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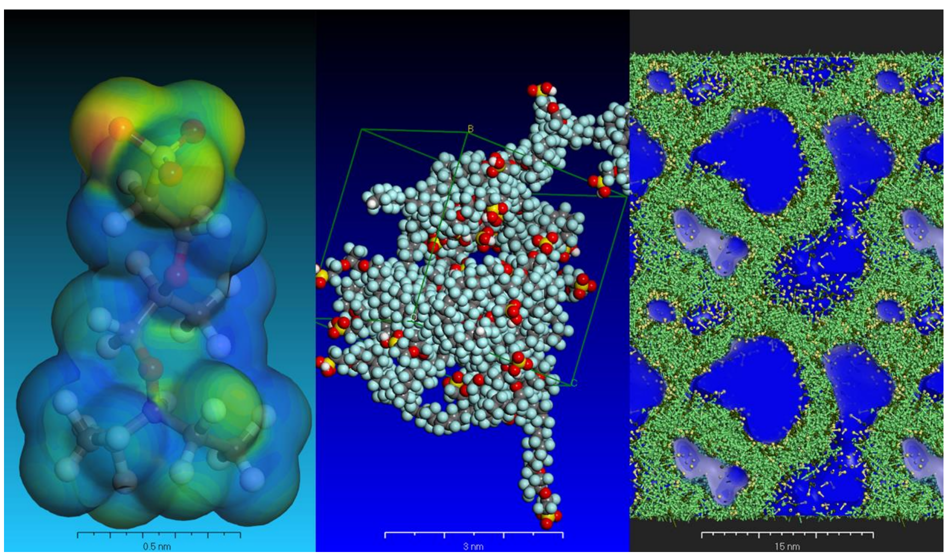
Materials Science: Changing the Face of the Next Generation of Makers

ARC Advisory Group

Next-Generation Composites are Changing the Auto Industry



Materials Simulation: Understanding the Building Blocks of Materials Properties

Executive Overview

Human history is intimately interwoven with the discovery and utilization of new materials. From stone to bronze to iron, each discovery catalyzed a significant advance in society, making new tools and technologies cheaper and more available. This is especially true today. New materials are modernizing everything from airplanes to smartphones. This creative churn has launched something of a global industry renaissance in materials science research.

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However, today's consumers demand continuous product improvement. Cars must drive farther using less gasoline, medical devices must become smaller and easier to manufacture, batteries must charge faster and last longer. But there are limits to what existing materials can provide. New technologies like additive or 3D manufacturing offer groundbreaking opportunities in product design, yet are restricted by the materials they can utilize effectively. Scientists and engineers must think outside the box and adopt novel materials and approaches to take on these challenges. What's missing to make this quantum leap forward is a thorough understanding of not only what materials could work, but also why they work. Technologies such as 3D materials modeling and simulation can nudge us toward this improved understanding.

Today's material science researchers are beginning to leverage 3D modeling and simulation to characterize bulk materials properties. By exploring their fundamental physicochemical interactions down to the subatomic level, they can gain an understanding of the material properties we can see and feel. Each interaction – from the wave functions that govern the movement of individual electrons to the interface stability of a resin and carbon fiber composite – begets the bulk properties we see. These models capture snapshots of these systems, helping researchers better understand how materials work in a relatively low resource environment. Armed with this knowledge, researchers can refine materials to fit the unique requirements of their projects to intelligently design the next generation of advanced materials and products.

Materials Science is Transforming Industry

New, high-performing substances from exotic alloys to super-strong composites underpin many of the industry-disrupting technologies of the past few years. As a result, companies face mounting pressure to create new, high-performing materials that can help them tackle today's greatest business challenges. These include developing modern transportation platforms, improved civil infrastructure, "smart" cities, and sustainable consumer products; dealing with harsh environments; and even exploring beyond our planet. Traditional research methods that rely on physical experimentation alone are struggling to keep pace with the shortening product lifecycles required to excel in our 21st century marketplace.

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Forward-looking manufacturers and advocates of nanotechnology envision the seamless integration of materials science into product design. Organizations that have adopted this philosophy are already advancing breakthrough technologies and new materials with novel applications. We're already seeing the effects of these technologies across the aerospace, automotive, industrial equipment, specialty chemicals, bulk petrochemicals, high-tech, and consumer packaged goods (CPG) industries. For example, aircraft manufacturers like Boeing and Airbus have introduced new airframe structures made almost entirely of carbon fiber composites that are strong, stiff, lightweight, and easy to manufacture.

Likewise, automotive companies are utilizing carbon fiber-reinforced thermoplastics to lighten the body of newer model cars. Precursor components can be heated, combined with resin, and injected into molds to form the components of the car body. Such techniques offer greater flexibility in body design while maintaining the strength required for passenger safety. Moving beyond traditional manufacturing techniques to additive manufacturing affords even greater flexibility in body design. New and recycled plastics create durable, aesthetically pleasing automobile components while also reducing noise, vibration, and production costs and improving fuel efficiency and sustainability. These and the other opportunities offered by additive manufacturing could significantly restructure the transportation and mobility industry as we know it.

In the same vein, new battery technologies are disrupting multiple industries. Beyond electric vehicles, which have already catalyzed a momentous shift in the automotive industry, consumers are placing increasing demands on personal electronics to keep pace with our increasingly digital world. Batteries must charge faster, last longer between charges, and offer extended lifespans. As a result, leading companies such as Samsung are exploring materials that improve upon traditional lithium-ion batteries. Lithium oxide batteries offer higher theoretical capacities and energy densities than their mass-market counterparts. However, they are also prone to shortened lifespan due to decomposition in their electrolyte formulations. To address this issue, Samsung is exploring hybrid organic-inorganic gelled electrolyte matrices that can improve electrochemical stability during cycling.[1] Such approaches demonstrate the promise advanced materials offer.

New Materials are Changing Industry, Products, and Society

Increasing demand for more advanced materials is driving researchers to explore unlikely sources of inspiration. Unconventional feedstocks, structures based on nature, and 2D materials provide the foundation for technologies such as flexible circuits for wearables, autonomous vehicles, and next-generation aircraft. Researchers will have to venture even further afield to answer today's most pressing materials science questions. Some examples of material science innovation that is having an immediate effect on industry include:

- **Carbon fiber composites**: Advances in carbon fiber composites are transforming transportation. Beyond lightweight structural components, which simplify construction and lower fuel use, composite materials improve the durability of aircraft like the Boeing 787 Dream-

[1] Kim H, Kim TY, Roev V, Lee HC, Kwon HJ, Lee H, Kwon S, and Im D. Enhanced Electrochemical Stability of Quasi-Solid-State Electrolyte Containing SiO_2 Nanoparticles for Li-O_2 Battery Applications. *ACS Applied Materials & Interfaces.* **2016**. 8 (2), 1344-1350. DOI: 10.1021/acsami.5b10214

liner, as carbon-based composites resist corrosion and impacts better than their metallic counterparts.[2]

- **Organic semiconductors**: The seemingly limitless variation available in organic compounds means that the work functions and electrical properties of novel molecular electronics can be "tuned" for specific applications, from OLEDs to solar cells to printable circuits.[3]

- **Catalysts for renewable fuels**: For decades, catalysts have streamlined the production of petrochemicals and fossil fuel-based energy. However, new catalysts offer the ability to split water into hydrogen and oxygen using only sunlight, potentially lowering the barrier to the economic production of clean burning, renewable fuel and energy sources.[4]

Advancing Materials Science Research for the 21st Century

The remaining question for materials scientists is "How do we effectively utilize the knowledge resources at our disposal to streamline the R&D process and advance science?" Physical experimentation alone is proving to be too resource-intensive to be economical. Some estimate as many as 40 percent of experiments are unnecessarily repeated because records are difficult or impossible to find. Likewise, new intellectual property can be poorly documented, creating the potential for hundreds of millions of dollars in legal damages.

A comprehensive software portfolio that digitalizes materials science research can help scientists better understand the properties that determine product performance such as loads, stresses, fluid dynamics, and thermodynamics. Software that helps them document and share this understanding has the potential to transform materials science R&D. Virtu-

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[2] https://www.boeing.com/commercial/787/by-design/#/advanced-composite-use

[3] Wrochem F, Gao D, Scholz F, Nothofer HG, Nelles G, Wessels J. Efficient electronic coupling and improved stability with dithiocarbamate-based molecular junctions. *Nature Nanotechnology*. **2010**. 5. 618-24. DOI: 10.1038/nnano.2010.119.

[4] Oshima C, Nishiyama H , Chatterjee A, Uchida K, Sato K , Inoue Y, Hisatomie T, Domene K. Photocatalytic activity of $ZnO/GaP_{1-x}N_x$ for water splitting. *Journal of Materials Chemistry A*. **2015**. 3. 18083-18089. DOI: 10.1039/C5TA04732C

al testing allows researchers to explore new ideas in a relatively low-resource environment. As a result, they can reiterate and optimize promising ideas intelligently while identifying those likely to fail earlier. Advanced analytics utilizes existing data to predict new courses of action. Centralizing knowledge management in a common electronic environment creates a shared knowledge base for researchers to track the development of new products. In effect, such a portfolio serves as a compass to guide materials R&D intelligently, pointing the way to the next breakthrough in materials research faster.

Virtual Testing via Materials Modeling and Simulation

Materials modeling and simulation provides the foundation for bringing materials science research into the 21st century. The few resources needed to build a model compared with physical experimentation allow researchers to explore a wider range of solutions to a given problem. Consider the "oxymoronic" nature of consumer goods research. A seemingly straightforward product like a laundry detergent must remove stains yet preserve colors; add fresh scents while eliminating unpleasant ones; and be strong enough to break down dirt yet safe enough for prolonged contact with skin. Each of these engineering contradictions is critical to the performance of the final product, yet also presents unique engineering challenges. Modeling and simulation allows these challenges to be examined down to the subatomic level.

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Due to the large variety of material properties, materials modeling must bring together a corresponding multiplicity of analysis tools to simulate and analyze mechanical and physical properties, from electronic and atomistic models to mesoscale models. Consider again the example of designing a laundry detergent: quantum mechanics simulations can explore the thermodynamic stability of the detergent ingredients; atomistic simulations can assess the surface and interface energies between the ingredients to predict miscibility; and dissipative particle dynamics can be used to evaluate their mesoscale structure and texture. Combining multiple approaches highlights different aspects of exploratory material formulation and thus builds the foundation for the *understanding* that scientists need to predict the properties of materials. Armed with this knowledge, they can better determine which materials (or combinations of materials) to test in the laboratory. In fact, virtual testing can (and should) precede and guide physical testing.

To achieve truly materials-based product design, researchers must at some point address the design of the structures and systems that will comprise the final product. As a result, numerical methods such as finite element analysis (FEA) can computationally determine the behavior of a completed part based on its shape and composition. Such computational approaches allow engineers to optimize the shapes and structure of new parts. Coupling this with modeling and simulation maximizes the use of materials developed upstream in the value chain. As a result, teams of modelers can attack design problems from multiple angles and collaborate to optimize parts and, eventually, systems without constructing a single physical prototype.

Materials Science Research, Artificial Intelligence, and Machine Learning

Modeling, simulation, and advanced analytics are excellent tools for transforming of data into knowledge, but that is only part of the story. Organizations must also manage this knowledge in such a way that it is available to all stakeholders across the product development lifecycle.

Beginning with the laboratory scientist's research, this process progresses through various lab teams for reviews and confirmations under the direction of lab managers who plan, assign, and schedule research activities. The process can generate a vast number of reports, reviews, models, and test results. Multiply this work by hundreds or thousands of separate material variations and the volume of data and knowledge quickly becomes enormous. Effectively sharing this knowledge among all participants at each point in the research process requires moving beyond siloed approaches and adopting a more digitalized approach using tools such as an electronic lab notebook (ELN).

With many disparate sources of information, only a centralized knowledge repository like an ELN can provide a common thread along the entire R&D lifecycle. By connecting all the research related to a given product in a unified, shareable environment, the ELN reduces much of the complexity and elucidates many of the interdependencies of product development. By providing traceability, the ELN establishes the chain of intellectual property development. It collects and connects all scientific, engineering, testing, standardization, certification, and manufacturing data in a single place, creating a knowledge base for every organization's most powerful asset, its people.

The Dassault Systèmes Portfolio for Materials Science

Dassault Systèmes leverages an extensive portfolio of scientifically-aware software, providing end-to-end support for advanced biological, chemical, and materials R&D. This would include the BIOVIA Materials Studio, a complete modeling and simulation environment designed to allow researchers in materials science and chemistry to predict and understand the relationship of a material's atomic and molecular structure with its properties and behavior. Its portfolio for scientific informatics captures each of the critical capabilities needed to advance materials science, from its comprehensive materials modeling and simulation environment and powerful framework for data science to its user-friendly, cloud-enabled ELN. Engineers can also simulate the performance of parts at the macroscale based on their structural and material properties. Each of these products provides a critical piece needed for the creation of a scalable portfolio for materials science research in the 21st century.

Driving the Global Industry Renaissance

As science- and process-based industries move into the era of advanced manufacturing, they are embracing emerging technologies that will drive the next generation of materials and products. As organizations assume greater responsibility for this end-to-end, "idea-to-product" lifecycle, they also exert greater control over new materials performance. Today's industry leaders must consider the energy, environmental, and health effects at every stage of materials development from extraction to production and recycling or disposal.

Powerful materials science modeling and simulation tools along with unified laboratory solutions like the ELN are transforming scientific data into valuable knowledge of unprecedented depth, breadth, and applicability.

Fortunately, the days of trial and error in materials testing are over. Powerful materials science modeling and simulation tools along with unified laboratory solutions like the ELN are transforming scientific data into valuable knowledge of unprecedented depth, breadth, and applicability. Most importantly, organizations can now leverage a unified informatics platform to move from document-based, siloed research to a data-centric, model-based work environment that combines multi-physics, behavior modeling and big data augmented by AI and ML.

The ever-advancing power of digitalization makes these research and development capabilities available to manufacturers of all sizes. New production processes such as 3D printing transform both the products and economies of manufacturing. Combining real and virtual knowledge and know-how is changing the face of materials science and driving the global industry renaissance of the 21st century.

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Acronym Reference: For a complete list of industry acronyms, please refer to www.arcweb.com/research/pages/industry-terms-and-abbreviations.aspx

API Application Program Interface
B2B Business-to-Business
BPM Business Process Management
CAGR Compound Annual Growth Rate
CAS Collaborative Automation System
CMM Collaborative Management Model
CPG Consumer Packaged Goods
CPM Collaborative Production Management
CRM Customer Relationship Management
DCS Distributed Control System
EAM Enterprise Asset Management
ERP Enterprise Resource Planning
HMI Human Machine Interface
IOp Interoperability
IT Information Technology
MIS Management Information System
OpX Operational Excellence
PAS Process Automation System
PLC Programmable Logic Controller
PLM Product Lifecycle Management
RFID Radio Frequency Identification
ROA Return on Assets
RPM Real-time Performance Management
SCM Supply Chain Management
WMS Warehouse Management System

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