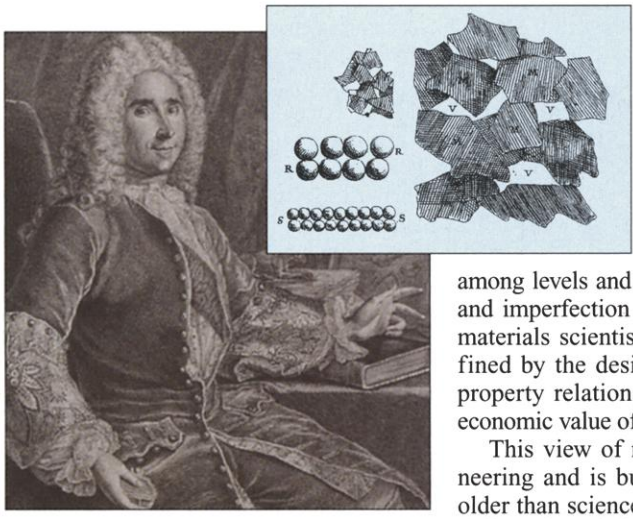
Designing a New Material World

Gregory B. Olson

Materials have paced the evolution of technology for millennia. Their importance in the advance of human civilization is apparent in the naming of historical epochs, from the Stone Age through the Bronze and Iron Ages and into the ongoing Silicon Age. The origin of diversity in the material world remains largely mysterious to the public, yet the specialists' ability to understand and manipulate the microstructures of materials has grown explosively over the past half-century. As the new millennium unfolds, a confluence of natural philosophies—one that combines reductionist and synthetic thinking—is ushering in an Age of Design marked by new materials and ways of creating them that go beyond the dreams of the medieval alchemists.



Materials savant. René de Réaumur and his 1722 sketch of steel's anatomy.

Materials as Systems

The modern view of materials structure was best expressed by the late philosopher-scientist Cyril Stanley Smith *(1)*. He described a universal multilevel nature of structure with strong interactions among levels and an inevitable interplay of perfection and imperfection at all levels. Smith argued that the materials scientist's distinct view of structure is defined by the desire to understand the structure and property relations underlying the technological and economic value of materials.

This view of matter integrates science and engineering and is built on a natural philosophy that is older than science. Smith identifies the origin of this philosophy within medieval alchemy, whose practitioners are mostly remembered for their attempts to "transmute" base metals into gold. They knew nothing about protons and electrons. Still, Smith asserts that their aspirations, motivations, and even concepts resembled the modern materials engineer's use of complex processing to "transmute" the multilevel microstructure of materials (from the atomic to macroscopic levels) to achieve the essential property of gold, namely, economic value.

The property-driven view of structure and processing for the creation of value, shared by modern materials science and alchemy, embraces an essential complexity of material structure. During the 17th century birth of modern science, Smith identifies a short-lived Golden Age of materials science under the leadership of René Descartes, whose "corpuscular" philosophy inspired the development of a multilevel view of structure to account for the diverse properties of materials.

The prescient grasp of materials achieved by the corpuscularians is well represented by René Antoine Ferchault de Réaumur's 1722 sketch of the structure of quench-hardened steel (see figure above). He proposed that a single grain of steel (G), if enlarged, would reveal a set of "molecules" (M) and voids (v). Higher magnification would reveal a substructure of the molecules (pp); and yet higher magnification would show an aperiodic arrangement of spheres. The finest scale Réaumur envisioned corresponds to a periodic packing of spheres, what we might think of as the nanoscale.

This elegant view contained many structural elements of modern materials science. There was no instrumentation with which to validate it, however, so the complex structural view was supplanted by more intellectually compelling but overly simplistic notions. One was Isaac Newton's continuum, which erased structural considerations entirely. The other was John Dalton's atomism, which held that there was only one level of structure that mattered. These conceptual idealizations were sufficiently compelling to divert the corpuscularian framework for 2 centuries.

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A Materials Science Timeline

1556
Georgius Agricola's *De re metallica*, a compendium of 16th century mining, metallurgical, and general materials production, is published.

1664
Cartesian corpuscular philosophy recognizes material properties as emerging from a multilevel structure.

1665
Robert Hooke publishes *Micrographia*, which reveals levels of material microstructure never before seen.

1722
René de Réaumur publishes the first technical treatise on iron.

1782
Josiah Wedgwood develops an early form of process control with his invention of the pyrometer for measuring furnace temperatures.

1808
John Dalton publishes his *New System of Chemical Philosophy*, which establishes atomic theory.

1824
Joseph Aspdin invents portland cement, which remains one of the most used materials in the world.

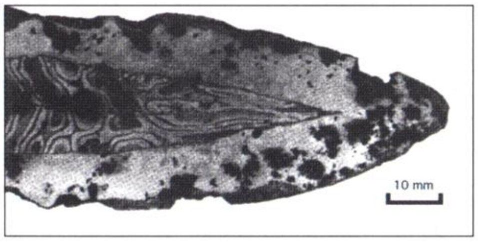
1839
Charles Goodyear accidentally discovers vulcanization, which ultimately renders raw rubber latex into a widely useful material.

1856
Henry Bessemer patents a process for large-scale steel production.

We have had the past century to reinvent materials science. The atom and the continuum remain dominant philosophical forces; they are the foundation of existing theoretical tools. But armed with the growing reservoir of structural facts gleaned from instrumentation and computation, the challenge now is to adapt these theoretical tools to understand and control the complex structures of real materials.

The modern view of material structure differs from Réaumur's mainly in the detailed morphologies characteristic at the different length scales of a material's hierarchical structure. In the case of steel, the most significant difference is the overestimation of porosity in the 18th century depictions. And if Réaumur's voids are reinterpreted as "free volume," his sketch becomes a reasonable model of polymeric materials. It shows the remarkable ability of the human mind to infer necessary structure from the contemplation of properties alone.

Smith made another important historical observation about materials development *(2)*. Since prehistory, people have put newly discovered materials to practical use long before they understood much about them.



Cutting edge. Etched and repolished tip region of a 6th century sword.

Consider the pattern-welded sword blades made and used by Merovingian Franks and Vikings (see figure above) as early as the 6th century A.D. By hammer-welding steels of differing carbon content (a technical feature unknown to the early sword smiths), a laminate composite was fabricated by labor-intensive "hand lay-up" to produce a hybrid structure with a tough core supporting a hard cutting edge.

The actual mechanism of the quench hardening of steel, which is responsible for the hardened sword edge, was hotly debated even in the early 20th century. There were two factions: the "allotropists," who favored structural transformation, and the "carbonists," who pegged the hardening mechanism on dissolved carbon. A crucial observation was the discovery by Floris Osmond in 1893 of "martensite" in steel, the microstructural form that iron assumes during the quenching process. We now know that the combination of a martensitic transformation and the redistribution of trapped interstitial carbon (along with ambient aging during which additional microstructural evolution occurs) underlies the edge hardness of the 6th century swords.

The ancient swords embody another illustration of how art and craft has traditionally preceded science. The sword smiths' use of chemical etching to bring out aesthetic metallic patterns set the foundation for modern metallographic observation of microstructure established by Henry Sorby in the 19th century. By etching metal samples with acid, Sorby revealed internal microstructures and correlated them with the properties and performance of the materials.

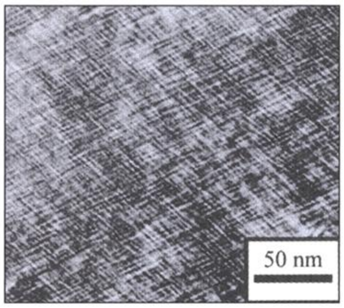
Transmission electron microscopy (TEM), a modern analytical cohort of metallography that reveals finer structural levels (see figure at right), suggests that the ancient swordmakers ever were accidental nanotechnologists. TEM analysis reveals nanometer-scale patterns of carbon in the hard edge of the sword. These patterns emerged from a process called "spinodal decomposition", in which a solid solution, such as the sword's high-carbon martensitic steel, becomes unstable and its constituents reorganize *(3)*. In modern parlance, the swordmakers' products could be described as "self-assembled heterophase nanostructures."

The spatial dimension of materials is only part of what makes them tick. There is a spectrum of characteristic relaxation times associated with the various chemical and physical processes operating at the material's differing structural length scales. This adds the dimension of time.

The resulting dynamic spatiotemporal hierarchy means that any material at any time has structural features, such as grain sizes and dispersed particles, that have not yet reached equilibrium. That is why a material's structure and properties depend on how it was made and what conditions it endured in service.

Also fundamental to this dynamic view of materials is a realization that structural defects play vital roles at all length scales. Defects can make things fail in a thousand ways, but they're also often what makes materials so valuable. Perfect silicon crystal without dopant ions is not the semiconductor that has changed society. Pure iron metal without the right spicing of carbon would never have become the steel backbone of the industrial revolution. Although "defect tolerance" remains a central tenet of modern materials science and is of incalculable commercial and safety importance, "defect engineering" is ascendant in the minds of many materials researchers. That's because defects on various hierarchical levels are a principal opportunity for controlling material behavior.

Because the personality of each material depends on all of these interacting spatial and dynamic attributes, it makes sense to approach materials as complex systems. Smith advocated such a systems view of materials decades ago. As more contemporary practitioners live by that insight, they are finding pathways to important new materials that can catalyze advances in manufacturing tools, computers, communications systems, and the myriad technologies whose very existence or improvement depends on more capable materials.



Inside steel. TEM reveals nanoscale structure of a quench-hardened steel.

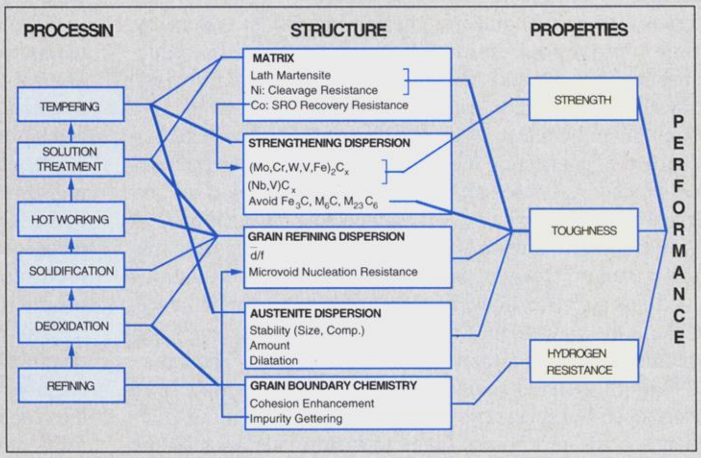
The Materials Discipline Comes of Age

Two principal branches of natural philosophy have evolved to form modern materials science. One is reductionist analysis, which takes nature apart to discern and understand its fundamental units. Reductionism has operated throughout the development of science. More sporadic has been the evolution of the synthetic systems view, which is better suited for understanding the connections holding nature together. In a new balance of these two philosophies, the systems view integrates the fruits of our investment in reductionism while replacing conventional discovery-based R&D with a far more effective and efficient design-based approach.

CREDITS: (TOP) *DE RE METALLICA*; (MIDDLE AND BOTTOM) G. B. OLSON

Materials by Design

To design a material is to try to meet a material user's need. A good place to start is with property cross-plots, like those of Michael Ashby, that graphically define property-performance relations *(12)*. These help engineers select materials for their product designs. They're useful for defining a quantitative set of property objectives that will sum into the materials performance needed by users. These performance specifications are determined by the role of the potential material in the wider system it serves. They also help define economic parameters, such as the cost of raw materials and processing, for the overall material design task.



Planning materials. Flow-block diagrams guide materials design.

With objectives and economic constraints defined, the linear three-link framework of materials science and engineering (see figure, p. 996) serves to guide the design and development phases. The Steel Research Group (SRG) (see main text) uses flow-block diagrams that represent 1) key microstructural subsystems (such as crystal grain sizes), 2) the primary links of these subsystems to the properties they control (such as strength and toughness), and 3) the stages of processing (such as tempering or reheating) that govern their dynamic evolution.

With these in hand, systems analysis is then applied to identify and prioritize key structure-property and processing-structure relations. Often, part of this exercise involves some additional modeling or empirical data gathering to fill gaps in the knowledge required for making practical decisions about composition and processing details. The systems view operates here at the strategic level, but it is supported by traditional reductionist analysis at a tactical level. On balance, the procedure greatly reduces the amount of costly experimentation in materials creation. Instead of making tens of prototypes along the way to a useful new material, SRG designers reach their target metal using only a few actual melts to refine the computation-heavy design efforts.

–G.B.O.

Although there were seeds of this turning point in materials science in early industrial laboratories at General Electric, Bell Labs, and elsewhere, the multifaceted field of materials research was deliberately synthesized as a single academic discipline in the late 1950s and 1960s with the founding of the first university materials departments *(4)*. Specialists in the science and technology of metals, ceramics, polymers, and composites collaborated in pursuit of unifying principles for the creation of materials of all classes. This meeting of minds helped lay the sociological and cognitive groundwork for a systems approach to materials.

The development of operations research in World War II and large-scale national missions such as the Manhattan Project and the Apollo space program were also important. It is estimated that at least 70% of our unprecedented economic boom of the past decade derives from technology, which in turn derives in good part from radically improved productivity via new systems-based methods of product development.

After World War II, newly formed government agencies, including the Office of Naval Research, the Defense Advanced Research Projects Agency, the National Science Foundation (NSF), and others also helped midwife the multidisciplinary sensibility needed for developing complex materials. The same was true in academe. Starting with Smith's Institute for the Study of Metals at the University of Chicago, a series of university materials research laboratories established a national infrastructure for the interdisciplinary enhancement of materials science. The private sector added sociological foundations for the emerging discipline through a diverse mix of professional materials societies, as well as the establishment of numerous materials-centered journals and conferences.

The field now consists of many thousands of practitioners who share a growing sense of community, yet whose collective expertise runs a stunning gamut of materials categories. There are synthetic diamond makers, metal alloy designers, polymer scientists, optical fiber experts, thin film ceramic makers, developers of compound semiconductors, and "biomimetic" materials researchers who aim to emulate or adapt biology's unmatched brilliance in materials innovation. The list goes on and on, with a diversity akin to the living kingdom's millions of species.

Over the past 4 decades in materials R&D, however, there has been a consistent emphasis on "good science," as defined by reductionism, rather than "good materials," which emerge when engineering, manufacturing, and economic factors are included in the mix. This bias has limited the technological impact of the materials science community, particularly the academic portion. And materials engineering per se has been left primarily to industry, which has yet to fully benefit from the expanded base of materials science.

There is a twist in store. The science of materials has reached a level at which it now can radically change engineering practice. The possibilities are akin to what has come from the relationship between the life sciences and medicine. Until the 19th century, there was little or no science to guide medical technology and practice. Since then, however, the ever growing corpus of biomedical knowledge has been leading to an ever more amazing stream of health care innovations. Here, a genuine desire to meet societal needs has produced a healthy mix of reductionist and systems viewpoints, yielding a culture that naturally integrates scientific understanding into practical use. The materials research community is poised to emulate this model.

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1860s
Henry Sorby applies light microscopy to the study of the microstructure of metals and rocks.

1869
John Hyatt successfully commercializes celluloid, an artificial plastic material.

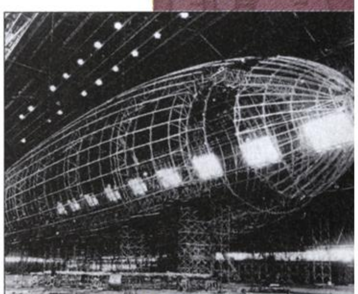
1869 and 1870
Dmitri Mendeleev and Julius Lothar Meyer publish versions of what will become known as the Periodic Table of the Chemical Elements.

1886
Charles Hall and Paul Héroult independently discover cost-effective methods for producing aluminum metal from ore.

1893
Floris Osmond discovers martensitic transformation.

1900
Max Planck formulates the idea of quanta, thereby setting the stage for the development of quantum mechanics.

1906
Alfred Wilm discovers age hardening in aluminum alloy, which is later used for making dirigibles and other aircraft.



1909
Leo Baekeland patents Bakelite, the first entirely synthetic plastic, and commercializes it widely.

1911
Heike Kamerlingh Onnes discovers superconductivity in mercury chilled to temperatures near absolute zero.

1911–12
The father-son team of William Henry and William Lawrence Bragg, along with Max von Laue, develops the basis of x-ray crystallography, one of the most important analytic techniques for studying material structure.

1921
A. A. Griffith postulates role of defects in fracture strength.

Late 1920s
Hermann Staudinger argues that polymers are made of small molecules that link to form chains.

1934
Wallace Hume Carothers invents nylon.

1940s
The wartime practice of organizing multidisciplinary research collaborations to achieve technological goals becomes a model for the subsequent organization of a field that later becomes known as materials science and engineering.

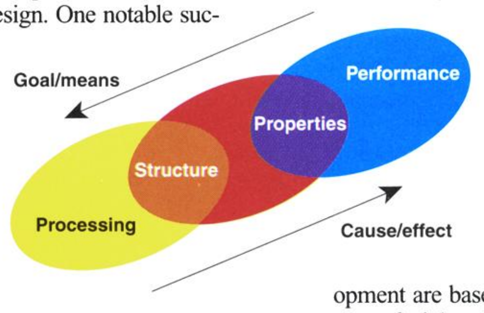
1947
John Bardeen, William Shockley, and Walter Brattain invent the transistor.

Materials by Design: Efficient Innovation

There is a general engineering design movement under way. It draws on the vast information pool generated by reductionist analysis, but adds the component of design, for which the systems approach is crucial.

Central to the materials design approach is a powerful logical structure connecting the "four elements" of materials science: processing, structure, properties, and technological performance (see figure below). By connecting adjacent pairs of these elements, a three-link chain representing a versatile materials paradigm emerges. The deductive, cause-effect logic of reductionist science flows from processing to performance. All along the way, science reveals the relevant structures and phenomena, often in astounding clarity and detail. The inductive logic of systems engineering flows the other way, from performance to processing, thereby enabling designers to arrive at specific procedures likely to yield materials with the desired sets of properties and performance.

Not often successful in terms of producing useful new materials, early efforts at materials design nonetheless were harbingers of what materials development is to become. Generally, what has made or broken past efforts was whether they included the element of design. One notable success is the work of H.K.D.H. Bhadeshia and co-workers at Cambridge University, whose ambitious assault on the complex problem of weld metal design has spawned productive efforts at several national laboratories in the United States and Japan.



Big four. Four-element paradigm of modern materials science and engineering.

The initiative I know best is the Steel Research Group (SRG) at Northwestern University, which my colleagues and I have continuously developed since 1985 *(5, 6)*. This university-industry-government program was organized within the context of systems engineering to explore general methods, tools, and databases for the design of materials, using high-performance steels as a test case (see sidebar on p. 995). There is a faith underlying this framework: The scientific knowledge base is now robust enough to supplant the traditional, empirically driven development of materials with a more efficient theory-driven and computationally based approach (see sidebar on p. 997).

In the SRG, we begin by combining the perspectives of materials users, suppliers, modelers, and designers into a set of specific materials property objectives. Those specifications, in turn, help us define how to use, adapt, or expand science-based models and databases of material behavior. We then use these models and databases to zero in on compositions and processing protocols that can transform those compositions into alloys fitting our specifications. In the past decade, we have used this framework to develop new alloys with unprecedented sets of properties. Some are now under evaluation by industrial and government partners for use in airplanes, power generators, aircraft carriers, and other applications.

Our own projects for designing steel are just a beginning. A recent NSF-sponsored workshop on Materials Design Science and Engineering *(7)* has called for broadening this approach to the design of all classes of materials. And in recognizing materials as one of five critical technologies for U.S. competitiveness, the President's Office of Science and Technology Policy *(8)* has identified computational materials design as a principal opportunity.

Opportunities abound for application of the new systems-driven computational design approach. Successful examples from our efforts include a stainless steel bearing for a space shuttle application, high-strength, high-toughness steels for aircraft landing gear and armor applications, and a new class of ultrahard steels for advanced gear and bearing applications. The more general validity of the design approach has been explored with computational design projects focusing on nonferrous alloys, hydrate ceramics, case hardening polymers, and nanostructured thin film materials for microelectromechanical devices and hard coatings.

The new design capabilities will also help realize the dream of biomimetic materials, which emulate the complex adaptive microstructures of the living world that are beyond the reach of traditional empirical development. One successful demonstration is self-healing metallic composites. These incorporate "shape memory" alloys that exploit martensitic structural transformations to change their shape controllably. Integrating such components into thin film electronic devices to create efficient microactuators is leading to smart materials systems that unite the worlds of structural and electronic materials. Here the growing philosophy of predictive materials design is now combining the electrical engineer's realm of perfection-driven, artificially structured microcircuits with the materials traditions of self-assembly *(9)* and defect tolerance *(10)*.

Following the same philosophy can reduce the cost of discovery. In contrast to computational materials design, the prevalent industrial methods of materials development are based on an intrinsically slow and expensive process of trial-and-error empiricism. Theoretical input has been qualitative at best. It typically takes tens of millions of dollars over 2 decades to fully develop and qualify a new material in a critical application *(11)*. This sluggishness stands out in an era when engineers are expected to deliver new generations of products, such as automobiles, on an 18-month cycle. What's more, under these competitive pressures many industrial materials-development groups have been severely reduced or closed over the past decade. A recent National Research Council study *(11)* has concluded that the greatest challenge to the materials field today is the short time and cost constraints of the full materials development cycle.

Another reason these industrial materials development efforts have been downsized is anchored in the old R&D model in which new materials are discovered rather than designed. A typical estimate is that $1 of discovery costs $10 of development. If eliminating that first dollar was the only advantage of computational materials design, its impact on the total discovery and development cost would be small. The real advantage of materials design is that good design in the first place requires much less development later. And rather than using materials design approaches simply to provide an initial prototype for subsequent empirical development, there's yet more to be gained by integrating predictive modeling throughout the full design and development process.

Consider two costly and time-consuming phases of the standard materials development cycle: process optimization and qualification testing. A major concern in process optimization is scale-up. Because processing phenomena such as heat transfer depend on product size, a prototype material investigated on a small scale is not likely to behave the same way when processed on a large scale. "Solidification design" can preempt

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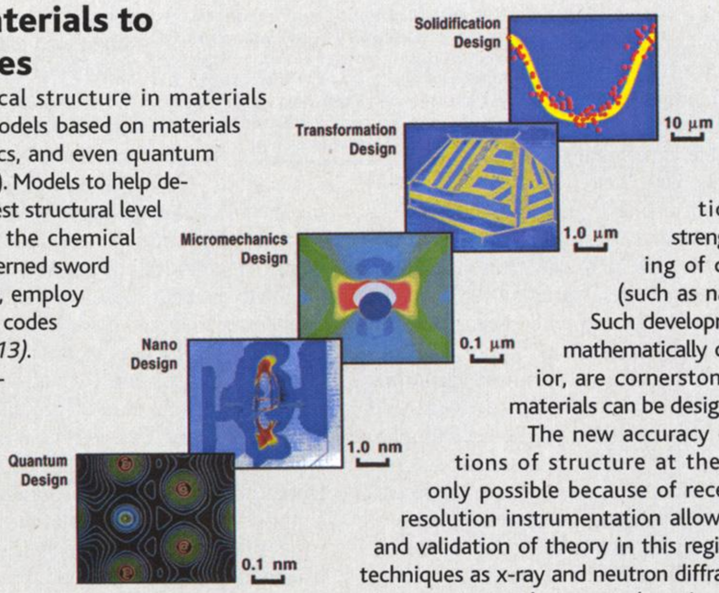
Virtualizing Materials to Create Real Ones



Model relay. Computational design of materials requires a hierarchy of models.

Design of the hierarchical structure in materials requires a hierarchy of models based on materials science, applied mechanics, and even quantum physics (see figure at right). Models to help design features on the coarsest structural level of solidification, such as the chemical banding visible in the patterned sword blades mentioned earlier, employ powerful thermodynamic codes such as THERMOCALC *(13)*. These models enable designers to simulate the 10-μm scale of structure. In metal alloys, this is the level at which the chemical partitioning between liquid and solid phases evolves during solidification processing. Application of these models aids decision-making about thermal processing details, a practice we like to call "solidification design."

At the 1.0-μm scale of structure, "transformation design" is the goal. This concerns the evolution of structural changes during quenching, whereby crystal grains present at high temperatures transform and subdivide as the hot alloy cools into a hierarchy of lower temperature crystalline units. The design goal here is to specify and control processing temperatures so that desirable microstructures will form, while hindering the formation of competing microstructures that are less beneficial.

The 0.1-μm scale represents the micromechanics design level. An example of the phenomena relevant at this scale is "grain refining," in which the large grains formed at high temperatures that can embrittle alloys are made smaller by more precise thermal or compositional control. There's a trade-off here, because more smaller particles can also catalyze ductile fracture (breaking, that is), as there are more interfaces that can separate from one another. Micromechanics models typically are based on continuum descriptions of mechanical phenomena that can simulate the evolution of microstructures during material deformation and fracture.

In recent years, an even finer structural level—the nanoscopic level—has become better understood and more controllable. The control of 1-nm-scale particle dispersions in alloys created through solid state precipitation during "tempering" at intermediate temperatures, for example, provides efficient obstacles for resisting plastic deformation. Said differently, this nanometer-scale structuring strengthens the metal.

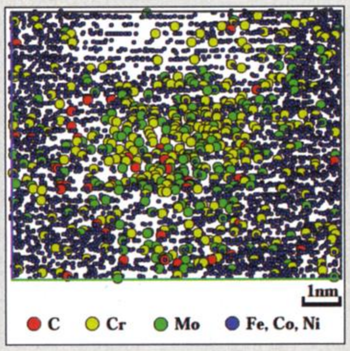
The development of design models for these diminutive scales builds on a half-century evolution of theory for both precipitation and strengthening in metals. A major materials science breakthrough of the 1950s was the identification of dislocations as the key defects that enable the sliding of crystal planes, which shows up as plastic deformation of many materials. While most structure-property relations, such as the Hall-Petch relation for grain refinement strengthening, are based on empirical correlations, a major triumph of the 1960s was the Orowan particle strengthening equation. Derived directly from dislocation theory, it relates strength to the inverse spacing of dislocation obstacles (such as nanoscale precipitates). Such developments in theory, which mathematically codify materials behavior, are cornerstones for the claim that materials can be designed largely in silico.

The new accuracy of theoretical predictions of structure at the nanometer scale is only possible because of recent advances in high-resolution instrumentation allowing precise calibration and validation of theory in this regime. This includes such techniques as x-ray and neutron diffraction, various electron microscopies, and atom-probe microanalysis. The latter is represented by the three-dimensional atomic reconstruction of a 3-nm strengthening carbide particle in an ultrahigh-strength steel shown below. Such new capabilities in structural and chemical analysis down to the atomic scale open a new era of quantitative materials nanotechnology.

The electronic level is the finest level relevant to real materials. This is the realm of quantum design. As acknowledged by the 1998 Nobel Prize in chemistry shared by John Pople and Walter Kohn, the development of computational quantum mechanics and its extension via density functional theory constitute a profound advance that already has had significant industrial impact. A collaboration of materials science, applied mechanics, and quantum physics has enabled some of us in the Steel Research Group (see main text) to apply computational quantum mechanics to engineer steel at the subatomic level.

Our approach was to recast models of the impurity-induced embrittlement of grain boundaries into thermodynamic terms *(14)* and to rely on precise models of the atomic structures at grain boundaries. As represented by the computed valence charge density contours for a phosphorus atom at the core of an iron grain boundary, total energy calculations are sufficiently precise and accurate to explain the known effects of interstitial components such as boron, carbon, phosphorus, sulfur, and hydrogen on the cohesion of iron grain boundaries. What's more, the calculations lead to new mechanistic insights at the electronic bonding level. Extension to elements that occupy substitutional Fe sites in the boundary has enabled us to predict new alloying elements for enhancing boundary cohesion in steels. This is creating a new generation of "quantum steels" that incorporate these properties derived directly from electronic-level predictions.

—G.B.O.



Atomscapes. A view of a Cr-Mo carbide particle that strengthens steel alloy.

1950s to 1960s
Much of the theoretical foundation behind the formation and evolution of material microstructure is developed. Among them is the Hall-Petch relation for grain refinement strengthening and the theory of diffusion of solids.

1953
Karl Ziegler develops catalysts that make it easier and cheaper to polymerize ethylene into stronger, more capable polymers.

1955
A team of scientists at General Electric combine high temperatures and enormous pressures to create synthetic diamond.

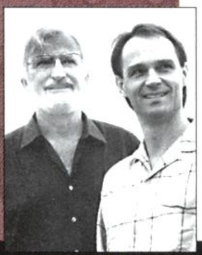
1957
John Bardeen, Leon Cooper, and John Schrieffer provide theoretical basis for superconductivity, discovered in 1911.

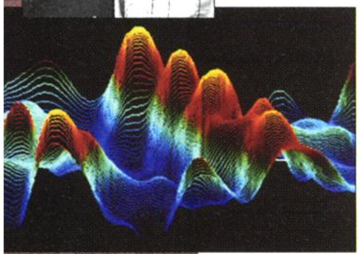
1959
The U.S. government funds the first IDLs, or interdisciplinary laboratories, which mark a beginning of the modern academic model of materials science and engineering.
J. W. Cahn and J. F. Hilliard develop theory of microstructural evolution in diffuse-interface systems.

1970
Researchers at Corning develop optical fibers transparent enough to make fiber optic communication practical.

1974
A study by an NAS committee, COSMAT, defines field of materials science and engineering, creating a community sensibility.

1980
Gerd Binnig (right) and Heinrich Rohrer (left)

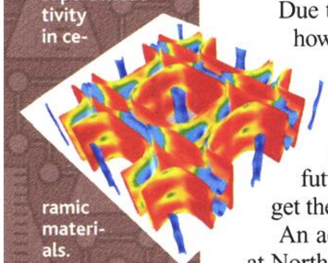




invent scanning tunneling microscopy, which has led to a family of imaging tools often capable of molecular- and atomic-scale resolution.

1985
First university "materials by design" initiatives attempt computational materials design.

1986
K. Alex Müller and J. Georg Bednorz discover high-temperature superconductivity in ce-



ramic materials.

1990s
The field of materials science and engineering begins shifting into a more systems-based approach to materials innovation and toward materials design in which researchers can predict new materials they would like to have rather than having to discover them.

this common showstopper. By using models that simulate how materials respond to processing conditions for designing a material at the ultimate process scale of interest, we can reduce the number of expensive large-scale experiments while shortening the development cycle.

Improving qualification testing is more challenging. To design with confidence, designers must know how properties vary within the materials they intend to use. Current practice requires much testing to define these variations statistically. But most structure-property theories provide mean values of the variables of interest; they do not tell a designer about location-to-location variations within materials.

Help is coming, however. Researchers are developing a probabilistic materials science whereby structural distributions are mapped into property distributions. These are the kinds of data designers can use to make better predictions about how different materials will affect their products. Models of this kind already exist for fracture properties and heterogeneous phase transformations, and more efforts are being planned for this vitally important area.

Structure of Education

Education offers the most leverage for moving materials R&D into the systems-based paradigm. In its post-Cartesian form, modern metallurgy began with an emphasis on the direct correlation of processing and properties. The advent of physical metallurgy a century ago opened the "black box" of structure and brought a revolution in the fundamental understanding of the mechanistic link between processing and properties. This understanding created the foundation for the more recent generalization to materials science, making possible the general materials design and systems engineering methodologies described in this essay. Given the demonstrated potential of materials design, institutionalizing it via education would result in many benefits to society.

Due to the historic dominance of reductionist philosophy, however, we now have in place an analysis-oriented education system. In the name of objectivity, we train students to shut down the more synthetic and emotional tools of thought, which are precisely the ones best suited for doing good systems engineering. The future of engineering education, therefore, ought to target these subjective reasoning powers.

An activity of our new materials engineering curriculum at Northwestern, the Dragonslayer Project, is designed to do this. The project explores the design of an "aesthetic" material through collaboration of freshman and upperclass design teams. The widespread presence of Western dragon combat in literature is used to integrate frontier steel technology with the history and legend of swordmaking to design an ultrahigh-performance sword that our market analysis shows would be of maximum value to sword collectors.

Much of the mystique of the legendary Samurai sword, which even 5 centuries ago achieved performance levels equivalent to those of a modern carburized blade, stemmed from its ability to cut through other swords of the day. The equivalent performance advance has been adopted as a benchmark for property requirements.

Fanciful as the project might seem, it's no different from the kind of materials design that goes on at the DuPonts and Cornings of the world. Searches of literature, albeit medieval literature, were used to determine technical specifications, including the need for flame resistance when fighting fire-breathing dragons. Historians of the Dark Ages helped to identify and select a historically accurate sword style—the patterned double-edge broadsword. And market analysis helped determine what the target buyers, sword collectors, would be willing to buy and how much they might pay.

Finite-element mechanics simulations of cutting through a modern carburized blade led to a conceptual design for radical surface-hardening technologies to achieve this ambitious sword-cutting objective. We also were guided by the unlikelihood that anyone would face supernatural evil armed only with technology. This led to an additional design parameter, which market surveys indicated would constitute an important attribute in a collectible dragonslaying sword: The sword should be made from material of heavenly origin, namely, meteoritic iron. This is a technical feature with historical and legendary precedent (including the Excalibur legend).

Our systems approach to materials design has established the feasibility of using tabletop-scale aqueous electrolytic refinement of available meteoritic iron to achieve the necessary purity for producing the unprecedented alloy steel performance needed for a sword fit to defeat the most evil of adversaries. The freshman design team's proposed market plan includes auctioning a single "techno-mystical" sword for publicity, followed by commercial marketing of a range of high-performance steel products, including the "Dragonslayer golf club."

In this millennium, a new architecture of synthetic thought will continue its symbiosis with modern computational capabilities. And an age of empirical exploration will continue to be superceded by an Age of Design. This will open up powerful pathways by which human creativity, fused with scientific knowledge, will bring new levels of control over the material world widely applicable both to society's problems and its ambitions. The manifestation of the design paradigm, whether in an undergraduate or corporate setting, corresponds to a form of transmutation beyond the alchemist's dreams: the creation of materials from thought.

References

1. C. S. Smith, *A Search for Structure* (MIT Press, Cambridge, MA, 1981).
2. C. S. Smith, *A History of Metallography* (MIT Press, Cambridge, MA, 1988).
3. K. A. Taylor *et al.*, *Metall. Trans.* **20A**, 2717 (1989).
4. I. Amato, *Stuff: The Materials the World Is Made Of* (Basic Books, New York, 1997).
5. G. B. Olson, M. Azrin, E. S. Wright, Eds., *Innovations in Ultrahigh Strength Steel Technology*, Proceedings of the 34th Sagamore Army Materials Research Conference, 1990.
6. G. B. Olson, *Science* **277**, 1237 (1997).
7. D. L. McDowell and T. L. Story, "New Directions in Materials Design Science and Engineering," National Science Foundation Workshop Report, Georgia Institute of Technology Materials Council, Atlanta, GA, 1999.
8. "New Forces at Work: Industry Views Critical Technologies," 4th Office of Science and Technology Policy Report on Critical Technologies, February 2000.
9. G. M. Whitesides, J. P. Mathias, C. T. Seto, *Science* **254**, 1312 (1991).
10. S. Williams, *Technol. Rev.* **102**, 92 (September/October 1999).
11. D. Stein, *MSE: Forging Stronger Links to Users* (National Research Council, Washington, DC, 1999).
12. M. F. Ashby, *Materials Selection in Mechanical Design* (Pergamon, Tarrytown, NY, 1992).
13. L. Kaufman and H. Bernstein, *Computer Calculation of Phase Diagrams* (Academic Press, New York, 1970).
14. J. R. Rice and J.-S. Wang, *Mater. Sci. Eng.* **A107**, 23 (1989).

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