Materials Informatics

John R. Rodgers and David Cebon,
Guest Editors

Abstract

Global markets are pressuring the materials industries to reduce the time span between materials research and materials development. In particular, current approaches to the development and insertion (deployment) of advanced materials in military systems are too time-intensive and expensive. Despite the large investments in defense systems, insertion is not certain, since materials development is often not linked to the system designer needs, with the results frequently being that the materials do not meet their requirements. There is potentially a high payoff for developing methodologies that will accelerate the insertion of materials, thereby saving millions of investment dollars. All industries engaged in developing advanced materials are searching for new methodologies to solve these problems.

Once a new material has been developed, it must be characterized and modeled. Otherwise, components using it cannot be analyzed, and consequently, it cannot be used in engineering products. Therefore, exploiting the full benefits of new (and existing) engineering materials requires specialized informatics tools for data capture, management, analysis, and dissemination. Advances in computing power, coupled with computational modeling and simulation and materials properties databases, will enable materials scientists and engineers to meet these challenges.

The articles in this issue of *MRS Bulletin* show a variety of applications of the methodologies that are employed in using materials informatics approaches to materials and engineering product development.

Keywords: *combinatorial materials science, informatics, performance, properties, simulation, structure, theory.*

The term "informatics" has been defined as the use of computer software to gather, store, manipulate, retrieve, and classify information. This issue of *MRS Bulletin* will focus on materials informatics—the application of computational methodologies to processing and interpreting scientific and engineering data concerning materials. Modern materials science and engineering research produces a large amount of heterogeneous data. Computational methods are then used to organize, manage, interpret, analyze, and visualize these data. Using a combination of computational methods, like density functional theory (DFT), to calculate structure and properties, combined with data mining of properties databases to identify trends and systematics in property data, it is possible, then, to identify suitable candidate starting materials for a variety of materials science and engineering applications. These computational methods are now becoming important tools for use by materials scientists and engineers in materials and product development.

Materials informatics can be broadly divided into three main parts: data generation (synthesis), data management, and knowledge discovery (analysis). New experimental methods, such as combinatorial materials science[1] and diffusion multiple approaches,[2] are synthesizing large amounts of structural and property data—physical, chemical, and engineering. Combinatorial materials science is an experimental approach to quickly analyze materials and to test for their physical and structural properties. A diffusion multiple approach is the result of an assembly of three or more metals, in close contact, that is subject to high temperatures to allow thermal interdiffusion. The large amount of data generated by these methods needs to be stored, analyzed, and mined for further applications.

More recently, "computational" combinatorial methods or high-throughput *ab initio* computations, based on density functional theory (DFT)[3] (see also the September 2006 issue of *MRS Bulletin*) are being employed to calculate the structure and properties of materials systematically across a wide parameter space.[4] DFT, based on quantum mechanical methods, is used in computational materials science for the calculation of structural, electronic, optical, and magnetic properties of materials. These advances, which have been made possible with increases in computational speed, and the parallel development of robust *ab initio* techniques, are also generating enormous amounts of property data.

The use of these complementary methods—computational experiment and theory—to generate data, coupled with methods for data checking and estimation[5] for the filling in of "holes" in materials property space,[6] are providing routes to predict new feasible materials compositions and their properties,[7–9] thus improving materials design and selection capabilities.

For the successful design of components for engineering applications, data, and knowledge relating to the selection of the material, the component geometry and the processing route need to be optimized to maximize performance and minimize cost and adverse environmental impact.[10] Other strategies for successful design consist of a systems approach that integrates processing–structure–properties–performance (PSPP) relationships where there is a need to link processing parameters of a material to its structure, properties, and performance.[11] From PSPP relationships, it is possible to establish links between properties and structure, and between structure and processing. Being able to extract such relationships from vast arrays of physical and engineering properties databases and materials processing data facilitates the materials design process.

In this century, materials science will become an ever more important factor in many technologies. The constant quest for new materials with better properties, improved performance of existing materials, decreased materials development costs, and reduced environmental impact ensure the continual and steadily growing importance of systematic materials development and selection.

The Edisonian approach (i.e., trial and error) has been widely used in designing materials. Relying on intuition and experiment, this approach can screen only as many materials for which it is practical to perform experiments. As an illustration, consider Table I, which compares the approximate number of experimentally known materials compositions with the maximum possible number. Most elements and binaries have been studied, but the number of experiments falls drastically

Table I: Distribution of Chemical Systems.

Systems	Experimentally Known	Percent Known	Maximum Number
Elements	100	100%	100
Binaries	4,000	81%	4,950
Ternaries	8,000	5%	161,700
Quaternaries	1,000	<1%	3,921,225

for ternaries (three elements), while the properties of quaternaries (four elements) and higher systems are almost unknown. The number of materials studied by this Edisonian process is usually tens, or possibly hundreds, as compared with the virtually infinite number of possible candidates representing tertiary, quaternary, or even more complex compounds, about whose properties we currently know nothing at all, that can be studied using combinatorial methods.

Materials informatics approaches, then, provide an effective way to interpret and use materials properties data in the selection and design of materials and products. The articles in this issue of the *MRS Bulletin* cover many of the methodologies that have been developed for this purpose.

Morgan et al.[12] introduce an essential item in the materials development process: crystal structure prediction. Crystal structures, which provide links between the components of the PSPP chain, are important in understanding many materials properties that are symmetry-dependent,[13] from mechanical to electronic. They show that the inability to predict the crystal structures of a crystalline solid from a knowledge of the chemical composition, alluded to by Maddox[14] as "one of the continuing scandals in the physical sciences," can be successfully solved using a combination of data mining and *ab initio* quantum mechanics methods. Predictions using these combined approaches result in ~90% accuracies if the five most likely structures at each chemical composition are used.

Bligaard et al. cover the applications of electronic structure calculations in the design of metal alloy catalysts. Applying a combination of computational and data-mining approaches, they show how the concept of a Pareto-optimal[15] set can be used to define alloys with favorable catalytic properties, by simultaneously optimizing a multiproperty data set. A Pareto-optimal set produces an infinite set of solutions from which a desired solution can be chosen.

Le Page, who has made significant contributions in the application of data mining and computational approaches to a number of topics—from the crystal chemistry of minerals[16] to structure types[17] and physical property calculations[18] using quantum mechanical calculations—describes a number of applications of the integration of crystal structure databases and computational methods for property data mining. This contribution provides an overview of informatics approaches that can be used in materials development at the crystal structure stage.

Wu describes a computational materials design platform to support materials design across adjacent length scales. This platform, an integration of a variety of computational methods and data-mining techniques, has been used to solve design problems.

Combinatorial materials science (CMS)[1] aims at discovering new materials using a combination of high-speed chemical synthesis, high-throughput screening, fast data-storing, data screening, and information processing. Takeuchi et al. describe this integration of experimentation and the related data-mining tools as applied to the prediction of new materials. They cover the underlying techniques for data analysis schemes for identifying materials compositions, structure, and properties.

Cebon and Ashby describe in detail the needs for materials data and related software in engineering product development. They systematically cover a number of topics, from data types and data evaluation for the engineering materials selection process to enterprise-wide materials data management. They show how quantitative engineering property data can be integrated with descriptive supporting information in the systematic optimal selection of materials. They also show the need for comprehensive data coverage to facilitate the selection process and discuss important topics such as the correlation between materials properties and the estimation of properties.[6,19] The application of these last two methods not only improves the quality of the database of materials properties but also makes it possible to include missing data to populate property space. The authors have also described the need for software systems that can automate the key data management tasks: data capture, analysis, deployment, and maintenance. Specific requirements of such systems are flexibility of data management, change control, version control, quality control, and traceability of information.

Arnold focuses on identifying what constitutes "sufficient" data content (i.e., quality and quantity) for developing, characterizing, and validating constitutive models for use in structural analysis—particularly finite element modeling. Constitutive theory concerns the mathematical modeling of the physical response (output) of a material to a given stimulus (input); that input can be a generalized force or displacement. He focuses on the materials information needs of sophisticated nonlinear time- and history-dependent (hereditary) constitutive models. Such models are needed for the accurate prediction of the performance and life of components under arduous operating conditions—for example, cyclic loading at high temperatures. He also describes the informatics infrastructure required for handling the potentially massive amounts of materials data needed to generate these models. Arnold points out that although data for simple materials properties (e.g., density, Young's modulus, ultimate tensile strength, yield stress, coefficient of thermal expansion, etc.) are widely available in the literature, often the corresponding response curves—needed for complex modeling—are not available. Furthermore, the detailed pedigree information that is needed to assess the applicability and quality of the information is often not stored or reported with it. Consequently, much existing materials property data cannot be used for generating the complex constitutive models needed for engineering analysis and design. To address these issues, a paradigm shift is needed in the way that engineering organizations collect, store, manage, and disseminate materials information.

In the aerospace industry,[20] the introduction of a new class of materials, including the time to develop design practices that fully exploit the performance of the materials, can take 20 years or more. Such development practices are now too long for aerospace materials industries to maintain their competitiveness. Similar issues exist in other materials industries. As a result, the competitiveness and success of materials development depends increasingly on the ability to utilize information, which is abundantly available, to think strategically, faster, and better than the competition and produce new products.

These challenges carry with them the cost of implementation. New technologies to manage information, on its own, do not give a competitive advantage, since information today is widely available and

technology alone cannot convert data into knowledge. There is thus a need for knowledge creation, and this involves data generation, gathering, evaluation, and organization, and the conversion of data/information into patterns, trends, systematics, and regularities. This can be achieved by domain experts who use the *science of the domain* coupled with the materials informatics concepts described in this issue in knowledge creation. The return on investment[20] in using materials informatics approaches in materials research and development makes its inclusion a key resource in product development.

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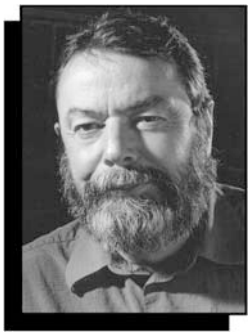

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topological transition in films adsorbed on quasicrystalline surfaces.

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