, the 2008 ICME study explains the initiative of the Ford Motor Company to develop cast aluminium engine blocks (Pollock and Allison, 2008). ICME has been strongly supported by industry, and serves to more closely integrate predictive computational materials science and engineering in materials design and development processes.

A foundational premise of the aforementioned US MGI is that the process of incorporating new and improved materials into products can be accelerated by promoting concurrency of the conventionally sequential and progressive phases of materials development and deployment shown in Figure 6.2 (adapted from Holdren [2014]). In other words, by anticipating downstream materials certification and manufacturing requirements during their initial development and laboratory-scale property optimisation, the time involved to deploy new and improved materials into products can be reduced from its historical average of 15 to 20 years down to perhaps 7 to 10 years or even faster. Moreover, costly and time-consuming iteration through steps 2 to 6 in Figure 6.2 can be reduced. Step 4 should consider specific manufacturing routes and product forms in the deployment phase.

The MGI contends that more seamless connectivity of experiments, computation, digital data and data science are needed both to speed up the pace of new materials discovery and to enhance concurrency of downstream steps. Materials discovery, traditionally serendipitous, is increasingly guided by combinatorial computational materials screening and can consider downstream integration and certification. In practical terms, the MGI is focused more on supporting materials discovery and early-stage development, while ICME is directed more towards accelerating the linkage from materials development through properties certification and product deployment. Increasingly, new materials are being developed for specific applications and products,[5] in contrast to the historical model of creating a range of available materials listed in a supply catalogue. This serves as a powerful driving force for the coupling of materials development into manufacturing, and requires incorporation of digital data in all phases.

Figure 6.2. **The historical sequential stages from materials discovery through deployment (from left to right)**



Source: Adapted from Holdren, J.P. (2014), "Materials genome initiative strategic plan", *https://mgi.nist.gov/sites/default/files/factsheet/mgi_strategic_plan_-_dec_2014.pdf*.

Important current trends in materials research and development enable the accelerated co-ordination of materials development and manufacture in the digital age:

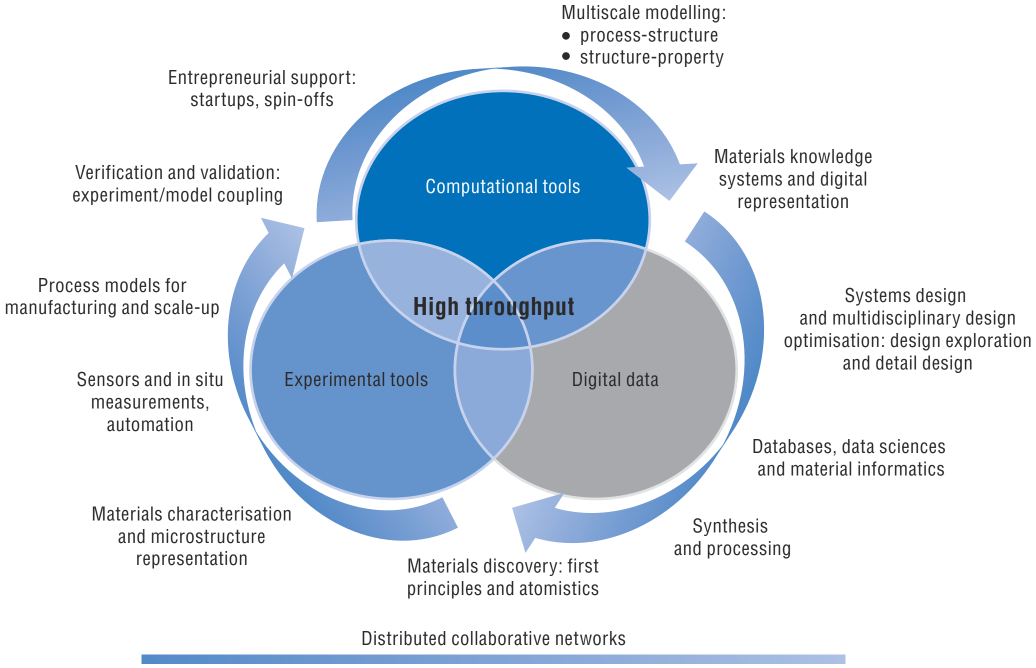
- **The democratisation of quantum mechanics:** 30 years ago, computational quantum mechanics was the province of physics and chemistry, but it now pervades engineering education and practice as a toolset to support materials design and development, even in disciplines such as mechanical, aerospace, and civil engineering, as well as manufacturing sciences. Combined with computational materials science, multiscale micromechanics of materials, and ubiquitous computing, the utility of computation to support materials discovery and development is apparent.
- **Recognition of the hierarchy of material structure**, from atoms (sub-nanometre) to molecules to interfaces between multiple phase states of matter, and its important role in tailoring material properties for desired performance.
- **The ability to play "what if?" games** to explore potential performance of new and improved materials via predictive modelling and simulation.
- **Advances in high resolution materials characterisation and in situ measurements**, along with digital representation of these levels of hierarchy of material structure as part of the information to be coupled with digital manufacturing, along with traditional solid geometry model information and tolerances.
- **Manufacturing's embrace of information regarding materials science, chemistry and physics**, enabling consideration of complex effects of environment, manufacturing processes, and service conditions.
- **Digital recording of workflows regarding the history of how materials are synthesised or processed**, how their structure and properties are measured, and how they are used in specific manufactured products, the traceable "fingerprint" of a material pedigree. This combines with an information infrastructure (information theory, databases and data registries, digital interfaces and distributed e-collaboration).
- **Formal theory and methods to support decision making in materials development** (considering utility or value of information in supporting design decisions, goal programming, information economics, and methods for uncertainty management), integrated with digital workflows.

Perhaps the most potentially transformational trend lies in the intersection of big data and materials, which facilitates the pursuit of several of the other key trends in this list. For example, the big-data revolution pervades prediction of weather systems, climate change projections and cybersecurity (see Chapter 2). But the digital materials enterprise also stakes a claim in big-data "territory", albeit often understated, in particular with regard to the large variety and volume of materials data (Mellody, 2014). Computational modelling of the dynamics of behaviour of all atoms within even a cube of a crystalline metal that is a mere 1 millimetre on one side (about 15 times the thickness of a typical human hair) is a challenge comparable to other big-data applications. When materials are processed or placed in service, their structure often changes with time in ways that are also quite non-linear and dynamic. Such applications demand coarse-grained representations and models to be utilised to gain predictive understanding. The historical focus of the materials community on reduced order material descriptors such as measured "properties" has perhaps obscured this big-data character, although terabytes of information being generated from in situ experiments highly resolved in time and space are now becoming commonplace. The old paradigm of property catalogues may suffice for materials that have a long track record of service, but does not suffice for materials yet to be developed. Digital representation of material structure from the atomic scale upward conveys a wealth of information that offers value in downstream integration with manufacturing and deployment, and we have barely scratched the surface. For these reasons, it is necessary to take a broadened view of the materials development enterprise, as discussed next.

The materials innovation ecosystem

It is evident that the 21st century will act as a bridge from the dawn of the digital age into the era of ubiquitous computing, sensors and networking via big data – we stand on the threshold of the "Internet of Things". The convergence of advancements in data science and informatics, computational materials science, multiscale and multiphysics modelling, digital representations of material structure and associated metadata, in situ measurements and in-line process/manufacture diagnostics, automation and controls, uncertainty quantification and management, and integrated systems engineering offers the prospect to "close the loop" between materials development, manufacturing, and new and improved product development (McDowell, 2007). The notion of manufacturing ecosystems[6] has gained considerable traction,[7] as has discussion of industry ecosystems,[8] yet these notions have largely excluded emphasis on the primal and enabling role of materials discovery and development. This leads to the recognition of the need for a new kind of materials innovation ecosystem that can alter the relation of the materials supply chain to OEMs, and change the character of the modern research university and its relation to industry and government. Such an ecosystem can serve the needs of more intimate coupling of materials discovery and development with product manufacturing. 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 data from results of simulations, experiments and various other sources of information and associated metadata (important additional information about the data), providing an objective basis for communication. These data are the "currency" of this ecosystem. As an example, the Institute for Materials[9] at the Georgia Institute of Technology (Georgia Tech) has fostered a vision for the materials innovation ecosystem shown in Figure 6.3 as a "test-bed" concept (McDowell and Kalidindi, 2016). The inner Venn diagram shows overlap of experiments, computation, and digital data, as per the MGI strategic plan (Holdren, 2014). It is at the core of a multidisciplinary, distributed, collaborative network that couples materials development with manufacturing. To accelerate materials development, the methods should have a high-throughput character, requiring a digital information infrastructure for connectivity. This is a key point of departure from classical approaches to developing materials. Building on a well-established foundation of materials discovery, synthesis and processing, characterisation and microstructure representation, this ecosystem wraps together elements of materials data science and informatics; multidisciplinary systems design optimisation; materials knowledge systems; digital materials data and metadata; multiscale modelling; sensors and automation; unit process models for manufacturing; in situ measurements and manufacturing scale-up; and principles of uncertainty quantification, verification and validation, with entrepreneurship to form networks that can develop and make use of templated workflows to carry materials from the invention to application stages. Finally, an e-collaboration platform is essential for co-ordination of activities of the various experts and stakeholders involved in this digital infrastructure, shown in Figure 6.3. Basic research at universities can adopt a "use-inspired" (Stokes, 1997) paradigm that seeks to link downstream materials advances to key gap technologies, as well as disruptive new materials technologies such as nanostructured batteries for energy storage, ultra-strong materials, and materials for separations (Pearce, 2013).

Figure 6.3. **Elements of the materials innovation ecosystem, a cyber-physical infrastructure generalising the central theme of the US MGI focused on combining computation, experiment and digital data**



Source: Adapted from McDowell, D.L. and S.R. Kalidindi (2016), "The materials innovation ecosystem: A key enabler for the materials genome initiative".

New materials can be disruptive

In many cases, developing new materials can have more disruptive potential than improvement of existing materials. New materials can drive innovation. For example, fixation of implants via bone ingrowth into porous material structures replaced cement fixation and revolutionised hip replacement technology decades ago.[10] According to information from the European Commission,[11] "70% of product innovation is estimated to be based on materials with new or improved properties."

Advances in vulcanised rubber[12] in the 19th century constitute an important historical example of a modification of a natural or synthetic rubber to achieve enhanced durability via the addition of sulphur or other additives that affect cross-linking of polymer chains. An extensive range of transformative polymer-based products have been developed, bringing about significant advances in automotive tyres, orthopaedic materials, composite materials, and many other applications. One goal of modern materials discovery and development in the next product revolution is to replace the trial and error discovery approach by a more systematic, computation-assisted strategy. As illustrated in Figure 6.2, discovery precedes materials development.

More systematic, scientific approaches to materials discovery are evidenced in two examples. The mission of the Materials Project[13] is "to accelerate the discovery of new technological materials through advanced scientific computing and innovative design." Important aspects of this effort include software, novel supercomputing strategies, and screening methods to assess new materials for specific applications. By pursuing scalable computational materials science over supercomputing clusters, the Materials Project has predicted several new battery materials which were made and tested in the laboratory. It has also identified new transparent conducting oxides and thermoelectric materials using this approach. QuesTek Innovations LLC[14] have combined ICME methodologies with their Materials by Design technology to rapidly develop new high-performance alloys, coatings and other materials. This is accomplished by coupling physics-based, cyber-enabled expertise and design tools with advanced characterisation techniques to minimise costly and time-consuming experimentation in order to rapidly focus on a few iterative prototypes that are scaled up. Examples of designed materials include commercially available Ferrium steels, as well as alloys under development based on aluminium, titanium, nickel, molybdenum, tungsten, niobium, copper, cobalt, and other materials. Their Fe-based Ferrium steels are being evaluated and used in a wide range of demanding and safety critical applications in aerospace and e.g. the oil and gas industries.

The importance of improved materials

A simulation-assisted approach to materials development can reduce time and cost as companies eliminate repetitive tasks with fewer iterations. ICME strategies that employ materials simulation to inform materials development decisions can facilitate better products, such as stronger and more highly complex hierarchical structures. Successful integration of materials modelling and data science into decision support for product development can also shorten the time between materials discovery and their commercial use. In the past, this period could stretch to 20 years or more (Holdren, 2014). The Accelerated Insertion of Materials (AIM) programme, run by the US Defense Advanced Research Projects Agency (DARPA) from 2000 to 2003 (McDowell and Olson, 2008; McDowell and Backman, 2010), had considerable impact as a case study by developing and integrating a suite of process and microstructure-property models along with uncertainty analysis to optimised forged nickel-base superalloy gas turbine engine discs. AIM demonstrated significant time savings. For example, in aerospace engine design, concurrent optimisation of design and manufacturing processes allowed the design of a rotor disc that was 21% lighter and 19% stronger than other models in half the time of a typical development cycle (Holdren, 2014).

This has the potential to transform the materials supply chain. Large companies will increasingly compete in the development of materials. This is because "if you have a proprietary manufacturing process which applies to proprietary materials, you are creating a long-lasting competitive differentiation" (The Economist, 2015). In other words, materials innovation within OEMs and their supply chains will provide the benefit of staying ahead of the competition in new product development. The resulting knowledge management systems are not only algorithmic in nature but also involve an embedded culture and cannot be easily reproduced. Furthermore, companies can identify future disruptive technologies while improving existing materials within their innovation ecosystems.

The digital materials and manufacturing thread

Digital manufacturing is defined as the use of an integrated, cyber-enabled system comprised of three-dimensional (3D) visualisation, simulations, analytics, and various collaboration tools to simultaneously create product and manufacturing process definitions.[15] An August 2015 McKinsey and Company article[16] states that "Industry and academic leaders agree that digital manufacturing technologies will transform every link in the manufacturing value chain, from research and development, supply chain and factory operations to marketing, sales, and service." The report goes on to say that manufacturing generates more data than any other industry sector, yet much of it is not harnessed. It states that "digital transformation of the $10-trillion-plus global manufacturing sector will play out over a decade or more," and that "Boeing developed its two most recent airframes, for the 777 and 787, using all-virtual design, reducing time to market by more than 50 percent." Airbus is actively pursuing development and implementation of composites and other advanced materials in aircraft design and manufacturing, developing technologies to improve the rate of composite manufacturing.[17] This runs entirely parallel with the materials development enterprise, which is most often viewed as part of the manufacturing supply chain, somewhat divorced from the datasets considered in digital manufacturing. The concept of a "digital twin"[18] has been introduced in reference to a virtual digital representation of a physical system, such as a 3D model of an object or collection of parts in sub-assemblies or assemblies, which can potentially be used to represent the form and function of physical objects in digital computing. The digital twin concept includes the possibility of using sensor feedback from the actual system as a means of monitoring and controlling the response of the virtual representation. Similar to the concept of augmented reality in video games, it is envisioned that the digital twin will faithfully represent all appropriate physics associated with the system response, complex interactions, and even degradation or failure. In other words, the digital twin can serve as a means to create, build, and test equipment and manufactured parts in a virtual environment.[19]

To deal with the deluge of information from sensors that will be gathered in future NASA and US Air Force vehicles under extreme service conditions, Glaessgen and Stargel (2012) have argued that traditional fleet management approaches are too limited, and uncertainty associated with limited data is too high given the time lags and limited data content involved in typical physical inspection schemes. The concept of a digital twin that links with the vehicle's on-board integrated vehicle health management system, maintenance history, and available fleet data, including historical data, to mirror the remaining lifetime expectation of the actual physical flying twin is envisioned as the basis for desirable future platforms. This digital twin concept has even been proposed for use in assessing the health and maintaining a fleet of military aircraft.[20]

To provide a realistic surrogate for the actual system, the digital twin concept must also material structure and behaviour. It is also clear that the uncertainty of models of material behaviour and in-service degradation of materials, either based on simulation or data correlations, should be incorporated within the digital twin concept. In the spirit of anticipating downstream certification for applications shown in Figure 6.2, materials can be designed or redesigned based on digital twin response and comparison with behaviour of fielded systems. This leads to the prospect of continuous improvement in fleet quality, e.g. by coupling new and improved materials development with critical fleet components. ICME (Pollock and Allison, 2008) involves the incorporation of computational methods and data science to inform decisions made in materials development for product applications. Digital representation of random microstructure and predictive computational structure-property relations over a range of realistic microstructures are key enabling technology components of ICME. This necessitates integration with manufacturing processes, including digital CAD files with both geometric and materials information related to manufactured components, along with supporting information regarding inspection, process control and quality control.

Additive manufactured parts for tooling, repair and replacement parts, and prototyping are excellent candidates for the digital twin concept. Additive manufacturing has the potential to create new material forms to enable new and improved products, and facilitates the realisation of location-specific properties that vary throughout the part in a manner that in some way optimises performance for a given set of system requirements (see Chapter 5).

Challenges for the future of accelerated materials innovation

As outlined in the introduction to this chapter, significant challenges must be address to realise the promise of cyber-enabled accelerated materials development and manufacturing. These are discussed in the remainder of this chapter, with major policy issues enumerated in the conclusions.

Building the culture of the materials innovation ecosystem

Economies that stand to benefit most from this emerging vision of the integration of cyber-enabled materials development and product manufacture are those that can most effectively develop and sustain the necessary culture of innovation. Key ingredients include a more robust materials supply chain, distributed service providers, and digital data and workflow tracking. This culture change will probably be led by universities via future workforce development and OEMs through embracing materials innovation in applications, leveraging government investment and influencing policy making.

The materials innovation ecosystem in Figure 6.3 is a human-centred, cyber-physical infrastructure aimed at providing decision support to processes of materials discovery and development. It does not replace best practices but embeds them. The necessary culture for this ecosystem to flourish emphasises distributed, collaborative stakeholders and experts in all phases shown on the periphery in Figure 6.3. The ecosystem is too extensive to be built around a single discipline such as materials or manufacturing. Universities will struggle with its scope, which tends to defy characterisation within individual academic units or even colleges. Small to medium-sized companies may wonder how to prioritise investments with limited resources or how to focus their own resources to collaborate with others. Large companies and industry sectors may wish to develop their own internal ecosystems as a subset approaching the scale and scope of the vision in Figure 6.3.

The digital data aspect is key not only to material structure representation and integration of materials and manufacturing, but also for tracking collaborations and communications for a given materials discovery and development effort – in other words, templated workflows of digital information and decisions. The entire process is quite amenable to modern data science. Pursuit of the materials innovation ecosystem will open many new opportunities for specialised service providers who can provide data, data science, materials synthesis and processing, materials characterisation and property testing, uncertainty quantification, modelling and simulation, and various other decision support tools on an as-needed basis. This can result in a recasting of the role of materials and manufacturing supply chains. It must be systemically and organically developed and sustained through education, training, and identification of best practices. Moreover, moving to an ecosystem for materials innovation enabled by a digital information infrastructure requires building on the emergent communities in data and data science, so that career categories such as “materials data scientist” will become commonplace. Along with high-throughput methods, there should be as much emphasis on a culture of connectivity between distributed experts in the ecosystem as on specific technologies. In this ecosystem, quantifying and managing uncertainty in data and models is essential to support decision making in materials development and investments in scale-up of manufacturing.

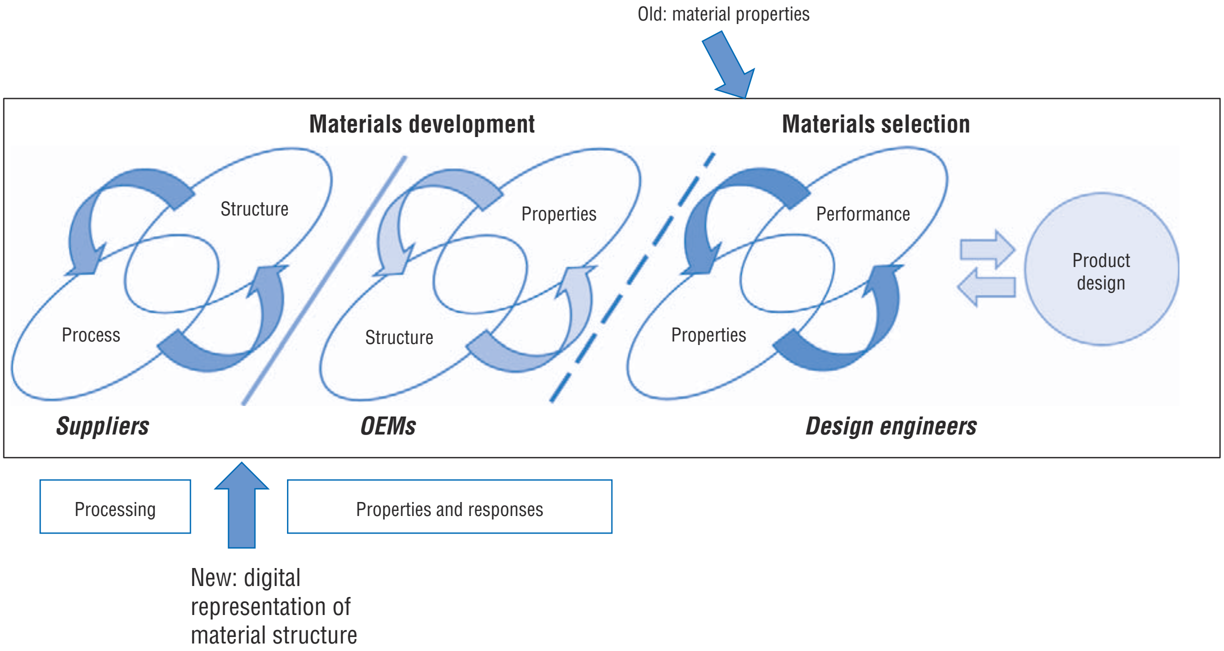
In addition to improvements in linking new and improved materials to enhanced product development and manufacture, there are other important capabilities that accrue to this technology, including but not limited to:

- Prioritising research and development initiatives in government agencies.
- Prioritising the blend of experiments and computational models in terms of their utility in supporting decisions in new and improved materials development, considering return on investment. Empirical routes to materials development that rely on time-consuming experimental protocols are costly. The question is how these protocols can be reduced by reliably supporting decisions in materials development based on information from modelling and simulation, as well as advanced data correlations.
- Prioritising mechanisms and materials science phenomena to be modelled for a given materials design and development problem.
- Conducting feasibility studies to establish probable return on investment of candidate new material systems.

Integrating a cyber-enabled materials supply chain

Figure 6.4 shows how a future emphasis on digital representation of material structure as a means to communicate with design and product development will change the role of the materials supply chain relative to historical practice shown in the lower right inset in Figure 6.1. With the focus shifted to emphasise digital representation of the hierarchical structure of materials (solid slanted line to the left in Figure 6.4), instead of the historical focus on properties (dashed slanted line to the right), materials suppliers are required to maintain and convey digital structure information. This disrupts and evolves the traditional supply chain-OEM-manufacture relationship based on meeting nominal structure metrics and property specifications from the OEM. In particular, digital information regarding the structure of materials, along with related structure-property information, will be the medium of communication to virtual design and manufacturing tools used by OEMs and other customers. This includes metadata regarding property measurements, models based on simulation and/or data analytics, and details of all the steps in the material's process history, i.e. how the material is made. This will also shift much of computational materials engineering onto the supply chain, with new demands to be met by digital materials service providers. Customisation of materials to address product-specific performance requirements can be addressed on a contractual basis within such an ecosystem (it is difficult at present), and small to medium-sized new companies specialising in customisation will populate the interface between materials supply and OEMs. A good example is QuesTek LLC, mentioned earlier. Data science companies can provide data services and analytics to assist in identifying potential new materials or improvements in coupling materials to manufacture. Public-private consortia and investment in future workforce development will be necessary to build the culture of this new paradigm.

Figure 6.4. **Shift from historical focus on materials selection to digital representation of the material's structure to support materials development**



Source: Adapted from McDowell, D.L. (2012), "Materials genome initiative: Implcations for university education and research", *www.brown.edu/conference/mgi-town-meeting/sites/brown.edu.conference.mgi-town-meeting/files/uploads/McDowell_presentation%20%5bRead-Only%5d%20%5bCompatibility%20Mode%5d.pdf*.

E-collaboration and web agent approaches to distributed materials and manufacturing

The materials innovation ecosystem shown in Figure 6.3, coupled with the manufacturing ecosystem within a given industry sector, is inherently distributed. Competition within the supply chain of the ecosystem for both materials and services (e.g. data, data science, experiments and computation) can serve to both accelerate processes and reduce cost.

Given the central role of digital information in materials innovation, the sharing of digital data is a key issue. Incentives are key to motivating the mutually beneficial sharing of information (McDowell, 2013). New journals such as *Integrating Materials and*

Manufacturing Innovation[21] will continue to be spawned that are expressly devoted to innovation at the interface of digital materials and manufacturing, as more established journals seek to identify their niches in this new digital materials era. In the United States, the National Institute of Standards and Technology (NIST)[22] is at the forefront of materials data registry and open data initiatives for the MGI. Related data archival activities are distributed across multiple government agencies involved in the Subcommittee of the MGI (SMGI).[23]

Clearly, it is difficult to comprehend how a single company could mount such a highly distributed arrangement that combines pre-competitive information and best-in-class service provider capabilities with proprietary datasets and applications. In the long-term, materials and manufacturing stakeholders will be globally distributed, and will assemble various elements of a cyber-physical infrastructure to support materials innovation. Still in its early stages, underdeveloped technology components of this infrastructure currently include i) high-throughput materials synthesis/processing, characterisation and property measurement; and ii) information infrastructure (McDowell et al., 2014). Distributed platforms and service providers can offer elements of materials information infrastructure that support many of the aforementioned goals. Such platforms and service providers could afford services ranging from modelling materials via quantum mechanics through finite element methods, high-throughput methods for discovery and development and modern data sciences applications. Relevant examples of platforms and service providers include, but are not limited to, the aforementioned Materials Project at the Lawrence Berkeley National Laboratory (LBNL), the Open Knowledgebase of Interatomic Models (OpenKIM) project on interatomic potentials at the University of Minnesota,[24] the NIST Center for Hierarchical Materials Design (CHiMaD)[25] at Northwestern University, Argonne National Laboratory and the University of Chicago, and the US DOE PRISMS Center at the University of Michigan.[26] Materials data registries and model repositories include those at NIST,[27] Citrine Informatics,[28] NanoHuB,[29] and the National Data Service's Materials Data Facility.[30] Similar nodes exist in Europe (e.g. the Novel Materials Discovery [NoMaD] computational materials repository[31]) and Asia (e.g. National Institute for Materials Science [NIMS] in Japan[32]). By and large, these platforms do not address distributed e-collaboration.

There are certain potential manifestations of the envisaged materials information infrastructure that have not previously existed and which create new market niches, most of which could be integrated within the e-collaborative framework. These include:

- digital material data registries and repositories
- web- and cloud-based data services and applications that add value by aiding interpretation of data to support materials discovery and development
- web agents and service vendors for modelling and simulation support tasks
- assignment and certification of the "readiness level" of data as well as modelling and simulation tools
- services vendors that couple materials to unit manufacturing processes (for example, computational models or advanced correlations for machining or processing of metallic articles).

This information infrastructure can be broadly distributed and leveraged, with extensive "plug and play" attributes.

Future workforce development

Examples of already existing academic course offerings and programmes that address materials innovation include the master's programme in Materials Science and Simulation at the Ruhr University Bochum,[33] ICME courses at Mississippi State University,[34] Northwestern University's ICME Masters certificate focused on design,[35] and the Georgia Tech From Learning, Analytics, and Materials to Entrepreneurship and Leadership (FLAMEL) programme (NSF IGERT).[36] Summer programmes include the Texas A&M IIMEC Summer School on Computational Materials Science Across Scales,[37] the University of Michigan Summer School on Integrated Computational Materials Education,[38] the Lawrence Livermore National Laboratory (LLNL) Computational Chemistry and Materials Science Summer Institute,[39] and the summer workshop from University of Florida Cyber-infrastructure for the Atomistic Materials Science Center.[40]

Box 6.1. **Imperatives for the future workforce**

The new materials innovation ecosystem will require major shifts and broadening of the skill sets of the materials development workforce. University curricula and instructional tools should be refined and extended to integrate various elements of the materials innovation infrastructure shown in Figure 6.3. This reformation must extend beyond traditional materials education to bridge across engineering and science academic disciplines that naturally foster various supporting elements. For example, there is a significant gap in curricula at universities in addressing uncertainty quantification and protocols for decision support in materials development. This gap has emerged from a focus in the materials community on the bottom-up scientific method to discover and develop materials, largely removed from consideration of product level systems engineering. Treatment of uncertainty generally falls under the categories of systems design, data sciences, and optimisation under uncertainty.

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 characterisation and property measurements, inverse methods and metamodelling, uncertainty quantification, verification and validation, data science, and systems integration with manufacturing. Quantifying uncertainty in materials process-structure and structure-property relations has a rich scientific depth, in addition to its economic imperatives. Addressing uncertainty quantification and its management in concert with systems engineering can dramatically accelerate materials innovation efforts, as outlined in a recent study[41] of The Minerals, Metals and Materials Society (TMS). As a service to future workforce development, Georgia Tech's Institute for Materials has produced on Coursera[42] two massive open online courses (MOOCs) supportive of the MGI. The two courses are Materials Data Sciences and Informatics[43] and Introduction to High-Throughput Materials Development.[44]

Data challenges offer incentives to develop mechanisms to gather all necessary elements of data science, experiment, and computation and draw the attention of the future workforce to accelerated materials discovery and development. A good example is the recent Materials Science and Engineering Data Challenge sponsored from 2015 to 2016 by the US Air Force Research Laboratory in partnership with NIST and the US National Science Foundation.[45]

Road mapping and capitalisation of the materials innovation infrastructure

The US MGI has clarified the core elements of the materials innovation infrastructure as comprising the intersection of experiments, computational modelling and simulation, and data (e.g. registry, storage, analytics). This is shown at the centre of the materials innovation ecosystem depicted in Figure 6.3. However, investment in materials research infrastructure to date in most developed countries has focused on high-end materials synthesis and characterisation facilities, with less attention devoted to high-throughput methods to process and characterise materials. Materials data science and informatics is in early, formative stages. Few universities in North America, Europe or Asia have well-developed curricula in this regard. Beyond digital information, the materials innovation infrastructure also requires physical infrastructure for: i) high-throughput materials synthesis and processing, ii) characterisation, iii) property measurement; and iv) high-performance computing and data storage.

Fortune 500 companies such as IBM[46] and small and medium-sized firms such as Wildcat Discovery Technologies, Inc.[47] have made initial investments in order to mount an integrated materials innovation infrastructure that couples experiment and computation with data science for materials discovery. Investment in related infrastructure necessary to produce manufactured goods in a variety of sectors – from transportation, to energy and security – has been slow. This is particularly true with regard to shared user facilities. Indeed there is a question of how to invest in new cross-cutting shared user facilities necessary for accelerated materials discovery and development, such as high-throughput instrumentation for materials characterisation, property measurements and materials synthesis and processing. In a manner analogous to high-end scientific infrastructure for materials research such as synchrotron x-ray and neutron diffraction, these facilities should be distributed in nature, i.e. regional, national, and even international. Corporate investment is likely to be sector- and even material system-specific. Private sector investment may not facilitate a broader development of the materials innovation infrastructure that serves the common needs of pre-competitive screening and scaled-up evaluation for materials solutions.

In many respects, the materials innovation ecosystem underlying the aspirations of MGI and ICME has analogies to the inter-agency National Nanotechnology Initiative (NNI)[48] begun in the late 1990s, an initiative that fostered distributed nanotechnology research throughout the United States. The MGI has been similarly framed in terms of fostering a distributed materials innovation infrastructure that aims to accelerate the pace of discovery, development and deployment of new and improved materials into products, with the objective of reducing the time and cost involved. But a key distinction between the infrastructure of the materials innovation ecosystem and the infrastructure initiative of the NNI is an emphasis in the former on high-throughput tools and strategies. In addition, the MGI focuses on "closing the loop" between experiments, computational modelling and simulation, and data sciences and informatics to promote concurrency of early-stage research and development (R&D) with considerations of certification, manufacturability, and long-term service requirements for materials systems. In the United States, much of this infrastructure already exists or is under active development, but lacks organised connectivity across materials classes, with limited support for access. Furthermore, there are no clear mechanisms to identify gaps and prioritise elements for inter-agency funding that cut across the broad materials innovation ecosystem. Efforts to date are most often localised in specific academic institutions, government research laboratories, and industries. There is limited awareness among the broader community of distributed capabilities or of how to combine them across the elements of the materials innovation infrastructure.

Important insights and perspectives can be drawn from the report of the workshop Building an Integrated MGI Accelerator Network, held at Georgia Tech, 5 to 6 June, 2014 (McDowell et al., 2014). This workshop assembled 150 thought leaders and stakeholders from academia, industry and government in the United States to explore how distributed experimental, computational, and materials information infrastructure might be further developed and collaboratively networked to most efficiently realise the vision of the MGI. Co-organised by Georgia Tech, the University of Wisconsin-Madison, and the University of Michigan under the auspices of the Materials Accelerator Network,[49] the event initiated a national dialogue regarding community MGI priorities and the path forward. A set of opening plenary talks outlined the government MGI strategy and shared industry and academic perspectives on accelerating materials discovery, development and deployment. Plenary talks were followed by breakout sessions organised to cover a broad range of application domains, including materials for organic and inorganic electronics, structural materials, materials for energy storage and conversion, biomaterials and bio-enabled materials, and materials and interfaces for catalysis and separations. Breakout sessions explored and discussed three specific themes: critical issues and technology gaps, infrastructure for MGI integration, and a strategy for road mapping a materials accelerator network.

Box 6.2. **Critical issues and technology gaps in accelerating materials discovery and development**

Summarising from the report of the workshop Building an Integrated MGI Accelerator Network (McDowell et al., 2014), some of the critical issues and technology gaps that must be closed to realise the vision of MGI cut across these application domains:

- **Materials information infrastructure**, particularly web-based environments for e-collaboration and data sciences.
- **High-throughput strategies for screening and development** that consider capabilities and constraints on available synthesis and processing routes, including fast acting modelling tools to assess the probability of meeting requirements.
- **Future workforce development**, with an integrated perspective on coupling of experiments, computation, and data sciences.
- **Fundamental understanding** of the **relations between structure at different length scales and materials properties/performance.**
- **Advanced diagnostic methods**, particularly in situ/in operando.
- **Consideration**, at early stages of discovery and development, of the **long-term stability of materials** under service conditions, environmental stability, degradation and performance lifetime.
- **Predictive simulation of metastable states and non-equilibrium trajectories** of evolution under service conditions for applications, enabling parametric exploration of candidate materials for product applications. Metastability of a material refers to its useful operation away from the system's state of least energy. Many useful engineering materials are metastable.
- **Measurement science and modelling and simulation of synthesis and processing.**
- **Principles of kinetic and thermodynamic control of process route/structure relations.** The challenge is knowing how to exert reliable control of structure over various length scales (nano-macro) during processing, including up to large scales.

New kinds of data science strategies and distributed user facilities are necessary to address the gaps identified in Box 6.2, in addition to education and training. High-priority recommendations to close key gaps identified in this workshop (McDowell et al., 2014) included the following:

- Focus on education and training of the future MGI workforce.
- Compile a knowledge base of existing MGI-related efforts in the United States.
- Link physical- and cyber-infrastructure that cut across materials classes and application domains.
- Establish working groups and networks in and across these materials domains.
- Define common foundational engineering problems for each materials application domain to rally MGI stakeholder collaboration and networking.
- Establish a stronger materials innovation infrastructure.

Conclusions

With the confluence of advances in predictive computational materials modelling, data science, and high-throughput methods for materials screening, significant opportunities exist to substantially decrease the time to bring new and improved materials to market in next-generation products. Emerging technologies such as on-demand 3D printed parts hint at the demand for mass customisation and rapid deployment of new materials. The rates of discovery and development of materials to enhance downstream product competitiveness can be accelerated significantly by coupling historically empirical, experimentally based strategies with computational simulation and data science strategies. Furthermore, new kinds of high-throughput shared user facilities are essential to rapidly make materials, measure their structures and properties, and screen for applications to refine for manufacturing scale-up. Unprecedented recent advances in combinatorial search methods for new materials can further interplay with accelerated materials development to revolutionise new product designs and performance.

The analysis of incentives for materials development in response to many 21st-century grand challenges largely revolves around economic viability, sustainability and evidence of societal impact. The design of the necessary incentives requires appropriate government strategies and policies. Moreover, the promise of "democratisation" of customised products offered by ubiquitous technologies such as 3D printing and incorporation of sensors and communications within materials to facilitate the Internet of Things (Burrus, 2014) has global implications, analogous to the profound influences of cellular smart phone technology and social media.

Given the strong competitive product edge that each new and improved material can confer for a limited period of time, it stands to reason that data and intellectual property (IP) challenges are critical issues. For major product innovation with new and improved materials, there is only a limited window of time after product release during which to gain market share. This window continues to shrink as the time to introduce new highly competitive materials is compressed. There are multiple IP-related questions. For example, who owns the data? Who owns the infrastructure? Who owns value-added information or capabilities? How are open development contracts differentiated from proprietary contracts? Materials are often core to new and improved product capabilities – will the existing international patent system be sufficient to protect competitive advantage? Suppliers can potentially control more IP in a state-of-the-art materials innovation ecosystem because they will be responsible for curation of the digital workflow documenting materials development. What is the background IP and how is it defined? How much pre-competitive collaboration is desirable to compete in the space of new products? Can development costs be shared? What are best practices models for pre-competitive development of shared technologies and cyber-physical infrastructure? How can companies differentiate based on downstream development and applications? There are no easy answers to these questions, but a competitive marketplace will inexorably drive the distributed materials innovation infrastructure forward in an increasingly connected digital world. It is clear that no single company or organisation will be able to "own" the array of technologies associated with an e-collaborative materials innovation ecosystem. Nor is this desirable, since the interconnected global economy can benefit broadly by contributing goods and services to the ecosystem. OEMs can focus on utilising this ecosystem to maximise benefit in new product development and reduce time to market, with the caveat that competitive advantage will focus more on increasing the pace of introducing new products and not relying solely on their intrinsic value, absent disruptive advances in new product capabilities and/or creation of new markets. Hence, a public-private investment model is warranted, particularly with regard to building the cyber-physical infrastructure and in future workforce development.

Appropriate, enlightened regulatory policies could help to foster this ecosystem, emphasising the need for maintaining a largely open and accessible cyber-physical infrastructure and still providing safeguards for product-specific information and workflows. There are currently major efforts to develop the early materials information infrastructure and associated data standards in professional societies[50, 51] (Robinson and McMahon, 2016). There is also a need for policy co-ordination across the materials innovation infrastructure at national and international levels. The need for policy co-ordination arises from the necessity of federating elements of the cyber-physical infrastructure across a range of European, North American and Asian investments and capabilities, as it is too costly and unnecessary to replicate resources that can be accessed via web services with user support. Ultimately, good policies are required because of the need to change the culture of sharing data and, in particular, to facilitate a pre-competitive culture of e-collaboration. This is a good example of where existing structures and regulatory policies may not suffice, as they were developed for a different era.

Cyber-enabled design and development of materials also raise entirely new policy issues. Some issues are of strategic character, even having security and stability implications. For example, the motivation for replacement of rare earths in magnets and electronic materials involves consideration of the stability of materials supply and associated geo-politics. Such considerations can drive the search for new materials. Moreover, new cybersecurity risks can be anticipated since a digital, computationally assisted materials "pipeline" relying on various forms of data could be hacked or otherwise manipulated. Well-conceived and designed policies are needed for open data and open science (e.g. for sharing simulations of materials structures, or for sharing experimental data in return for access to modelling tools) (McDowell, 2013). Principles for negotiation of IP rights in the new materials innovation ecosystem among distributed stakeholders are a pressing short to medium-term issue, as new kinds of agreements will probably be necessary to distinguish open-source, shared data design environments from design and development scenarios with closed and proprietary character. Progress on new materials requires close collaboration between industry, universities, research funding agencies and government laboratories. Steps are also needed to foster interdisciplinary research and education, because materials research is inherently multidisciplinary (beyond traditional materials science and engineering, contributions come from physics, chemistry, chemical engineering, bio-engineering, applied mathematics, computer science, and mechanical engineering, among other fields).

In addition to changes in university curricula, as well as a shift from traditional modes of interaction of materials suppliers and OEMs in industry, proprietary information and licensing issues, etc., there are a number of potential technology barriers to further development and use of these kinds of methodologies. Often, models are either non-existent or insufficiently developed to support decisions to select among various potential designs or development routes. This includes models for both process-structure relations and microstructure-property relations. A particular need is the co-ordination of model repositories for rapid availability to support design optimisation searches. A complicating factor that is rarely addressed is the quantification of uncertainty of model parameters and model structure as necessary to support robust design of materials (McDowell et al., 2010). Uncertainty quantification of models is best performed during model construction and calibration or fitting of parameters by model developers, rather than by downstream users. It is incumbent upon funding agencies and review processes to require uncertainty quantification (UQ) of models and data as part of R&D proposals. This will require much more emphasis on UQ in the materials community, including new courses and emphasis on UQ in related university curricula. There is a pressing need for methods and policies governing access to distributed service providers, or "web agents", for models (McDowell et al., 2010), along with definition of "readiness levels" for these services addressing provenance, degree of validation, and support for usage and sustainment, analogous to well-known technology readiness levels (TRLs) in the US Department of Defense (US DoD).[52]

Deliberation between research bodies, firms, government research laboratories, standards organisations, and professional societies working on development of new and improved materials have predominantly been concerned with the compatibility of data formats. But this needs to evolve towards a focus more on how to use these data to support decisions in materials discovery and development, along with considering many of the foregoing policy issues. Data formats and protocols vary widely and digital platforms and data structures change rapidly. Access to and dedication of high-performance computing and cloud storage resources is an important element to which pre-competitive public-private consortia and government policy can contribute. Initiatives such as ICME in the United States and the Integrated Computational Materials Engineering expert group (ICMEg)[53] in Europe are all wrestling with these issues to some extent. In addition, cyber-physical infrastructure relating to high-throughput methods for rapidly making new materials and assessing stability, performance and suitability for products is of high value to a range of stakeholders; there is a need for broad community access to user facilities.

As discussed in this chapter, large-scale initiatives are under way in North America (MGI, ICME), Europe (ICMEg, Horizon 2020)[54] and Asia to systematically build the science base and infrastructure to support more rapid materials innovation and linkages to manufacturing (methods and tools, materials data infrastructure, shared facilities, and future workforce development). Progress is inexorable but its rate is currently limited by lack of co-ordinated planning and investment. Policies and regulations must be updated to reflect the modern era of materials development in which high value is placed on digital data and its co-ordinated, collaborative exploitation to support materials design and development decisions. Policy making at national and international levels can strongly influence the rate of development of the materials innovation ecosystem, broaden the potential pool of collaborators, and promote adoption of more efficient investment strategies. Some of the key policy requirements may be summarised:

- Allocate R&D investment in pre-competitive materials data registries, high-performance computing, and high-throughput experimental infrastructure. This investment is necessary to cultivate and support the culture of the materials innovation ecosystem.
- Empower the materials supply chain through policies that promote digital representation of material structure as specifications beyond an exclusive focus on property sets.
- Promote and reward efficiency of distributed e-collaborations of industry, government, and academic stakeholders involved in materials development.
- Encourage accessible digital data as a product of publicly funded research.
- Develop strong incentives for researchers and developers to share materials data by adding value to the curation, analysis, and management of the data provided, including access to state-of-the-art advanced correlations and UQ methods.
- Address the IP barriers to sharing data and data analytics that may affect specific product development or competitive advantage to industry by fostering development of an extensive pre-competitive common infrastructure that can accelerate materials insertion.
- Establish incentives for universities to adopt cross-cutting curricula and other educational or training platforms that support and nurture the materials innovation ecosystem across e.g. engineering, the sciences, computing and management.
- Road map the development of the materials innovation infrastructure and prioritise investments at regional, national, and international levels.
- Foster formation and development of distributed small to medium-sized companies with specialisations ranging from materials data services, high-throughput screening, materials computation and design, to materials suppliers that can provide services upon demand to support accelerated discovery and development of materials for manufacturing.
- Develop regulations and certification protocols governing engagement of distributed web- or cloud-based service providers in materials discovery, development, and scale-up manufacturing.
- Emphasise the need for sustainable materials and product solutions.

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