New Directions in Materials Design Science and Engineering (MDS&E)

Report of a Workshop Organized by the

Georgia Institute of Technology Materials Council and Morehouse College

Sponsored by the U.S. National Science Foundation

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EXECUTIVE SUMMARY

New Directions in Materials Design Science & Engineering (MDS&E) Report of an NSF-Sponsored Workshop

The development of new materials and the capability of tailoring existing materials to meet new and demanding applications will be a key to continued improvement of the quality of life for Americans in the 21st century.

Traditionally, **design with materials** has been a sub-discipline of design engineering which addresses materials selection issues for various applications, quite distinct from materials science and engineering. The fields of materials science and materials engineering have been predominantly concerned with processing of materials, establishing structure-property relations, and measuring properties. This traditional empirical approach is increasingly shifting towards **design of materials** to achieve enhanced (or optimal) functionality, driven largely by advances in theoretical modeling, process modeling and resolution of analytical characterization. In recent years, science-based tools for analysis of structure-property relations have advanced significantly. These tools support the prediction of specific pre-synthetic material properties, of both structural and functional nature.

Engineering and science are on equal footing in their contribution to the design of materials. Engineering synthesis is essential to match material performance requirements with properties, and to identify "subsystems" of material microstructure which control these structure-property relations. On the other hand, science-based tools of quantum mechanics and various longer range approximations as well as continuum kinetics, thermodynamics and computational solid mechanics provide means of quantitative analyses of these subsystems, the key to designing their architecture in a manner which optimizes performance objectives. Various high resolution characterization tools may be used for quantifying subsystem geometries and composition, along with properties at related length scales. All of these elements acting in concert lead to the field of **Materials Design Science & Engineering (MDS&E)**, the topic of this workshop. MDS&E is the invocation of science and engineering principles to tailor material structures to achieve a high degree of predictable, controllable functionality in applications. By necessity, MDS&E is a multi-disciplinary enterprise, with interactions of materials science and engineering, engineering science and systems design, materials chemistry, physics and biology, the computing and information sciences, and applied mathematics.

Materials design is accompanied by a ubiquitous integration of information technologies within the materials sciences and manufacturing multi-disciplines. The requirements of simulation, visualization, distributed information flow and ready access to vast databases are introducing rapid change to materials and manufacturing technologies. Manufacturing and materials design are increasingly interwoven with
information technology to facilitate rapid prototyping to reduce the materials development and design cycle time for products. Accordingly, there are at least two very significant implications of developing a rapid and reliable capability to design materials, both of which have far-reaching economic consequences in a highly competitive 21st century global economy:

- Revolution of the materials supply/development industry
- Realizing the potential for true virtual manufacturing

A change of culture is necessary in U.S. universities and industries to cultivate and develop MDS&E to reach its potential for enhancing our materials supply economy. In recognition of this shift towards materials design, it is imperative that the broad materials community enunciate a vision inclusive of both the scientific and engineering aspects of MDS&E.

To refine this vision, develop a common understanding of its fullness, and chart out a conceptual roadmap necessary to pursue it within the broad materials education and research community, the Materials Council of the Georgia Institute of Technology, in collaboration with materials faculty at Morehouse College, hosted a workshop October 19-21, 1998 in Atlanta. The workshop engaged a diverse set of keynote speakers and panelists in each of four themes:

- Structure-Property Relations Across Length Scales
- Materials Synthesis and Design
- Elements of Process Design Science and Engineering
- Multi-disciplinary Materials Education

The discussions led to recommendations for a national roadmap to pursue MDS&E, potentially requiring the support of a range of federal agencies. These include:

Follow-on workshops specifically devoted to:

- Databases for enabling materials design
- Principles of systems design and the prospects for hierarchical materials systems
- Identification of opportunities and deficiencies in science-based modeling, simulation and characterization “tools” to support materials design

Federally Funded MDS&E initiatives, including:

- Materials Design and Manufacturing (MDM) research projects involving a vertical integration of materials design concepts, toolkits and prototype development in a joint university/industry venture
Creation of a university-based MDS&E Institute to foster the development of curricula and capstone design courses to address materials design, and to advance principles for integrating engineering systems design concepts with basic science toolkits to design materials.

Focused investigator grants for undergraduate and graduate program development to provide support in the “trenches” for directing materials science and engineering design curricula towards materials design, involving the basic sciences and engineering disciplines.
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The October 1998 MDS&E Workshop

Traditionally, design with materials has been a sub-discipline of design engineering which addresses materials selection issues for various applications; it is quite distinct from materials science and engineering. The fields of materials science and materials engineering have been concerned with processing materials, measuring properties, and somewhat more recently with establishing structure-property relations. The traditional empirical approach of these fields is increasingly shifting towards design of materials as designers strive to achieve enhanced (or optimal) functionality. This shift is driven largely by advances in theoretical modeling, in process modeling and in resolution of analytical characterization. In the past decade, science-based modeling has advanced to the point where it can effectively merge with engineering system design methods to yield significant improvements in existing materials while yielding the ability to synthesize and process new materials to better serve our needs. U.S. industry and universities have only begun to recognize the potential of this materials design revolution.

In recognition of this fundamental shift of materials science and engineering towards materials design, the Materials Council of the Georgia Institute of Technology, in collaboration with materials faculty at Morehouse College, hosted a workshop October 19-21, 1998 in Atlanta at the Georgia Center for Advanced Telecommunications Technology (GCATT) near the campus of Georgia Tech. The primary objectives of the workshop were:

- to evaluate the status, strengths and limitations, of predictive capabilities for materials design across various disciplines,
- to identify intersections of disciplines and methods of training/education which might address limitations and expand applicability,
- to identify potential implications of materials design on science and engineering education and research, and
- to identify obstacles, challenges and opportunity areas for future focus.

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- Structure-Property Relations Across Length Scales
- Materials Synthesis and Design
- Elements of Process Design Science and Engineering
- Multi-disciplinary Materials Education

This report summarizes some important topics of clarification and some key points of consensus, and it recommends a specific roadmap to pursue MDS&E. In the last section of this report, we will outline a set of recommended national level initiatives concerning MDS&E.
Appendix A lists the itinerary of the meeting. Distinguished speakers and panelists in each theme were drawn from a broad range of scientific and engineering disciplines. A complete listing of participants appears in Appendix B.

Why Design Materials?

A material is a complex system in its own right.

Materials have conventionally been discovered by chance. After its discovery, a material’s properties were determined and only then would people invent uses to exploit these properties. This conventional approach to materials is too labor-intensive and too unreliable to address the challenges of our economy at the dawn of the 21st century. We can no longer rely on chance to lead us to new materials, and we can no longer wait for random research to provide the tools we need in order to fit an new material to an existing need or to improve existing materials to better meet our requirements. Rather, we want to define an application for a material and to define necessary properties, thus defining a range of material structures that might suffice. Indeed, we want to develop an overarching strategy for the design of materials; without such a strategy, we may be unable to compete in the future with the emerging European materials supply market and with aggressive Asian investments in materials technologies.

We address a problem that is not peculiar to materials suppliers; it affects the manufacturing enterprise related to consumer goods as well. It is true that major breakthroughs in the last decade have ushered in a new era in the development of new materials and materials processes to be used in products with commercial and defense applications. However, in order for Americans to continue improving the quality of their lives in the 21st Century, we will need to be able to create new materials and to tailor existing materials to meet new and demanding applications. Our experiences in the 20th Century offer many examples of the ways that new materials have improved our lives. In the modern kitchen, for example, the appliances we use to handle, prepare and refrigerate food have become lighter and more durable as plastics have supplanted metals. Our business productivity and efficiency has been enormously enhanced by the discovery of transistors and of semiconductors that can be produced only by revolutionary advances in material process control and high resolution characterization. The Titanic likely would not have sunk had it been made with today’s steel processing methods. And Leonardo da Vinci’s dream of human flight has been achieved with an unimaginable degree of safety and regularity because today we use materials and manufacturing methods that he could never have imagined.

We may overlook these examples because we have become blanketed by the convenience that new materials have afforded to us. However, we must
understand that our standard of living cannot continue to improve if we do not rise to the challenge of changing the way we approach business in the materials supply industry, of changing the way we view materials in design, and, most fundamentally, in the way we educate people who deal with materials.

In recent years, science-based tools for analysis of structure-property relations have advanced significantly. These tools support the prediction of pre-synthetic material properties, of both structural and functional nature. Theoretical and applied solid state physics is now poised to predict the structure of presently unknown materials possessing desired properties at atomistic/molecular scales. These approaches achieve excellent descriptions of ‘perfect’ material structures. Yet these approaches remain in an embryonic stage when it comes to predicting the properties of ‘real’ materials; our tools are not yet well enough developed to support the design of complex new material structures of highly heterogeneous nature for applications at higher length scales and over long time scales.

While our atomistic simulation tools provide a predictive undergirding to support materials design, a systems approach is required to address the nonlinear, hierarchical nature of imperfectly processed real materials. Systems-based engineering design principles have developed substantially in the last 20 years. Materials typically used in applications today have complex, heterogeneous microstructures with different characteristic length scales, and these microstructures affect both processing/manufacture and in-service performance. We advocate a hierarchical, systems-based approach in which such materials would be designed to suit their functions. This approach would be analogous to the way we design aircraft or automotive engines, and from such an approach, new and exciting possibilities emerge. One way to meet this goal is to use modeling and simulation, applied judiciously in support of engineering systems-level analysis, which invariably includes considerations of feasibility, cost, stability, relative influence of structure at different scales, degree of imperfection, statistics of random microstructures, performance requirements, and so forth.
An Example of Materials Design

Our vision of MDS&E is best illustrated with an example. Workshop participant G.B. Olson has discussed aspects of Computational Design of Hierarchically Structured Materials in a recent article in Science (Vol. 277, 29 August 1997). Olson’s discussion of material design begins with the linear structure of interconnected processing-structure-properties-performance, and it adds to this structure Cohen’s assertion of reciprocity in the relation between structure and properties. Olson demonstrates that the cause and effect logic of science flows from processing to structure to properties to performance, while the inductive, goal-means relations of engineering flow in the opposite direction. Based on this general approach, Olson and co-workers have developed new designs of high-performance alloy steels once their performance objectives and property sets have been identified. Olson’s work was part of a multi-laboratory research effort undertaken by the Steel Research Group (SRG) which received initial NSF funding in 1985 (see http://mtl.ms.nwu.edu/srg_home.htm).

The SRG objective was to develop martensitic steels with combinations of strength, toughness and corrosion resistance that would allow a major advance in the useable strength level of structural steels, beyond the levels that could be achieved by empirical alloy development over the same timeframe. In support of a materials design approach to this problem, basic science modeling tools such as quantum mechanics and continuum micromechanics were used to facilitate the evaluation and analysis of ‘subsystems’ related to local ‘architectural features’ of microstructure which relate to interface strength and the effects of strain-induced phase transformations. Such subsystems typically correspond to various length scales in heterogeneous materials, some controlling strength and others controlling toughness, for example. In evaluating such subsystems, transformation kinetics are modeled using a separate code with model predictions validated using metallurgical quenching dilatometry, differential scanning calorimetry, light microscopy, and transmission electron microscopy. Pertinent diffusionless martensitic transformations occur at a length scale on the order of micrometers. To refine alloy carbide precipitate size at the nanometer scale, characterization tools such as x-ray diffraction, small-angle neutron scattering, atom-probe field-ion microscopy and analytical electron microscopy are combined with elastic energy calculations from continuum mechanics along with thermochemical software and related database to compute interfacial energies. If we can enhance our control of particle size, we can develop efficient strengthening dispersions, leading to 50% increase in strength at a given alloy carbon content.

Toughness subsystems of material architecture are dominated by yet another characteristic length scale. Continuum mechanics analyses are performed for ductile fracture associated with microvoid formation and growth at the interfaces on the order of 100 nanometers; these particles are introduced to decrease grain size in order to inhibit competing brittle fracture mechanism. The measured fracture energy and strain localization in shear are used to validate the results of the models. Finally, embrittlement resistance subsystems that govern
environmental cracking are manifested at atomic scales of 0.1 nanometer through the effects of environmental hydrogen and the prior segregation of embrittling impurities, acting in concert to produce intergranular fracture. Quantum mechanical calculations are employed to predict the segregation energy difference necessary to evaluate embrittlement potency. Moreover, these quantum-based tools offer a means to introduce new generations of “quantum steels,” in which grain boundaries are doped to attain desired electronic structures to enhance intrinsic cohesion and alter impurity interactions to affect improvements of environmental resistance.

In this example, it is important to point out that no attempt is made to somehow bridge all length scales through massive computer simulations based on multi-scale extensions of interatomic potential concepts. Rather, the design was performed largely with judicious choice of characterization tools along with continuum kinetics, thermodynamics and solid mechanics. Atomistics played a key role in both the evaluation of interface strengths and angstrom level design of composition to resist grain boundary embrittlement.

Implications of MDS&E

We envision a widening use of this approach to materials design. If we first develop models using this innovative merging of first principles analysis tools with engineering science approaches for analysis of continua and for multi-scale design of material microstructure, and if we then verify these models using state-of-the-art characterization tools, we can develop new ways to meet the challenges of previously formidable applications such as elevated temperature superconductors, durable heterogeneous ferroelectric, piezoelectric and shape memory materials, and improved refractory alloys for engines and power generation. Equally important outcomes would include significant improvements in existing materials and enormous decreases in the cycle time and cost for development of materials that are tailored to serve specific applications. Materials design is accompanied by a ubiquitous integration of information technologies within the materials sciences and manufacturing multi-disciplines. The requirements of simulation, visualization, distributed information flow and ready access to vast databases are introducing rapid change to materials and, more generally, manufacturing technologies (cf. 1998 National Research Council report on Visionary Manufacturing Challenges for 2020). Manufacturing and materials design are increasingly interwoven with information technology to facilitate rapid prototyping to reduce the materials development and design cycle time for products. Our vision of developing a robust, rapid and reliable capability to design materials has at least two implications, both of which have far-reaching economic consequences in a highly competitive 21st century global economy:

Revolution of the materials supply/development industry. It is likely that a new industry in design of materials will emerge to augment material
processing to provide users with innumerable options and high quality, engineered materials and material/structure systems. Already, we see the introduction of new companies which provide engineering and information science services in materials design. These services rely heavily on science-based design tools, consistent with the theme of MDS&E. New approaches such as combinatorial design permit a more rapid assessment of the material structure in meeting performance requirements, but they are yet in their infancy.

These new approaches to design of materials will supplant the more traditional materials development in a process that is already underway. Traditionally, certain classes of existing materials, such as metal alloys, have been improved incrementally, requiring large commitments of time and money from materials suppliers and clients. This slow, deliberate development process has resulted in sets of generic materials which serve as a ‘database’ from which materials are selected for design of engineering systems. Occasionally, however, the need has arisen for new materials having properties that cannot be attained from the set of existing materials. Systematic development of new materials has been relatively rare in the past - rather, the discovery of new materials has primarily been a hit or miss proposition. This laborious approach cannot survive into a future which will be dominated by information over-flow and rapid product development cycles which incorporate new sets of properties as part of the design specifications. It is no secret that major suppliers of metals have already suffered economically due to the largely empirical, costly and time-consuming nature of the conventional alloy development cycles. For example, large company holdings in the U.S. steel industry have declined, while small to medium size specialty suppliers have expanded marketshare. We observe further that the number of small to medium size specialty alloy suppliers has increased significantly over the past few decades. Supporting modeling and simulation tools have flooded the materials processing marketplace in the last decade, lending enormous potential benefits to decreasing the product development cycle. This indicates a developing trend towards new industries that embrace such tools (e.g. small to medium size suppliers for specialty applications).

Why will design of materials become critical to the success of these industries? Simply put, the market is pulling technology towards rapid new material development cycles. This market force is powerful, and it is absolutely necessary for us to use this technology in order to remain competitive in the international marketplace. The joint application of science-based design tools and computation and information technologies can revolutionize the pace of discovery of new materials.

**Realizing the potential for true virtual manufacturing.** When we eliminate laborious prototyping of systems in favor of enhanced modeling and simulation of materials processing and structure-property relations, we will reap an
enormous increase in the efficiency of product development and total life cycle engineering. Much has been written about the roles of geometric modeling, stress and transport analyses, dimensioning, etc. in realizing the dream of virtual manufacturing. However, we make things from real materials. We must be able to assign accurate material properties based on an in-depth understanding of process-structure-property relations across time and length scales as part of our vision of virtual manufacturing or prototyping.

Long term performance of components must be addressed at the virtual manufacturing stage. While advances in geometric modeling, numerical analyses and visualization of complex structures and systems are enabling technologies for virtual manufacturing with idealized materials, they are only useful for a part of the picture - assembly, cost analysis and conceptual design - without the accompanying understanding of material properties and implications for durability, repair, recycling, and so on. Increasingly, the processing of material is part of the process of manufacture of components and structures. For example, composite materials are processed during component manufacture. Likewise, thermal processing of components alters the material microstructure and resulting properties. These are essential components of engineering life cycle design.

The Roles of Science and Engineering in Materials Design

In our vision of MDS&E, science and engineering are on equal footing. Each contributes essentially to the field. One should not categorize materials design as only science-based design, but also systems-based design. The systems integration aspects and the “art” involved in the design process cannot be overlooked. To the extent that materials chemistry and physics can address the complexity of real materials, they can play a useful role in this dual scientific and engineering enterprise.

The recent report “The Physics of Materials: How Science Improves our Lives” (National Academy Press, 1997) provides a compelling overview of the many ways in which materials impact our everyday lives. This report was authored by the Committee on Condensed-Matter and Materials Physics, a group involved with fundamental atomistic and molecular studies of near-perfect materials. Promising future research areas mentioned in the report include the investigation of nonequilibrium phenomena, artificially structured materials such as Fullerenes and carbon nanotubes, high temperature superconductors and macromolecules as future research areas of high potential benefit. Indeed, these areas focus on basic technologies that involve critical, high-payoff applications.

The materials physics community addresses certain aspects of the overall scope of materials design. Scientific principles will continue to advance in time to treat real materials as complex systems in a more rigorous manner. The current program on large scale parallel computing funded by the DOE, Accelerated
Strategic Computing Initiative (ASCI), is an example of a national initiative to pursue this kind of “grand challenge” class of problems. It was formulated to address aging stockpile issues, including material aging and degradation, using science-based analysis tools. The report of a recent DOE Workshop (May 4, 1998) on Computational Materials Science on the worldwide web recommends that we develop initiatives to leverage ASCI in order to broaden the scope to multi-scale materials design of photovoltaics and structural materials such as steels, Mg and Al alloys, polymer composites and high temperature materials such as Ni-base superalloys (see http://www.er.doe.gov/production/bes/May4Report.htm). It is unlikely, however, that the kinds of nonlinearities and non-uniqueness inherent in processing and applications of these materials at length and time scales of most practical applications will fully yield to computational materials science tools based on first-principles types of atomistic or molecular analyses except in a few special cases of practical importance:

- compound semiconductors
- design of macromolecular materials such as pharmaceuticals, filter or sieve polymers, etc.

These special cases have a common feature - the length scale of the application is at or near the length scale of the analysis. Toolkits and integrated design approaches are relatively well developed for these specific applications (e.g. integrated circuits and pharmaceuticals). In this sense they are good case studies to learn from. However, they do not involve some of the very challenging scale-up issues faced by a host of other applications. For example, even extending electronic materials design to MEMS devices involves some uncharted territory associated with scale-up issues.

It is probably neither practical nor desirable to use federal funds to develop a “brute force” means to extend the tools of quantum mechanics or molecular dynamics to span all length and time scales in order to design materials. Rather, materials physics has yielded tremendous fundamental advances in descriptive models for ideal, small systems; the tools thus developed have now filtered into the materials chemistry and materials science communities which have traditionally focused on realistic, large systems. It remains in the future for the materials science community to embrace the complexity of many-body problems using multi-scale materials design for function. The recent DOE Workshop report on Computational Materials Science reports that “… collective and complex phenomena need to be described by additional mathematical models that do not simply emerge from the atomic scale theories and models. Nevertheless, they require information and input data from the theories and models at ever finer length and time scales…” The point here is that materials design is not pure scientific recipe, but it can benefit enormously from a new level of quantitative, predictive insights that it has rarely enjoyed.

The role of material system designers is to identify those selective aspects of the multi-scale material design that require use of these first-principles tools.
These aspects most often focus on surface or interface thermodynamics and related transport problems. Surface thermodynamics is much more complex and intimately related to details of structure than is bulk thermodynamics. Since the former deals with directional aspects of transport, it offers an ideal application domain for quantum or molecular dynamics models. In fact, such analyses can assist in the prediction of structure-property relations for interface structures at even much higher length scales. For example, weldments form connections between structural members in piping, offshore structures, automobiles, and many other applications and have been designed and analyzed to date purely with continuum mechanics modeling tools. Truly predictive tools are lacking. Real materials are characterized by having impurities and imperfections at interfaces. Often, these must be understood, controlled and tailored to design materials effectively.

Practical Considerations: Implementing Materials Design

A number of practical issues arise when we consider moving towards materials design:

How do we educate students to meet the challenges of designed materials, given the dual roles of science and engineering?
How do we rapidly identify candidate new systems which are sufficiently far from those with which we have experience, and perhaps embody microstructures and compositions that are non-intuitive and often far from equilibrium?
How do we integrate new material classes or certain desirable subsystems into existing materials?
How do we accelerate the identification of those length scales and associated transport or kinetics processes that most strongly affect desired properties for a candidate material system?
Is it possible to develop objective schemes to model the collective effects of lower scale subsystems at higher scales, thereby enabling the prediction of the response to candidate (even virtual) materials to loading conditions, environments, and process histories?

From a materials design perspective, it is likely just as important to develop science-based tools to address distributions of microstructure and resulting properties as it is to apply first-principles calculations for thermodynamic properties of surfaces or interfaces. There can be no such thing as a deterministic design approach for materials, just as there can be no deterministic design approach for any other complex, heterogeneous, hierarchical system, such as an automobile or an airplane, with enormous sets of interactions among components. In any domain, probability issues are to be embraced and addressed as part of the design process. Of course, differences in time scales in synthesis or
processing and during subsequent service raise important concerns about long
term integrity, stability or durability of a material system. Scientific tools are
not available to address this issue. In most practical applications, the length or
time scales and many-body complexities are well beyond those that can be
considered by self-contained, first-principles approaches applied to all scales.
This problem was recognized long ago in the field of engineering design, a
discipline which routinely addresses complex, hierarchical, heterogeneous
systems such as aircraft engines, pumps, highway and bridge structures,
skyscrapers, etc. Although the scales of interest to designers differ entirely from
those of material microstructures, designers in the two domains face analogous
problems. Engineering principles are used to support each level of such a design
approach, along with axiomatic or optimization principles. While we must
respect and appreciate complexity, it must not stop us from designing!

Design makes selective use of science-based analysis tools. But it is
fundamentally an engineering-driven or synthetic enterprise. Design is not
purely analytical. Hence, the human factor is inseparable from synthesis of
new materials or improvement of existing materials.

Small companies are now being formed to address materials design in its
embryonic stages. For example, QuesTek Innovations LLC (Evanston, IL)
dresses a set of applications for materials by design, including proprietary high
performance alloys suited to advanced gear and bearing materials and stainless
steels, custom alloy design, materials modeling, and process simulation. In
addition, the tools for a virtual design environment are being developed,
including software for Computer Integrated Manufacturing Systems, project
management services, and technical and financial management for research and
development projects. QuesTek just received the Technology of the Year Award
from Industry Week magazine for their materials-by-design technology. Co-
recipients included IBM’s copper interconnect technology and Apple’s iMac
computer. The QuesTek web page (http://www.questek.com/) lists a set of case
studies that are available for demonstration of materials by design concepts. As
another example, the National Research Institute for Metals (NRIM) in Japan
(http://www.nrim.go.jp/) has an open materials design web page, complete with
case studies, a recent trend that should continue to grow with time. The linkage
between information technology and materials design is obvious.
The systems integration that is necessary to conduct materials design must be recognized as part of the materials education enterprise. This has not generally been the case. Case studies such as those reported by QuesTek and NRIM will assist enormously in reformulating multi-disciplinary curricula in universities to better respond to this changing environment and to opportunities in materials design. This is not to diminish the role of basic scientific principles in design of hierarchical materials systems; rather, the challenge is to identify how the design process can strategically benefit from these basic science tools.

The design of a new, high performance steel, described earlier in this report, provides an excellent case study of a materials design project that begins with identification of a discrete set of length scales within the microstructure (subsystems) which control strength, toughness, environmental resistance. The designer then followed up with a selective application of science-based analysis tools and supporting high resolution characterization and experiments for validation. That example pointed to the need to develop comprehensive case studies for each material system of interest in order to uncover high payoff modifications of structure. With time and investment in materials design, it should be possible to similarly develop case studies for new materials that have never before been envisioned or processed to meet more severe or peculiar service requirements. It is also clear that such approaches can involve rather large scale efforts to build the foundation of materials design.

Thermodynamics is perhaps the unifying element for multi-scale design of materials. We must recognize that the non-equilibrium character of many of the highly un-natural systems we can consider to meet functionality requirements demands the development of tools to address long term stability as well.
Educational Imperatives of MDS&E

Materials design is a discipline that is already "out there" in an embryonic stage, and it is not well-integrated into the curricula of U.S. universities. There is a disconnect between emerging characterization and simulation tools and the kind of design experiences we offer our students in materials science and engineering departments. Embracing MDS&E means a revolutionary change in materials education and multi-disciplinary interactions of materials science and engineering, engineering science and systems design, materials chemistry and physics, biology, the computing and information sciences, and applied mathematics.

A change of culture is necessary in U.S. universities and industries to move in this direction. It is imperative that we educate a new "breed" of engineers and scientists who are well versed in materials design. Only through such changes can we facilitate revolution in materials development/supply and in virtual manufacturing as we look to the 21st Century. The new and improved materials needed to fuel our economy will be developed primarily through university-based design projects and through development of MDS&E as an academic pursuit.

The discipline of materials science and engineering has gained significant recognition for its role in providing the educational foundations in materials within the past two decades. There has also been an historical interest in basic phenomena of materials among the sciences. Meanwhile, commerce in various material classes - metals, ceramics, polymers and their composites - has become quite competitive from the perspective of suppliers. Further, performance specifications have become more demanding. The challenge to U.S. universities is to integrate those aspects of the sciences which have not conventionally been so directly integrated into the mainstream of materials education and multi-disciplinary materials research in order to realize the full vision of materials design.

Materials Science and Engineering (MSE) is the logical discipline to serve as a focus for university education in materials design. Several preceding reports have laid the groundwork within MSE for a more highly integrated approach to materials design. The Grinter report, published in 1955 by the ASEE Committee on Evaluation of Engineering Education, strongly coupled science with the field of
materials engineering and formed the foundation for changes of expectations and guidelines of the Accreditation Board for Engineering and Technology (ABET) in the 1960’s. The integration of science into the academic programs was a part of the plan to ensure a broad program of study that involved non-technical subjects. This plan involved specific subject areas of study to meet the new goals for engineering education: (1) humanities and social sciences, (2) mathematics and basic sciences, (3) engineering science, and (4) engineering specialty subjects and electives. The Grinter report significantly influenced all of engineering education including the evolution of materials science and engineering education programs, and it influenced how these programs and related research are embedded within the university setting.

The 1974 COSMAT report, entitled *Materials and Man’s Needs*, moved recognition of the MSE discipline forward. At that time, national goals revolved around natural resources, energy, and the environment as well as defense. The COSMAT report dealt with materials issues in the context of the public awareness of the finiteness of the earth’s resources. Further, it was one of a series of reports on major fields of science and engineering, and it focused only on materials science and engineering. It was the first study to embrace both science and engineering in its coverage, and it recognized the strong coupling and inter-relationship of structure and properties as a basis for the design, preparation, and utilization of materials. The study amplified the strong need for a phenomena-driven approach to education in the field, and it provided the concepts for new directions towards interdisciplinary approaches to education and research in the field. This study also provided the background and directions for major changes in the way materials funding was viewed in federal agencies, including organizational changes within the NSF.

A decade later the MSE report, *Materials Science and Engineering for the 1990’s: Maintaining Competitiveness in the Age of Materials* (1989) was prepared at the request of Don Fuqua, then chair of the House Committee on Science and Technology, because MSE had changed dramatically since the COSMAT report. Again it was recognized that the interdisciplinary aspect of materials science and engineering is a critical component of the field. A key conclusion of this study was the definition of the field in terms of the integration of four core elements: structure, properties, processing/synthesis, and performance. Educational directives that evolved from this study provided the basis for the new directions of undergraduate education in the field. Engineering programs that had been materials class specific type programs migrated towards materials science and engineering programs that embraced the integration of the four elements of the field. Accreditation requirements emerged from the profession to mandate this integration in the undergraduate degree programs in the field. As with previous studies the interdisciplinary aspect was recognized with the recommendation for cooperation across the disciplines impacted and with the need for interdisciplinary teams to address many of the problems. Following the historical evolution of these studies, our MDS&E workshop was organized into sessions along the lines of the four elements defined by *the MSE report*. These four elements
form the core of materials design and life cycle engineering. Especially important is the recognition of the need to understand and develop predictive models for behavior at various length and time scales.

It is logical to expect an inertia of materials programs that resists reformulating curriculum to address MDS&E goals. This is the case when any significant “cultural” changes are required. There will be a “learning curve.” This requires communication and buy-in of faculty, students and administrators. It will require an infusion of resources rather than just reallocation of existing resources to accomplish such a cultural change. It will be necessary to make trade-offs in academic programs to incorporate and provide proper support for MDS&E.

Materials design is a broad interdisciplinary enterprise, extending beyond the borders of traditional MSE departments to include Materials Physics and Chemistry, the Engineering Sciences and Applied Mechanics, Applied Mathematics, Biology, the Computing and Information Sciences, and engineering systems design theory. In a sense, we may speak of this broader context of materials science and engineering as the “core” of MDS&E. Emerging science-based tools for materials simulation should be integrated into the education of materials designers in each of the four elements. These include new techniques for characterization and control for processing, as well as new tools for synthesis and modeling of evolving microstructures.

Given the kind of quantitative reasoning skills and creative attributes that our students will need to raise materials design to maturity, as well as the inherited boundaries that have been set among disciplines in most universities, we may identify rich target sets of opportunities to begin to structure our education to meet the demands of MDS&E. With regard to undergraduate and graduate education, these include:

- Developing a centralized, commonly accessible database for instructional materials
- Pursuing multi-disciplinary team-taught courses
- Developing instructional media, focusing on case studies that demonstrate materials by design as part of a larger component or system design rather than just materials selection
- Developing philosophical and axiomatic systems-based approaches for functional design of materials, as well as decision-based design concepts
- Developing modules for science-based modeling of core phenomena to be used in supporting the materials design process (e.g. atomistics, molecular dynamics, finite elements, quantitative image analysis, characterization,
and other modeling and simulation tools), with cooperation of all relevant programs/disciplines

- Developing virtual instructional tools to expose students to complex operations in processing, characterization and structure-property relations; design tools should be available for use in various materials-related disciplines

- Expanding capstone design experiences to more fully integrate materials design throughout the undergraduate program, with open-ended design covering the matrix of the four elements and the material classes

- Changes to titled academic degree programs in materials that consider alternatives to the conventional classification of academic majors related to specific materials or classes of materials such as structure/properties correlation, development of microstructure (thermo/kinetics), modeling and simulation, and materials characterization.

- Exploring novel minor program of study options and cohesive cross-disciplinary graduate courses which introduce science-based tools as well as over-arching systems design principles

- Interacting among disciplines to provide leverage; e.g. MSE departments could provide minors for various other departments, while other departments could provide focused topic courses within a coherent university-wide materials design program

- Aiming graduate research towards complex materials design problems, resulting in case studies, user interfaces for science-based toolkits, and advances in approaches for materials design

- Exploring possibilities of practitioner degrees and team projects or thesis work with materials design as the central theme of the research.

The NSF Materials Research Center at Northwestern University provides a good example of the way instructional modules for materials design can be developed to appeal to a wide range of students. As part of this program, “Materials World Modules” have been developed focusing on individual topics within materials science such as composites, biodegradable materials, biosensors, smart sensors, concrete, polymers, food packaging materials, sports materials and ceramics (see http://mwm.ms.nwu.edu). These instructional modules are principally directed towards middle and high school science classrooms to supplement the students’ regular curriculum. The Materials World Modules explore various aspects of design with materials and design of materials to demonstrate how materials are developed and exploited in order to satisfy certain performance goals related to practical, everyday consumer needs such as fishing poles, coin counters, roofing tiles, monitoring cholesterol and glucose levels, controlled release of medicine, humidity sensors, environmentally friendly food packaging, voltage protectors and new sporting games.

Such programs represent one element of a “front end” strategy for opening possibilities for the new era of MDS&E and to pique the interest of new generations of students. They also foster recognition of the connections between
the sciences and engineering in the general enterprise of materials design. The program has pushed teachers to teach differently, has demonstrated gains in the quality of the science content of the curriculum, and has been rated by students as enhancing their critical thinking skills and prospects to pursue the sciences.

To lay the foundation for this new approach to education, it must be acknowledged that the general public requires reinforcement of the importance of materials to the economy and our way of life. We must be forthright in educating them on how this is actually done in practice - through the joint efforts of the engineering and science enterprises involved in materials research and development, as well as designers that conceive new uses for existing materials and specify requirements for new materials based on market demand. In this process, the economic, social and political dimensions of design decisions also come into play in a way that challenges traditional educational approaches at this level. Primary and secondary education in the U.S. is not typically delivered with multi-disciplinary character. Rather, the focus is on the presentation of each subject in isolation from other subjects. Design of materials cannot be approached in this manner. In fact, it can be argued that our present shortcomings in the multi-discipline of materials design traces to this origin, as well as to lack of quality offerings of the sciences in U.S. middle and high schools. To begin to clear the path for a mindset of integration of disciplines that will be necessary for future generations of materials designers, it is essential to reach out to the public and K-12 faculty to convey an image for the materials field and to portray opportunities in MDS&E in practical terms: real world examples such as those used in the aforementioned modules developed at Northwestern University are of high potential value, for example.

Research Imperatives of MDS&E

The **MDS&E Grand Challenge** posed to the broad materials science and engineering community is to develop *general methods* for preparing materials with particular properties to meet functional design requirements in a flexible and efficient manner. This includes all aspects of synthesis and processing, coupled material/product design, certification and maintenance of properties, and systems considerations. These methods should be highly synthetic and predictive, moving away from the empirical methods of the past.

The major technical milestones or **MDS&E target technologies** required to address this grand challenge include:

1. **Principles and approaches for more quantitative materials design.** Design must be based on a collection of principles (qualitative concepts with quantitative “clothing”) that can be used to suggest possible processing and synthesis strategies to achieve the desired structures and properties using efficient manufacturing processes which minimize economic and environmental costs. This builds on the concepts currently used by creative designers of materials and products, but will be enhanced by the improved modeling and
simulation capabilities. These tools will be used increasingly as they become more reliably predictive. We must develop concepts and principles, simulation and modeling tools, and synthesis and characterization techniques that can transcend the length and time scales from electrons and atoms to those of macroscopic structures and products. A key component is the identification of scales at which basic scientific tools may most strategically benefit materials design. The development of hierarchical averaging principles for scaling up over length and time scales, stemming from statistical mechanics or Gibbsian thermodynamics, must take great strides in the coming decades. To this end, consideration of the statistical aspects of microstructure morphology and its impact on kinetics and structure-property relations is of first order importance.

2. Enhanced modeling and simulation tools. Lack of verification by unambiguous experiments is perhaps the greatest shortcoming of the existing state of modeling and simulation. Modeling and simulation of evolving material microstructure, including self-organizing phenomena, is essential to specify processing and to support in-service applications. Further, appropriate characterization tools must be coupled with modeling and simulation to verify predictive quality. These modeling and simulation tools must cover a wide range of length and time scales. Some must be based on first-principles quantum mechanics, while others are to be based on simplified interatomic potentials or mechanics of continuous media. Hybrid approaches may make use of features and capabilities of disparate model sets. Critical requirements include:

Accuracy: modeling and simulation must be sufficiently accurate that the results can be trusted even in the absence of experimental confirmation over the entire space of predictions

Speed: the time scale for making these predictions must be short enough to be useful for design.

Visualization of solutions and design options: ultimately the designer needs concepts, not just numbers, in order to evaluate trends and to consider a range of possible choices. To develop new concepts from complex simulations will require clever ways to visualize the essential characteristics while ignoring other details. This will require progress in the logic and heuristics for extracting information and in graphically formatting this information for purposes of building intuition. There are many existing codes that are now utilized in analysis of material processing and durability. “Toolkits” to support materials design should be user-centered and user-friendly and will be application-dependent. They cannot be developed in the abstract.

3. Validated, reliable and comprehensive databases. It is necessary to develop and maintain validated databases for material systems that are well characterized and reproducible. These databases can be used initially to validate the modeling and simulation tools, which in turn can be used to supplement the databases with structural and property data created by validated modeling and
simulation tools. Presently, data are scattered throughout the literature. Further, data are accumulating daily from sources as broadly ranging as combinatorial synthesis and atomistic simulations. The challenge is to make this data accessible to the designers and modelers in a systematic way that abides by standards and testing. Sorely lacking here are critical expert evaluations of widely accessible data. The development of world wide web-based tools and prolific access to data provides an opportunity to build expert systems that could utilize expertise and knowledge in new ways; this would help modelers to validate their software tools and help the designers access data that can decrease the costs of processing and synthesis, testing, and manufacturing. Unless the data are validated and carry a "stamp of approval," this information may impede, rather than assist, design. In addition to properties related to interfaces, data are needed to support the assessment of long term impact of materials on the environment (toxicity and bio-degradability) as well as long term degradation of performance (deterioration in properties).

4. Methods for in situ characterization and testing. Performing characterization during materials synthesis or processing will allow the designer to evaluate modeling tools for multi-scale materials design. For example, modeling of interfaces and defects is absolutely critical to the design of process route that leads to a given material structure with desired properties. We desperately need new data from in situ characterization to be used jointly with modeling and simulation to provide new insights into the structures and properties of interfaces and defects achieved by various methods of synthesis and processing because it is very difficult to obtain reliable information about the structure and properties of interfaces from experiments. Thus we must develop modeling and simulation tools that can reliably predict the structures and properties of interfaces and we must develop in situ characterization tools for testing these predictions. This will also benefit feedback control algorithms for intelligent manufacturing.

To identify compositions of most interest, we can use combinatorial materials synthesis or processing with rapid, simultaneous in situ characterization, and we can follow these steps with focused optimization. We can apply the concepts and predictions developed with our modeling and simulation tools in conjunction with a multi-scale materials design methodology. When we use these tools and methods together, we may be able to identify the most rapid, cost-effective and environmentally conscious ways to generate new compositions having the desired structures and properties. There are some limitations on such combinatorial approaches to materials design, since they are flavored with empiricism. However, there are specific applications to which these approaches may be well suited, such as preliminary process identification and costing.

Recent developments give us confidence that the U.S. can meet the challenges of MDS&E and take a leadership role:
Recent progress in theory and simulation coupled with the dramatic improvement in computer hardware and user-friendly software provides an excellent starting point for developing the modeling and simulation tools. However, an intense, focused effort to validate and develop these methods into tools which are useful to a new generation of Materials Designers is required before these methods will have a real impact upon materials development or virtual manufacturing. Their science base must be strengthened. These tools will likely be competitively licensed to commercial software vendors that will market and maintain them in a form suitable for application by designers and manufacturing engineers. These tools will also be utilized in university curricula as part of teaching new generations of interdisciplinary engineers and scientists.

There has been enormous progress in synthesis, processing and characterization techniques and strategies that could build on new modeling and simulation tools to develop better libraries for discovery of new material systems.

Tools for geometric modeling, image analysis and associated automated meshing must be extended to properly support multi-scale computational analyses for materials design.

Software for materials selection is now widely deployed and used in university curricula, such as the Cambridge Materials Selector software (http://www.granta.co.uk) or the ASM Materials Data Selection software (http://www.asm-intl.org), offering valuable concepts and user interfaces to build on for materials design.

New technologies for in situ characterization based on MEMS technology are being developed to measure the evolving structure of materials for a wide range of applications and may provide valuable support for validating predictive capabilities of simulations and for providing material constants for high fidelity models.

A discussion of research imperatives leads naturally to graduate level research experiences in universities. It is at the graduate level where strong multi-disciplinary aspects of science-based materials design can best be addressed, since it is essential to develop a strong disciplinary background within the undergraduate program along with a framework of design of complex systems. The present system of graduate thesis work in materials emphasizes in-depth, scientific investigation of relatively narrow, well-defined aspects of given materials systems, characterization tools and so on. This is true for both the science and engineering academic enterprises. We must therefore promote new modes of graduate thesis problem solving, consistent with the philosophy of materials design. These will stress:
team efforts with multi-functional requirements (e.g. MSE, materials physics and chemistry, computing and information sciences, engineering sciences and applied mechanics, mathematics, communications, sociology, and management),

highly complex, multi-level, multi-dimensional problems that cannot be treated by any discipline in a self-contained manner, and

industrial connectivity to ensure realistic constraints and problem sets, as well as contributions to teaming efforts.

Intellectual property rights issues associated with design concepts and products of conceptual designs will have to be dealt with in order to foster productive and open relations between universities and industries.

A Recommended “Roadmap” for MDS&E

In this section we chart a course to pursue and exploit the opportunities offered by Materials Design Science and Engineering. With the recognition of scarce resources, we must make choices in each area that build the general reservoir of knowledge and the necessary tools while directing the effort toward design of materials and manufacture of relevant and timely products.

Because of the embryonic stage of MDS&E, research and education initiatives must be linked. At present, only a few materials science and engineering departments teach design of materials. Very few large-scale industries have identified design of materials as an integral and essential part of their enterprise. Hence, any initiatives must promote new modes of student problem-solving in academia, leading to new generations of engineers and scientists capable of addressing design of material systems. This initiative must be linked to industry so that realistic constraints of time and cost are part of the mindset of solving this class of problems, with full recognition of the importance of basic research in developing the science base essential to MDS&E. The “value-added” perspective is critical to design of materials.

We begin this section on recommendations by identifying some follow-on workshop topics that are essential to clarify and pursue the four MDS&E target technologies:

1. Principles and approaches for more quantitative materials design
2. Enhanced modeling and simulation tools
3. Validated, reliable and comprehensive databases
4. Methods for in situ characterization and testing

In addition we suggest educational initiatives to build and support the academic foundations of MDS&E. Finally, we close by recommending specific programs and funding levels for MDS&E, whether to be pursued by the NSF or as a multi-agency venture.
A. Follow-On Workshop Topics

Scientific and engineering societies can play an important role in fostering MDS&E by sponsoring symposia and short courses which address various aspects of materials design. There is a need for selective follow-on workshops which address specific issues related to MDS&E.

A1. Databases for enabling materials design

At our workshop, the issue of databases arose as an area of fundamental concern to materials design. The goals of this follow-on workshop would be to identify fundamental database needs, to identify critical experiments to support science based modeling and simulation, to identify who should develop, validate and maintain the database and to determine what level funding should be devoted to do this. It is believed that the required funding levels will be significant. NIST was mentioned as one logical possibility to manage this activity, but there may be other possibilities, including collaboration with a conceptual MDS&E Institute to be discussed later in this report.

There are many voids in our databases; consequently, there is much uncertainty in our first-principles science toolkits with regard to predicting structure-property relations. For example, phase diagrams are known only for historically common ternary and higher systems. Thermodynamic properties are virtually unknown for many possible systems, including many that can be predicted by emerging modeling and simulation tools. We thus have little verification of these models, so we cannot effectively benchmark design approaches and confidence levels for complex, hierarchical systems.

A2. Principles of systems design and the prospects for hierarchical materials systems

Proper design always includes the recognition of customer needs, preferences, and specifications along with economic, social and environmental constraints and technological capabilities. The “design” of materials approaches should therefore acknowledge applications to other similar classes of problems and draw from these, building in the essential and unique aspects of complex material systems. We must ask the question ”are we making use of all design tools that are available”? This topic is intended to explore among experts in systems design the various existing and emerging systems design approaches, with an eye towards materials by design.

A3. Identification of opportunities and deficiencies in science-based modeling, simulation and characterization “tools” to support materials design
This workshop topic focuses on the identification of the most fruitful and supportive applications for first-principles modeling and simulation tools of materials physics, materials chemistry and the engineering sciences in the materials design enterprise, as well as supportive application domains for high resolution characterization or needs for coupled characterization/simulation tools.

It is possible that all three topics could be addressed within one or two dedicated, cross-cutting workshops that focus on the materials design perspective. We recommend that these topics be addressed by workshops in the near future with specific objectives that support MDS&E. There is no apparent reason to continue to hold workshops reaching beyond these topics prior to developing new initiatives in MDS&E.

B. Recommended Funded Programs in the MDS&E Initiative

B1. Materials Design and Manufacturing (MDM) Research Projects

To achieve a measurable impact in the near future we recommend an integrated systems approach feature projects that couple fundamental research with development of essential educational materials and programs in a manner that is directed toward specific manufacturing goals of sufficient practical and economic importance. These Materials Design and Manufacturing (MDM) projects would be vertically integrated and would be directed towards specific applications. Clearly there are major opportunities in every area of materials, including biomimetic materials, composites, nanostructured nanophase materials, electronic packaging material systems, processed foods, civil transportation materials, cast alloys, and so on. Indeed, many of the challenges lie in developing heterogeneous systems that might combine ceramics, polymers, metal alloys, semiconductors, and biomimetics in self-organized systems that achieve very specific properties (including structural, mechanical, electrical, thermal, magnetic, chemical, acoustic, sensor) while minimizing manufacturing costs.

An annual funding level of $1M to $2M for each MDM project is deemed necessary to support the kind of coordinated, multi-disciplinary team effort that will lead to significant advances of materials design and that will form in-depth case studies to help undergird education in the field. In our view, considerable up-front industrial buy-in is essential, with at least 20% matching fund expectations from industry. The MDM projects should identify benchmark materials systems to verify principles of materials design and to facilitate virtual manufacturing/prototyping. Activities in these MDM projects should run the gamut from building basic science toolkits (modeling and simulation, correlations with databases, etc.) to database development (identifying, enhancing, validating and cataloging) to production of prototypes. The key goal is to demonstrate how integration via a systems level approach can affect improvement of materials/component within a reasonable timeframe. MDM projects are expected to provide working systems materials design algorithms and
to address the multi-scale modeling issues that are core to advancing the MDS&E target technologies.

Five year MDM projects should be evaluated for convergence towards end goals in the third year.

MDM projects should:

1. identify performance objectives
2. define a figure of merit for performance based on collaboration with systems designers and industrial experts
3. utilize a highly multi-disciplinary approach
4. emphasize systems design for functionality, and explore other engineering systems design approaches
5. identify reliability in terms of failure modes, long term durability and distributions of material structure and properties
6. emphasize predictive approaches as much as possible; employ and develop quantitative tools
7. identify related databases and verify integrity
8. identify when and where simulation is needed (also which kinds of simulation)
9. identify limitations of modeling and simulation tools and point to critical areas for improvement
10. include consideration of process route and structure/property relations as well as cost/demand factors
11. address the integration of materials design with concurrent engineering and virtual manufacturing
12. identify the degree of scale-up required from laboratory characterization and controlling microstructure length and time scales to application time and length scales
13. transfer technology transfer via case study modules to support MDS&E education
14. identify tightly targeted goals for future research

A more detailed example of one possible structure for MDM projects which emerged from our discussion appears in Appendix C.

B2. MDS&E Institute

In addition to the need for MDM projects, we see a pressing need for national coordination of MDS&E efforts related to advances in materials design concepts, case studies, instructional materials, workshops, short courses and exchange programs for faculty, students and industrial collaborators. In addition, the development and validation of databases for use with science-based toolkits is of significant national interest. It seems logical to establish a national center for MDS&E activities. This center would focus on the full range of educational and research goals in order to facilitate reform of the multi-disciplinary materials
curricula at universities, as well as to support curriculum development in undergraduate materials programs.

The objectives of the MDS&E Institute would be to foster development of academic programs to incorporate MDS&E and to support basic advances in materials design approaches, case studies and novel concepts for teaming within multi-disciplinary materials design environments. All four MDS&E target technologies would lie within the responsibilities of this Institute.

The suggested annual funding level is $1M to $2M with in-kind matching funds from industry to support the integration of essential industrial perspectives within the effort.

The MDS&E Institute should:

1. involve multiple institutions (preferably both research and primarily undergraduate) and explore various teaming arrangements/approaches
2. emphasize a systems approach, with an appropriate breadth of multi-disciplinary involvement
3. emphasize teaming of students, faculty and visiting industry representatives
4. host workshops, colloquia, short courses, and visiting positions on MDS&E
5. create subject matter for distance learning and virtual education
6. develop MDS&E multi-disciplinary case study modules for different material systems
7. develop, catalog and communicate use of science-based design tools
8. foster development of “virtual” materials design instructional tools
9. foster development of virtual manufacturing case studies and applications
10. identify tightly targeted goals for future research

The expected outcome of the MDS&E Institute is to directly promote and facilitate development of new generations of students who are more sophisticated in design of materials, including the use of basic science tools, who are familiar with databases and characterization/validation, who recognize financial and time constraints in design, who understand the entrepreneurial nature of the global competitive environment in designed materials, who have a broad perspective, and who are highly motivated to bring the MDS&E perspective to industry.

B3. Focused investigator grants for undergraduate and graduate program development

The lack of instructional materials is a potential stumbling block for development of a MDS&E-oriented curriculum because such a curriculum represents enormous changes in the teaching of design to undergraduates in U.S. materials programs. Recognizing the cost factor involved in these program changes, development of course modules, education of faculty and the human effort-intensive nature of teaching design, it is essential to provide support for the educational infrastructure in addition to the foregoing programs in order to
foster MDS&E within academic programs. In addition, at the graduate level it is necessary to embark on experiments involving teaming of graduate students in M.S. and Ph.D. research, working with faculty teams composed of various disciplines on complex MDS&E projects. Hence, focused investigator grants should be made available in connection with the MDS&E initiative to support development of a self-sustaining materials design component in the curriculum.

We recommend that funding be made available through competitive, peer reviewed proposals to reasonably address the initial stages of curriculum reform and instructional innovation over a broad range of institutions. This funding will help to establish a “critical mass” necessary to embed materials design within university curricula. Without such monies, MDS&E will be the province of a handful of visionary schools, subject to the specific nuances of their administrative and faculty structures and to their specific faculty preferences and talents. Such an ad hoc approach is unlikely to lead to a consistent national effort to teach materials design or to provide long term positive impact on the materials supply and virtual manufacturing communities.

It is also emphasized that these programs should couple with and derive mutual benefit from concurrent research programs within these institutions.

Bibliography


“Visionary Manufacturing Challenges for 2020,” report of the Committee on Visionary Manufacturing Challenges, Board on Manufacturing and Engineering
Appendix A - Workshop Itinerary

Local Organizing Committee

Co-Chairs: D.L. McDowell, Georgia Tech and T.L. Story, Morehouse College

Structure-Property Relations Across Length Scales
A. Saxena, K. Schwan, C. Lynch, R. Gerhardt, A. Zurieck

Materials Synthesis and Design
W. Rees, A. Rohatgi, N. Haque, P. Ludovice, N. Thadhani

Elements of Process Design Science and Engineering
W.J. Lackey, H. Paris, C. Summers, P. Kohl

Multidisciplinary Materials Education
T. Sanders, R. Talreja, A. Abhiraman, A. Erbil, M. Waugh

Program Advisory Board

Structure-Property Relations Across Length Scales: T. Eagar, MIT

Materials Synthesis and Design: W. Goddard, Caltech

Elements of Process Design Science and Engineering: H. Palmour, III, NC State University

Multi-disciplinary Materials Education: G.L. Liedl, Purdue University

Itinerary

Sunday, October 18, 1998
pre-workshop reception
5:00 pm at the GCATT building

Monday, October 19

Opening comments (8:30 am)
(W. Massey, Morehouse College and M. Thomas, Georgia Tech)
Introduction (8:40 am)
(D. McDowell, Georgia Tech)

Session I: Theme I - Structure-Property Relations Across Length Scales
Session Chair: A. Saxena, GT 9:00-9:05 am
Keynote Presentation: A.G. Evans, Princeton 9:05-9:35

Panelists: L. Kimerling, MIT 9:35-9:50
J. McGrath, VPI&SU 9:50-10:05
D.L. McDowell, GT 10:05-10:20
A. Gokhale, GT 10:20-10:35

Coffee Break 10:35 am

Panel Discussion, moderated by A. Saxena 10:50-12:00

Catered lunch (noon)

Afternoon

Session II: Theme II - Materials Synthesis and Design

Session Chair: W. Goddard, Caltech 1:10-1:15 pm
Keynote Presentation: M.A. Ratner, Northwestern 1:15-1:45

Panelists: D.A. Tirrell, Caltech 1:45-1:55
B.J. Evans, Morehouse 1:55-2:05
R. Haushalter, Symyx Technologies 2:05-2:15

Panel Discussion, moderated by W. Goddard 2:15-2:45
Identification of small groups for evening discussion/report writing (2:45 pm)
Break at 3:00 PM

optional GT/Morehouse tours

Evening

Small breakout group discussions/report outlines (7:00 pm)
Reports/recommendations to overall group (8:30 pm)
Summary discussion (9:15 pm)
Tuesday, October 20

Morning

Session III: Theme III - Elements of Process Design Science and Engineering
Session Chair: Hayne Palmour, III, NC State Univ. 8:30-8:35 am
Keynote Presentation: G.B. Olson, Northwestern 8:35-9:15

Panelists:

M.D. Allendorf, Sandia 9:15-9:25
S.M. Johnson, SRI International 9:25-9:35
J.M. Woodall, Purdue Univ. 9:35-9:45
W.L. Johnson, Cal Tech 9:45-9:55
A.S. Abhiraman, Georgia Tech 9:55-10:05

Coffee Break 10:10 am

Panel Discussion, moderated by H. Palmour, III 10:35-12:00

Catered lunch (noon)

Afternoon

Session IV: Theme IV - Multi-disciplinary Materials Education

Session Chair: G.L. Liedl, Purdue University 1:10-1:15 pm
Keynote Presentation: M. Flemings, MIT 1:15-1:35

Panelists:

R. Chang, Northwestern Univ. 1:35-1:45
R.W. Heckel, Mich. Tech Univ. 1:45-2:00
J.P. Schaffer, Lafayette College 2:00-2:15
P. Ludovice, GT 2:15-2:30
T.H.B. Sanders, GT 2:30-2:45

Panel/group discussion, moderated by G.L. Liedl 2:45-3:05
Identification of small groups for evening discussion/report writing (3:05 pm)
Break at 3:15 pm

optional GT/Morehouse tours

Evening

Small breakout group discussions/report outlines (7:00 pm)
Reports/recommendations to overall group (8:45 pm)
Summary discussion (9:30 pm)
Wednesday, October 21

8:30 - 9:15 am

Finish up the discussions from Tuesday on:

1. Materials education related to MDS&E
2. Materials process design

9:15 - 10:15 am

Group discussion on identifying

a. potential impact
b. critical issues, obstacles and opportunities

10:15 am - break

10:30 am - noon

writing - stage II
break up into small groups according to theme area (or other), develop and incorporate potential impact, critical issues, etc. Identify specific recommendations for university initiatives, university-industrial initiatives, and programmatic/funding initiatives relative to MDS&E. Identify specific recommendations for selective, critical areas for follow-on workshops. Objective: Develop theme summary reports.

Noon - catered lunch

1:00 pm - presentations of theme summary reports

2:00 pm - summary discussion - overall perspectives in integrating themes. Audience for report. First draft comprehensive roadmap for MDS&E

3:00 pm - closing comments, John Hopps, Morehouse College

Adjourn at 3:15 pm
Appendix B - Participants

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Appendix C - An Example Profile of the MDM Project Concept

One possible model for multi-disciplinary MDM projects emerged from our Tuesday evening workshop discussion. It considers a multi-disciplinary and multi-agency approach organized as follows. Teams of leading engineers and managers from industry who are able to identify the critical products and processes sufficiently valuable to serve as Commercial Manufacturing Targets would be brought together along with key managers from the Defense agencies (DARPA, DOE, and the DOD) to identify the Critical Manufacturing Targets. These should be targets that might be achievable, at least in a prototype form, within a five-year project of moderate budget dimensions. The community of research scientists and engineers from academia, government labs, and corporate research labs would then be allowed to form vertically integrated teams that would propose Materials Design and Manufacturing (MDM) Projects that would combine research and development in the four MDS&E target technologies:

1. principles and approaches for more quantitative materials design,
2. enhanced modeling and simulation tools,
3. validated, reliable and comprehensive databases, and
4. methods for in situ characterization and testing,

all goal-directed to achieve a Critical Manufacturing Target (CMT). These MDM Groups would be funded initially for three years with options for extending by an additional two to four years, contingent upon approval from review teams representing both the research science and engineering community and by review teams representing the commercial and defense communities. The MDM groups would be expected to make alliances with at least one U.S. industrial manufacturing company in which the company (or companies) would provide direct matching funds plus coordinating personnel. Successful tie-ins to manufacturing would be required among criteria in extending the MDM Group past the first three years. Each MDM Group would involve four co-PI's from academia and government laboratories (one of whom serves as Coordinating PI), each representing one of the four areas, plus one PI representing systems engineering and manufacturing (he/she could be from the manufacturing industry). The systems designer or manufacturing co-PI would be expected to provide the overall manufacturing design objective that would drive the research and engineering developments. The four co-PI's could each be in a different institution and might each direct an interdisciplinary team located at more than one site. The five PIs would meet regularly at one of the sites involved to discuss progress and specific plans for the next quarter. An annual meeting would be held at one of the sites which would feature talks and posters by the graduate students and postdoctoral fellows being trained; this meeting would be attended by a review committee consisting of four representatives (one representing each of the four MDS&E target technologies) from the academic and government lab
communities, plus a representative of the manufacturing community different from that of the manufacturing co-PI. The operating budget for the MDM would be between $1M and $2M per year, with at least 20% from direct matching by industry (this could be delayed as long as three years, but would be a requirement for extension past the three years). This direct industrial funding could come partial from SBIR or ATP funding obtained independently by the Industrial co-PIs. By the end of three years, there should be a plan for scaling-up the designs and demonstrations from the laboratory and computer to manufacturing. By the end of five years, there should be demonstrable progress toward these ends.

By the end of the first two years, each MDM group would be expected to form a collaboration with at least one other MDM group in which they would exchange information and collaborate on joint projects.

The success of each MDM Group would be judged equally on the progress toward practical manufacturing of valuable new products or processes and on the progress in developing the four MDS&E target technologies in a manner which is valuable to the other MDMs and to the general materials community.