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The Impact of Supercomputing Capabilities on U.S. Materials Science and Technology (1988)

Committee on Computer Simulation and Analysis of Complex Material Phenomena; National Materials Advisory Board; Commission on Engineering and Technical Systems; National Research Council

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The Impact of Supercomputing Capabilities on U.S. Materials Science and Technology

Report of the

Committee on Computer Simulation and
Analysis of Complex Material Phenomena

National Materials Advisory Board
Commission on Engineering and Technical Systems
National Research Council

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Abstract

A committee was formed under the auspices of the National Academy of Sciences to identify areas of materials science and engineering where a major impact might be realized, resulting from the emergence of supercomputer technology. The committee was broadly based, representing universities, industry, and national laboratories in the related fields of materials science, chemistry, and physics. A workshop provided experts from a wide variety of disciplines to aid in uncovering possible opportunities.

Not surprisingly, a great number of examples of exciting individual computational science were easily identified: Atomistic and electronic structure calculations on metals, semiconductors, and polymers; statistical mechanical studies of alloy phase diagrams; and fundamental modeling of fracture and deformation in metals, ceramics, and glasses are among those that are vigorously utilizing supercomputer technology. Not so immediately obvious were the cases where a hierarchical approach is being applied to solve a complex problem. Electronic structure effects on a scale of angstroms are being coupled with microstructural aspects on a scale of micrometers, and these are further coupled to continuum effects on a scale of centimeters. These complexities require the multidisciplinary efforts of materials scientists, chemists, physicists, metallurgists, fluid dynamicists, and mathematicians. Supercomputers are emerging as powerful and cost-effective tools, not only for the furtherance of materials science, but also for linking this science with engineering, design, and manufacturing.

From these examples the committee drew a number of conclusions and made recommendations aimed at improving the state of the art of supercomputing for materials science and engineering, especially in those areas where an interdisciplinary approach promises major technological impact.

In the report each two-page example stands alone, with the left-hand page providing a brief technological background and the right-hand page the specific supercomputer examples.

Acknowledgments

A great many people assisted the committee in conducting the study and preparing the report. We wish to express our genuine appreciation for their efforts.

A major forum for discussing experience and directions for using supercomputers in materials science and engineering was a workshop held at the National Science Foundation's San Diego Supercomputer Center on March 24-26, 1987. Sidney Karin, Director of the Center, was most generous in allocating staff time and building space needed by the workshop. Beverly Brown, a member of his support staff, was thorough and resourceful in handling the logistics for the workshop. Each workshop participant had an influence on this report and deserves thanks. It is impractical to mention all by name here, so we ask that the workshop program and roster, reproduced at the end of this report, be accepted as our acknowledgment to them. In addition, Kenneth G. Wilson, Cornell University, provided the participants with a thought-provoking presentation on needs for supercomputers in the future.

Critical suggestions and supplementary material were obtained from a number of people not able to attend the workshop: D. D. Chambliss, Cornell University; Barbara Cooper, Cornell University; Sam R. Coriell, National Bureau of Standards, Gaithersburg, Maryland; Paul R. Dawson, Cornell University; Tarasankar DebRoy, Pennsylvania State University; Anthony G. Evans, University of California, Santa Barbara; Robert M. Fisher, Lawrence Berkeley Laboratory; Arthur J. Freeman, Northwestern University; Massimo V. Fischetti, IBM Research Center, Yorktown Heights, New York; Howard Heinisch, Westinghouse Hanford Company, Richland, Washington; John Hutchinson, Harvard University; R. V. Kasowski, E. I. duPont de Nemours & Company; Alan Needleman, Brown University; C. Paulson-Boaz, Cornell University; T. N. Rhodin, Cornell University; S. L. Sass, Cornell University; S. F. Shen, Cornell University; Subra Suresh, Brown University; R. H. Wagoner, Ohio State University; James A. Weeks, Cornell University; Alex Zunger, Solar Energy Research Institute, Golden, Colorado; and Nicholas W. Winters, Lawrence Livermore National Laboratory.

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We could not have produced this report without several excellent efforts. At Sandia National Laboratories, Livermore, Joan Bersie and Bernie Marx coordinated communication among committee members, efficiently arranged the committee meetings, and assisted with the preparation of the manuscript; Jack Bishop handled the report's design and artwork; Sandra Simmons and Nancy Hunt assisted with its composition; and Robert Tucker attended to editing details. At NMAB, Jennifer Tilles handled key aspects of logistics for the workshop, Cathryn Summers and Susanna Clarendon provided secretarial support for committee records and sections of this report, and Steve Montgomery provided extensive editorial assistance.

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Background:

Executive Summary

The primary task of this study was to identify key opportunities that would make a major impact in materials science and engineering, exploiting the emerging capabilities afforded by large-scale supercomputers. The committee applied rigorous criteria: The equations or algorithms should be known well enough that progress can be demonstrated today and the future reasonably and credibly predicted. Examples of how "given a computer ten times faster, it will be possible to..." were discarded if not preceded by "we have shown, in agreement with experiment, that...."

Our committee was selected to represent universities, industry, and national laboratories from a broad geographical base and a wide variety of disciplines. We began by bringing together, at an intense workshop in San Diego (March 21-24, 1987), experts from the wide variety of disciplines comprising materials science and engineering (materials scientists, physicists, chemists, metallurgists, engineers, polymer scientists, etc.). Papers were solicited before the meeting, presentations were made, and follow-up discussions pursued. The vast amount of material collected was reduced to a manageable level at a committee meeting in July 1987.

We found early on that the computational capability of supercomputers (the largest and most powerful computers in existence at any time) is continuing to increase rapidly at roughly constant cost. Cray Research has announced the Cray-3; ETA, Inc., the ETA-10. NEC and Fujitsu appear committed to becoming the world's supercomputer manufacturers, utilizing parallel processors to achieve their performance goals. Simultaneously, massively parallel processing machines are being designed that are capable of unlimited growth in computing power. It is clear that for the first time in history a tool has emerged that can aid in understanding materials processes at the level of complexity required to make an impact.

We made a strong distinction between the *capability* of supercomputers and the *capacity* that can be gained by less expensive mainframes and workstations. We recognized that a hierarchy of computing architectures needs to be employed (e.g., workstations are more efficiently used for graphics than mainframes are), but we restricted ourselves to the kinds of problems that cannot be done any other way. The scientific and engineering complications are so great that, in many cases, computation is the method of choice over experiment.

We found molecular mechanics calculations on polymers being performed that could predict the elastic properties of a complex polypropylene glass or the heat capacity of polyoxymethylene. Such calculations are ultimately capable of predicting the constitutive laws necessary to design polymer-forming dies by computer, with enormous cost savings.

We found that supercomputers have become powerful enough to predict phase diagrams of simple alloys from first principles, in agreement with experiment, giving the historic field of alloy development its first real hope of designing alloys by computer. Although it is not possible to design complex alloys by computer today, the economic impact of being able to design specialty alloys by computer for a declining steel industry is large enough to drive continuing work in this area.

The economic advantages of silicon semiconductor technology are being exploited by growing layers of germanium on silicon substrates, a nonequilibrium thermodynamic process now capable of being understood computationally. The layer thickness at which deleterious misfit dislocations are introduced in the growth process can be predicted by supercomputer. "Band gap engineering"—the ability to tailor the band gap of a semiconductor to technological needs—is within reach. Already electron localization effects in superlattices can be predicted from first principles, in agreement with experiment.

An important first step has been made in understanding the complexities of adhesion, a problem that permeates nearly all manufacturing processes. A universal adhesive energy relation was discovered by extensive computation of the energy required to separate metallic surfaces. Surface science and engineering is at the heart of many present and future technologies (e.g., semiconductor interfaces and corrosion) and is particularly ripe for computation. Quantum chemical (*ab initio*) and solid state (local density functional) techniques have impressive successes to report.

One area that Japan dominates is the manufacture of the equipment for producing semiconductors. We found that supercomputing has already been successfully applied by U.S. researchers to the design of chemical vapor deposition equipment, specifically to the rotating disk reactor. Efforts such as this could enable the United States to regain its processing advantage.

Fundamental deformation and fracture mechanisms in metals, alloys, and ceramics are being studied extensively by supercomputing. The ability to describe the complex deformations of metals can lead to dramatic improvements in the design of forming processes. The atomistics of dislocation generation at a crack tip, including the effects of impurity atoms such as hydrogen ("hydrogen embrittlement"), can be calculated using realistic interactions between the atoms. Continuum models of microcrack density and propagation have reached a stage where numerical simulations can play a major role in design and performance assessments of, for example, tough new ceramics. The supercomputer will make it possible to link methods such as these, thereby significantly changing the way materials design is carried out.

Pharmaceutical design, although not traditionally a materials problem, is becoming progressively more supercomputer-oriented because of the costs and risks associated with human experimentation. Lest it become lost, one example of the enormous strides being made in the design of chemotherapeutic drugs by supercomputer has been included in this report.

The list of examples here is by no means exhaustive: We found ourselves "stopping the presses" a number of times as still another paradigm of supercomputing in materials science came to our attention, and we recognize that some areas of computational materials science and engineering may not be covered. Yet we felt convinced by the number and depth of examples to come to several conclusions:

1. Supercomputer simulation will serve as a powerful and cost-effective link between materials science and engineering, design, and manufacturing.
2. New theoretical methods, algorithms, and approaches for analyzing the individual components of complex materials systems are rapidly evolving.
3. To exploit opportunities in computational materials science and engineering, the United States must invest heavily in the science underlying the methodologies, in developing software to make these methodologies useful to engineers and technicians, and in providing adequate hardware to scientists and engineers at universities and in industry.
4. To remain a leader as materials simulation moves out of the laboratory and into the industrial plant, the United States must act decisively now to stimulate the development of these methodologies and to develop turnkey simulation systems for industrial plants.
5. Simulations can reduce design costs and the time from concept to market.
6. Supercomputers allow the use of hierarchical design tools.
7. Supercomputer simulation is a powerful design tool that can increase U.S. economic competitiveness today.

Based on these conclusions, the committee has the following recommendations:

1. Focused multidisciplinary research initiatives in selected areas of materials science and engineering should be started in order to integrate design and manufacturing with the underpinning research base.
2. A Supercomputing Center for Materials Applications should be created. Such a center would provide a better means for conducting pioneering research and moving the results of basic research into turnkey systems suitable for wide use in U.S. industry.
3. Existing supercomputer centers must be kept at the state of the art.
4. Multidisciplinary materials simulation groups should be formed.
5. The infrastructure of local computing associated with advanced simulation must be strengthened.
6. These initiatives should be implemented in a manner balanced to preserve the research strengths that are central to the success of materials engineering and processing in the future.

Introduction

Over the next few decades the use of computer simulation in the design and manufacturing sectors of the U.S. economy will be driven by heightened international economic competition and rapid increases in computer capability. An enhanced understanding of key technical disciplines such as materials science and engineering will be essential.

Materials science and engineering have historically provided fundamental technologies for transportation, industrial production, defense, construction, and other areas throughout a nation's economy. The vitality of a nation's industrial base has rested on its materials development capabilities: In ancient China the production of iron weapons and tools on a monumental scale enabled that society to expel indigenous barbarians. In the 19th century, British steel processing methods enabled a small nation to dominate the industrial revolution. Today, we find another small nation, Japan, relying on materials science and process engineering to dominate the steel and electronic industries.

In the United States, materials technology has often been superseded by that in other advanced industrial nations. Although there is hope that concentrated research and development programs will produce significant improvements, it is not clear that traditional methods will move U.S. industry ahead fast enough. An additional tool for attacking today's complex research problems, which could provide the needed edge, is the supercomputer.

This study focuses on opportunities for the simulation and modeling of materials behavior made possible by the rapid and continuous increases in supercomputer capability over the past few years. Sophisticated simulation and modeling can now describe complex materials phenomena on a physically realistic basis. These phenomena include deformation and fracture of structural engineering alloys, local chemistry and phases caused by multicomponent diffusion of chemical and defect species in alloys, and electronic behavior of metals, ceramics, and semiconductors. In certain areas, it may even be possible to predict material properties.

These scientific and engineering advances are made possible by significant developments in the hardware (computing machines), software (theoretical methods and algorithm development), and strong experimental database underlying the supercomputing environment. Several manufacturers have already announced machines, available within the year, with an order of magnitude speedup in the time to perform a calculation and nearly two orders of magnitude increase in central memory. These developments coincide with those in the microelectronics industry in general.

Mathematical algorithm development has also been proceeding at a rapid pace. The time needed to solve a typical partial differential equation (such as Poisson's equation) with *algorithms in common use 30 years ago* (such as Cramer's rule) on a *modern computer* would be longer than the time needed to solve the same equation with *modern algorithms* (such as preconditioned conjugate gradients) on the *computers of 30 years ago*.

The experimental database underpinning supercomputer computations is deep enough to allow progress; further experimental work must be incorporated into any believable simulation.

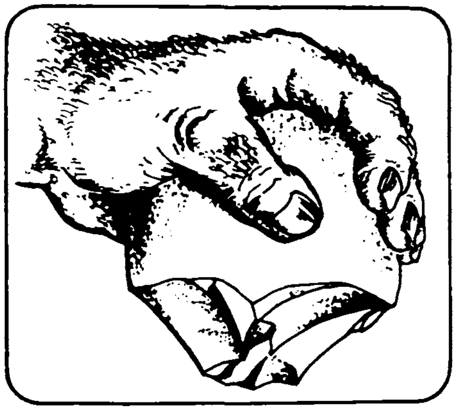
Concurrent with these increased technical capabilities has been the increase in international competition in materials-related and manufacturing markets. This competition is recognized as critical in the lucrative markets of electronic and optoelectronic devices for computer surveillance, telecommunication, and diagnostic systems, among others. Reliable design, manufacture, and performance of these devices will continue to limit system performance, and materials behavior will be the pacing factor in the rapid development and commercialization of new devices. Computer simulation is essential for development and commercialization and may offer the United States the opportunity to restore its competitive position in this arena. A parallel need and opportunity exists for structural materials, where computer simulation can integrate materials processing with manufacture and design to significantly reduce cost and lead time for product commercialization.

What follows is the main substance of this study, the examples. By no means inclusive, they nevertheless represent clear evidence of the emergence of this powerful new tool, the supercomputer, to simulate a wide range of materials phenomena, from the manufacture of automobile components and electronic devices to calculations of fundamental structure and thermodynamic relations. Each two-page example stands alone, with the left-hand page briefly describing the technology and the right-hand page the specifics of the calculations. Ancillary information is provided in blue background. The committee's conclusions and recommendations regarding technical and institutional issues are presented following the examples.

New Materials and Methods of Materials Processing Are the

In the beginning, materials were simply found—picked up and utilized in their natural state. We do not know when the first stick, stone, or bone was purposefully altered to assist in some task, but the origins of technology certainly date back to long before the evolution of *homo sapiens*. The earliest surviving examples of materials processing, from East Africa, are over 2 million years old. They are river pebbles of a size to fit in the hand, crudely shaped with a few intersecting breaks to form an edge at one end. Since that time, the ability to modify materials and grasp the potential usefulness of new material forms has set mankind apart from all other forms of life. Moreover, the success of individual groups and in many senses the fullness and success of their societies have been strongly influenced, if not controlled, by their mastery of the materials of technology.

Early technology was largely characterized by methods for modifying a material's shape without changing its material state. Rare flashes of keen empirical perception set standards for tens of thousands of years. A distinctly different technological revolution came about, some 9000 years ago, with the realization that readily deformable clay would harden to stone when baked. Unlimited formability in one state was replaced by stability in the final state. At the same time, there was no understanding of the complex chemical changes and recrystallization that take place in forming ceramics at elevated temperatures.



Oldowan Chopper

An even more significant technological revolution probably originated with the finding of beads of copper in the ashes of fires built against certain brightly colored rocks. Experimentation led to the concept of smelting, the intentional reduction of ore to its base metal. This development was of vast economic significance: A new material was not invented; rather, a new, more efficient materials process was discovered. It was then a relatively small step from smelting to alloying—to discovering that the simultaneous smelting of the ores of copper and tin produces bronze, a stronger material than copper and one that is also more easily cast into many desirable shapes. Without any understanding of the underlying reactions, persistent experimentalists discovered a new material that became the metal of choice. The earliest synthetic materials technologies, then, were metallurgy and ceramics. Both contributed to the rise of rich and complex civilizations.

The first (unplanned) smelting of iron may have taken place as much as 7000 years ago. Any efficient copper smelting operation requires a co-smelting of copper and iron oxides. If iron oxide is not naturally present, it must be added to increase the copper yield. Under certain temperature conditions, lumps of iron grow at the copper-slag interface. Their value as decorative items probably encouraged experimentation with this metal, which led to the discovery that iron oxide itself can be smelted.

As forged, iron is essentially carbon-free, soft, and ductile. Its mechanical properties are generally inferior to a good tin-bronze. It was the making of steel, the alloying of iron with small amounts of carbon, that was the crucial materials processing step which made iron-based alloys preferable to those of copper. Its pre-eminence among metals—combining hardness, toughness, and response to heat treatment with widespread availability and affordable cost—revolutionized civilizations.

By the early 1800s, steel could be made in quantity but only by ruinously expensive methods. In 1856 Bessemer (British) introduced a processing technique that involved shooting jets of compressed air into the molten metal and significantly lowered the cost of steel production. A decade later Siemens (German) pioneered the open-hearth process of steelmaking, which was appropriate to a different kind of ore. As a result of these new materials processes, the world output of steel increased tenfold between 1865 and 1880. A new material was not developed, but the means of production, the materials process, was made more efficient and cost-effective.

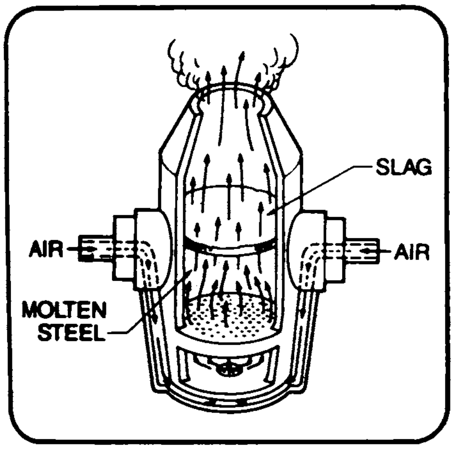
The United States became the world's largest steel producer until after the Second World War, when Japan invested heavily in steel production equipment. By making furnaces twice the size of American counterparts, the Japanese were able to produce high-quality steel at a lower cost. Again, it was not the invention of a new material; rather, it was the investment in the materials processing that gave Japan technological leadership.

It is not only in the development of the material that technological revolutions have continued to come

Fuel of Technological Revolutions . . .

about, but also in the forming and shaping of materials into useful end products. The 13th century tilt hammer, for example, was a boon to blacksmiths because it relieved them of much of the heavy labor required to forge metals. Today, metals are shaped by compressing them between specially designed dies, modern tools at the heart of materials processing. Precision dies are just as important for injection molding and extrusion in the polymer industry. Since 1920 modern methods of physical and chemical analysis have created a new industry, which produces billions of pounds of plastics and resins each year. Nylon, polyethylene, and polyvinylchloride (PVC)—unheard of 60 years ago—are now replacing steel and aluminum for many applications. For metals as well as polymers, however, die design is carried out painstakingly by trial and error; it is a materials processing area ripe for revolution.

Another area that grew out of modern technology is nuclear energy. It is perhaps not recognized that the Manhattan project was largely a task with unparalleled materials processing problems. One material (plutonium) required a nuclear reactor (which had yet to be constructed). Another (uranium-235) required the separation of two of the heaviest isotopes known to man.



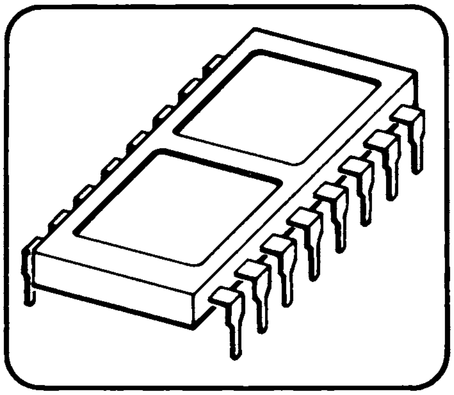
Bessemer Process

The invention of the transistor in 1947 at Bell Laboratories led to a quantum increase in interest in semiconducting materials, principally silicon and germanium. By the late 1950s, transistors, resistors, capacitors, and their interconnections were being incorporated on a single "integrated circuit" semiconductor "chip." In 1962 another U.S. invention, the laser diode (a light-emitting, solid-state device made of gallium arsenide), gave rise to the photonics industry. We have all felt the effects of the explosion in the electronics industry—communications, computer technology, information processing—brought about by the invention of these new materials and devices.

An unprecedented sophistication in commercial materials processing has been brought about by this latest technological revolution. Single atomic layers of silicon are deposited from chemical vapors onto substrates. Silicon is doped with ions implanted at precise distances below the silicon surface. "Clean rooms" keep submicrometer-size particles out of the processing environment. The Japanese have not only excelled at applying these techniques in capturing the world market, they have succeeded in dominating in the manufacture of the fabrication equipment necessary to apply these materials processes. This is the ultimate in holding the keys of production in one's hand.

Most recently, a serendipitous discovery of high-temperature superconductivity in ceramics has excited the materials community with prospects of zero-loss long-distance electrical energy transmission, superconducting computers, and railless trains levitated on magnetic fields. Once again, however, it will not be the inventor who profits from this discovery but the materials processor who develops the material and brings it to the marketplace.

We have progressed a long way from finding the materials of our culture lying on the ground. Carefully controlled processing methods are transforming existing materials into precise geometries and microscopic structures. At the same time, materials processing advances still depend largely on experimental development, aided by theoretical insight, although it would appear we have an adequate understanding of the underlying physics and chemistry to carry out development theoretically, aided by a few well-chosen experimental checks. What has been missing is a sufficiently powerful computational tool that will let us define the need and then carry out the design, atom by atom.



Semiconductor Chip

. . . Which Create National Needs for Competitiveness

The technological advantage gained with new materials and processes can dramatically enhance a nation's competitiveness. Historically, such a competitive advantage has often led to market dominance by a single nation. In the mid-1850s, Britain became the first nation to master the technology of economical steel production on a large scale. As a result, not only did Britain increase the number of miles of train track linking her industrial centers by a factor of 30 in as many years, but she also became the premier supplier of locomotive technology to the rest of the world.

Today there is fierce international competition for dominance in materials-intensive areas such as transportation, communications, and information processing. In the area of transportation, for instance, airframe materials technology is being driven to an extreme level of sophistication by economics. The manufacturer who can most efficiently produce the lowest-weight, highest-strength structural alloy may well dominate the market.

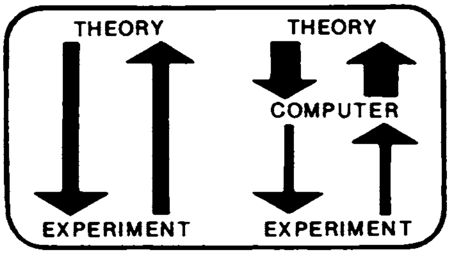
Alloy development and processing have become high-payoff endeavors in this arena. Metal forming, including the composition and thermomechanical processing of an alloy, is a highly competitive materials processing problem in the aircraft industry. Airframe design in particular is also driven by economic factors. While the aerodynamic shape of an automobile might influence fuel economy to a small extent, on an aircraft the shape of wings and fuselage are vital to performance. Multimillion-dollar wind tunnels have been constructed to provide design engineers with a tool for optimizing performance parameters before final production.

The need to be competitive in communications technology is emphasized by the 430 million telephones, 364 million television sets, and 100 satellites in use throughout the world. The materials on which this communications explosion is based were invented more than 20 years ago, but the processing techniques have become vastly more sophisticated in recent years. This phenomenon is true not only for the semiconducting materials in integrated circuits but also for the interconnection medium itself. Improvements in the processing of glass have reduced light transmission losses to such an extent that glass fiber has replaced copper as the material of choice for communications.

Perhaps the most intense area of competition involving materials and materials processing is that of information processing, which is the circulatory system—the blood supply—of a modern economy. No industrial nation can hope to be competitive without widespread application of this technology. For the past several years, automated information systems have handled airline reservations, kept business records, executed banking transactions, and paid the work force. Today, information systems control aircraft traffic patterns, assist with medical diagnosis, help fight crime, and model investment decisions. Tomorrow, we will manipulate knowledge on a grand scale, as digital storage media (polymers, alkali halides, etc.) and computer technology integrate on-line databases with real-time decision-making capabilities—opening up applications that are as yet unanticipated. The impact of superconducting ceramics on information processing has yet to be realized. The need for new materials and competitive processes to support this information revolution is recognized by every developed country. The nation with superiority in knowledge manipulation will be a formidable competitor indeed.

Supercomputing Can Enhance U.S. Economic Competitiveness . . .

The design of new materials and materials processes vital to the nation's economic competitiveness is an immensely complicated technical problem being addressed today as much by art as by science. When a process is too complicated to understand on a fundamental level, we traditionally perform experiments or tests on the process, which we then compare to a hypothesis or theory. The theory is modified accordingly. This is the essence of the scientific method in use since Francis Bacon proposed it. On its highest plane, the theory includes fundamental equations such as Newton's Laws. When the level of complication is beyond our ability to write down the equations, we make suppositions or guesses and gather data. If we can gather enough data in one place, we might be able to make correlations that enable us to make progress. Niels Bohr studied the 30 years of data on atomic spectral lines and made important correlations that led to his atomic model.



Computers bring a new methodology to science.

Supercomputers bring a third methodology to theory and experiment. When enough knowledge exists, in the form of fundamental equations for example, computers become a tool capable of yielding insight otherwise unobtainable. Knowing the equations is not even enough: F = ma does not tell us whether an automobile will be crushed upon impact.

For the complicated materials processes addressed here, there are many equations arising from different scientific and engineering disciplines. Chemical, physical, and metallurgical processes must be coupled to fluid dynamical equations, for example, in order to understand the chemical-vapor-deposition process used by the semiconductor industry. Supercomputers facilitate this multidisciplinary effort by threading together in the same program inputs from the different disciplines. We finally have a tool to help us accomplish the goal of coordinating otherwise splintered efforts.

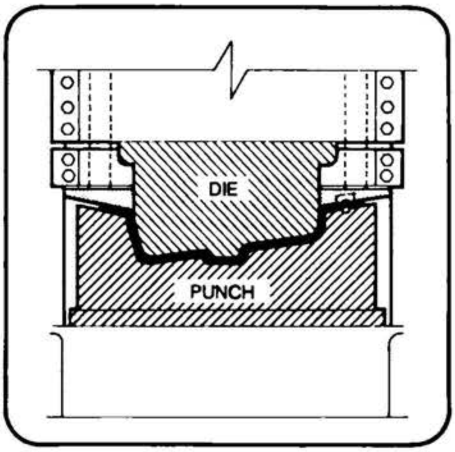
This multidisciplinary approach to large-scale computations was recognized early in the nuclear weapons program as being essential to making progress in such a complicated area. Hydrodynamics, neutronics, fluid mechanics, chemistry, physics, and transport phenomena are all coupled in elaborate computer codes. Designs that formerly required hundreds of expensive and time-consuming tests are now done better by computer along with a few critical experiments. It is not that nuclear design can be done without experiment, it is simply that computation minimizes the number of those experiments.

It is important not to confuse supercomputing with other high-level computation. A *supercomputer* is the most powerful computer in existence at any time. The supercomputer of the 1950s had the power of a hand calculator today. A factor of 10 increase in supercomputer power every 5 to 10 years has been and continues to be achievable. It is the capability of these supercomputers we wish to exploit; adding together a great many smaller machines will increase our capacity to compute but will not give us what is needed. A VAX-8800 may have the power of one-tenth of a Cray, but ten (or even twenty) VAX-8800s cannot do the calculations one Cray can (see page 50).

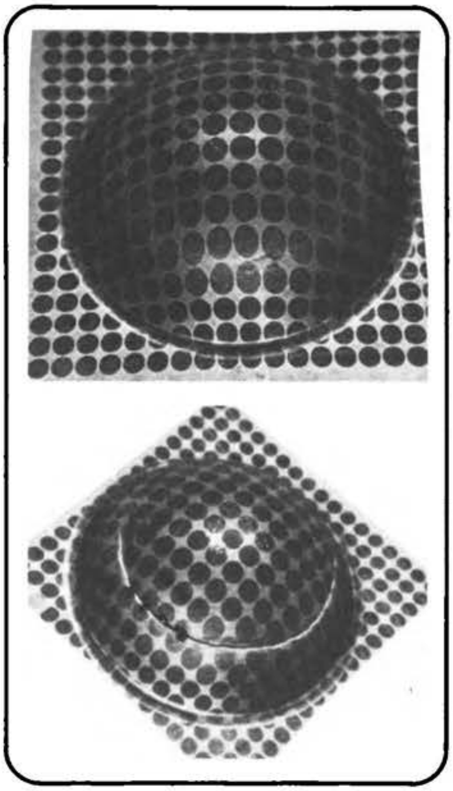
As in the weapons design program, the knowledge exists to enable us to use supercomputers to enhance our competitive position in the design of materials and materials processes. There are many illustrations of this, some of which are included in this report. Where large, long-term, multidisciplinary efforts have been undertaken, remarkable results have been achieved. It is essential that there be a long-term commitment: The weapons program began its supercomputing effort at the very beginning (1943) of nuclear weapon development and has led the world, indeed has been the driving force, in the use and development of supercomputing.

A national effort is needed in materials science and technology to awaken the research and development communities in industry and academia to the realization that supercomputers offer a new tool for unprecedented materials analysis, development, and processing simulation. To demonstrate that this opportunity is already within reach, our committee has assembled in this report a selection of ongoing research and development projects that show the power and future promise of supercomputer simulation in materials technology. Each example demonstrates in a particular way that today's supercomputers can synthesize various interrelated phenomena at all levels, from the electronic to the macromechanical, and thus describe material behavior during processing and manufacturing as well as material performance.

Developing Metal Forming Procedures and Dies Is a Billion-Dollar Industry . . .



Schematic of a typical die for sheet-metal forming.



Metal coupons with dot patterns such as these are used to measure the strain in a deformed metal sheet up to (top) and including (bottom) ductile tearing.

The forming of sheet metal into parts—from cans to automobile fenders to airplane foils—is a major manufacturing activity. Processes involving drawing, stretching, and bending of metal sheets, for example, require precisely shaped dies as well as carefully designed sequences of individual steps to achieve the final shape. This procedure costs the automotive industry alone on the order of a billion dollars annually. The same is true of the legion of other forming processes involving forging, extruding, etc. At present, however, most forming procedures are designed by trial and error, which limits the quality of the finished products and the cost-effectiveness.

One of the reasons that designing forming procedures is difficult is that the *formability* of materials depends not just on the amount of deformation in an operation but also on the history of deformation and on the ability of the material to resist fracture. For decades, *forming limit diagrams* have been developed to indicate the maximum amount of deformation, under simple deformation histories, that can be sustained by a material before failure. Parallel to this effort, constitutive equations based on continuum theories for plasticity have been developed to describe the relationships between stress, strain, and strain rate for metals. These constitutive laws have not, until recently, included descriptions of material failure, nor have they accounted for the history-dependent material response that is important for predicting failure.

What limits the strain to failure is typically the development of *failure modes*. These may include the formation of bands of intensely concentrated plastic deformation caused by the confinement of microscopic processes of *slip* to narrow zones within the individual grains of a metal, or by the development of microscopic damage involving the initiation of cracks or voids. In addition, metals are often highly anisotropic (their properties depend on direction within the material); the process of deformation itself results in the development of *textures* that induce further anisotropy.

The figure on the upper left illustrates a typical, but simple, sheet-metal forming process. Here the metal sheet is stretched over a die whose dimensions and shape are important design parameters. The middle figure illustrates the deformed shape of a similar sheet part formed by a similar process. The lower figure illustrates a typical failure mode—ductile tearing—that limits the ability to successfully form materials in this way.

Current understanding of metal plasticity, including failure, provides the basis for an unprecedented capability for designing forming procedures. The necessary analyses will, however, require next-generation supercomputers so that a complete account is taken of a material's behavior and of the actual three-dimensional forming process. Simulated forming on a supercomputer will not only save time and money, but also lead to revolutionary methods of shaping metals.

We Can Predict Two-Dimensional Material Response Today. . .

There are two phenomena that influence the tearing of a metal sheet during forming: flow localization and microvoid formation. These occur in both two and three dimensions, but today's supercomputer capabilities limit simulations to two dimensions. Two-dimensional (2D) modeling, however, is well established, as is seen from the following discussion.

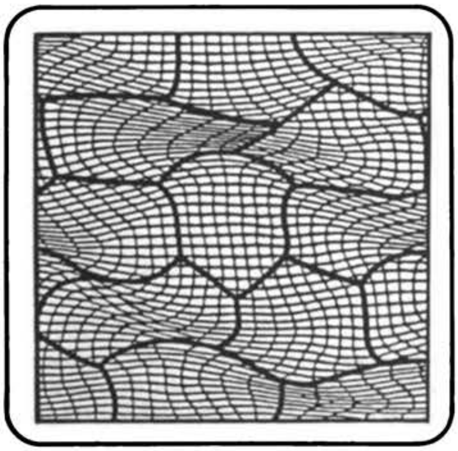
The development of advanced constitutive theories to describe the detailed behavior of materials depends on models that can simulate the deformation response of microstructures. In metals these microstructures consist of aggregates of grains and dispersions of particles of other materials that impart increased strength and stiffness. The boundaries of the grains, as well as the second-phase reinforcing constituents, are typical sites for the initiation of failure modes. Detailed simulations are needed that allow for strain compatibility between the various phases and incorporate realistic descriptions of the atomistic deformation mechanisms.

The figure on the left below is a supercomputer simulation of the 2D deformation of a polycrystalline aggregate subjected to compression. It illustrates how localized deformation, in the form of shear bands, occurs naturally and leads to failure of the material. Included are the predictions of material texture so that account is taken of the evolution of history-dependent anisotropy.

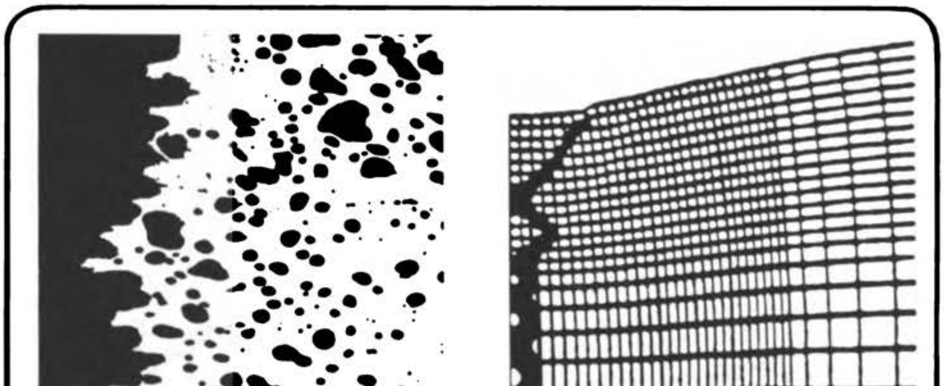
The figures on the right illustrate ductile rupture that occurs by microvoid formation. One is a micrograph of the fracture surface of an iron specimen that underwent ductile rupture through the initiation and growth of microvoids. The other is a computed ductile rupture pattern using an advanced constitutive theory developed for metals that undergo damage through microvoid formation. Damage through the formation of such microcracks can result from the earlier formation of shear bands or can, in turn, induce localized deformation that accelerates microvoid growth, leading to complete rupture of the material.

In both sets of figures the simulations accurately describe the complex events that occur on the microstructural and macroscopic scales. In particular they illustrate how fundamental descriptions of microstructural behavior can now be incorporated into simulations of complex macroscopic behavior and of macroscopic processes.

It is clear that enormous capability now exists for making fundamental improvements in the way we design and analyze technological forming processes. All the pieces are in place; we await the next generation of supercomputers.



Deforming finite element mesh for a polycrystalline metal. Nonuniform grain deformation and shear bands are computed along with the polycrystal's stress-strain response.



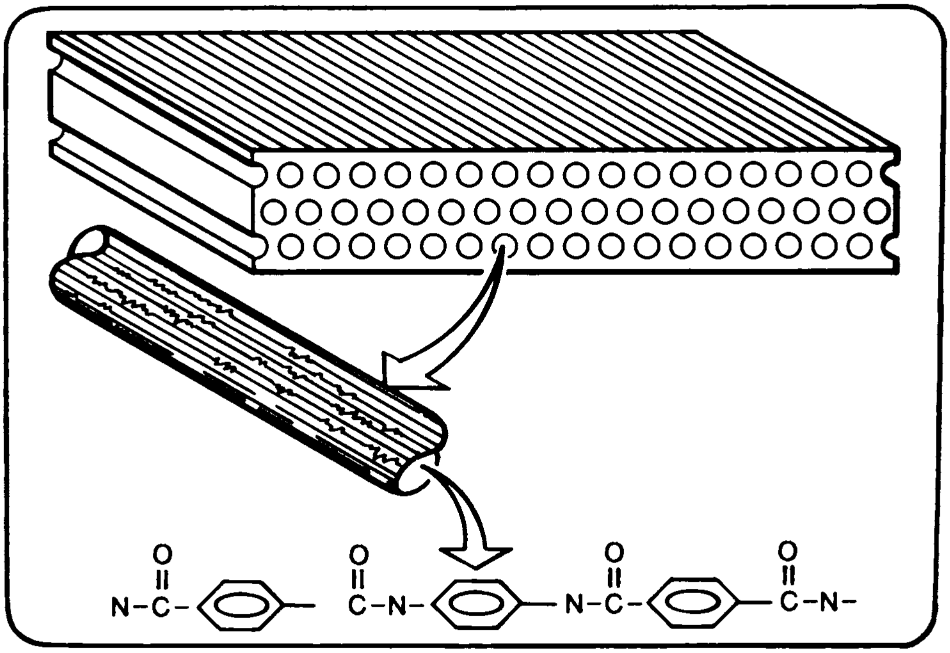
Microvoids (left), seen here enlarged in an iron specimen that failed through ductile rupture, reduce the amount of elongation before fracture. When the effects of microvoids are included in the deformation law, then the reduced ductility and rough fracture surface are reproduced in a 2D finite element analysis (right).

The Importance of Polymers Is Driving Us to a More Detailed Understanding of Structure Versus Properties . . .

Polymers are the major chemical constituents of plastics, elastomers, adhesives, and some fibers and coatings. On a volume basis their production and utilization in the United States has exceeded that of steel for some time, and their growth rate is 4 times that of steel and nonferrous metals. The design of new polymers and modification of existing ones for new uses are obviously important undertakings. Accomplishing these tasks depends not only on understanding the relation between the chemical constitution of a polymer chain and the properties of the ensuing material but also, ultimately, knowing the structure-property relationships for the bulk materials.

In the past much of this understanding was developed qualitatively and through empirical correlations. More progress is needed at the atomistic and molecular levels. For some properties and phenomena better theories are required. However, even where the interactions are well understood, it is difficult to account for the complex assembly of atoms in a bulk polymeric system.

From a structural point of view there are two main classes of solid polymeric systems: those that have chemical structural regularity (crystals) and those lacking chemical structural regularity (amorphous solids and glasses). Both classes are important. Designing and modifying polymers will be significantly aided when the static and dynamic properties of crystalline and amorphous polymeric solids can be accurately calculated.



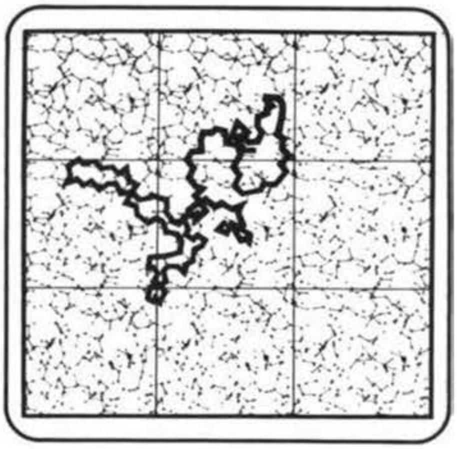
This composite of embedded Kevlar aromatic polyamide fibers is one example of a strong, lightweight material made possible by a synthetic polymeric fiber with stiffness and strength comparable to that of steel, but with much lower specific gravity.

Detailed Atomistic Simulations Can Predict Polymer Properties . . .

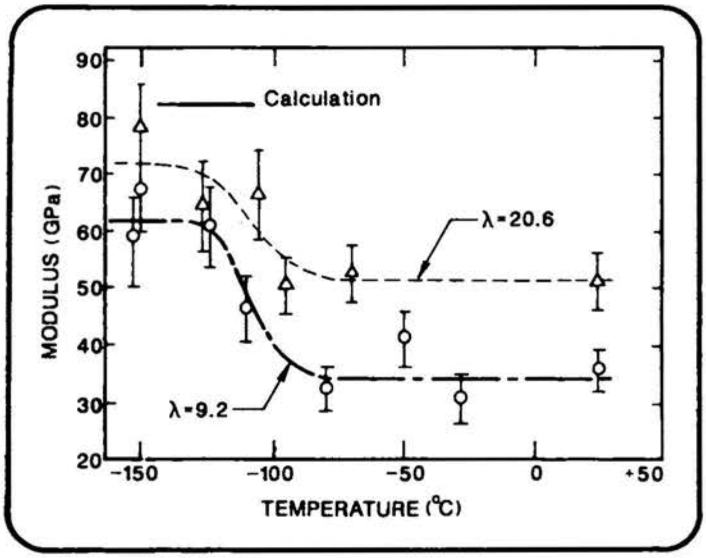
The calculation of static bulk properties of polymers is largely a problem of complexity, not of principle. The forces between atoms can be modeled by molecular mechanics. The energetics of bond stretching, bending, and twisting, as well as spacially dependent interactions between chemical building blocks in the same and different chains, can be represented by empirical functions (such as Lennard-Jones potentials), with parameters transferable among different polymer chains. While analytical calculations are unable to cope with the full complexity of the problem, supercomputer simulations incorporating these ideas (see figures below) have constructed minimum-energy structures for amorphous polymeric glasses and determined their bulk elastic properties.

In the area of crystalline polymers, molecular mechanics simulation techniques have been applied to energy minimization. These techniques include the internal molecular degrees of freedom and crystallographic packing parameters, allowing a calculation of the mechanical and thermodynamic properties of crystals.

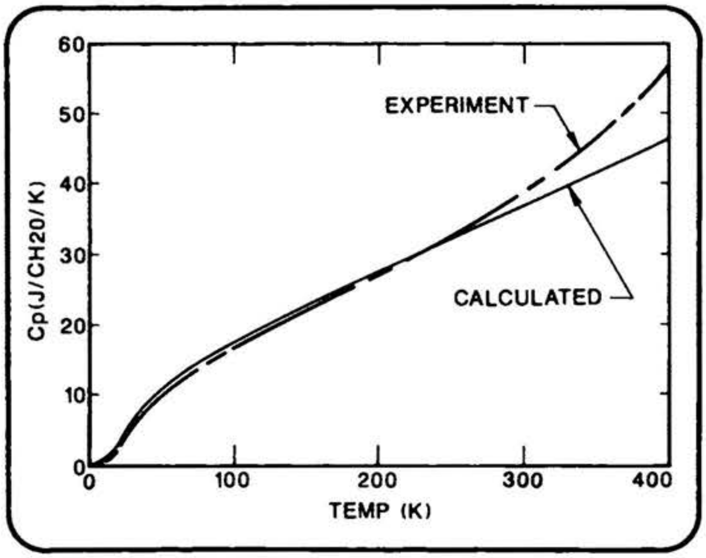
In the future, supercomputer calculations that simulate molecular motions in polymeric solids will lead to an understanding of time- and temperature-dependent properties. Coupled with advances in supercomputer technology, these techniques will at last allow the exploration of new polymeric materials with specifically tailored properties, before painstaking synthesis is actually attempted in the laboratory. For example, to study the viscoelastic response of a polymeric material, one needs to carry out a molecular dynamics simulation of a few hundred polymer chains comprising a few million atoms over an actual time period of 10 ns. One way to accomplish such a simulation would be through massively parallel processing coupled with performance improvements in each processor.



Calculated structure for atactic polypropylene glass. Parent chain is boldface; others are images. The calculated Young's modulus (not shown) is in good agreement with experiment. Note the highly disordered entangled structure, a difficult phenomenon to simulate properly.

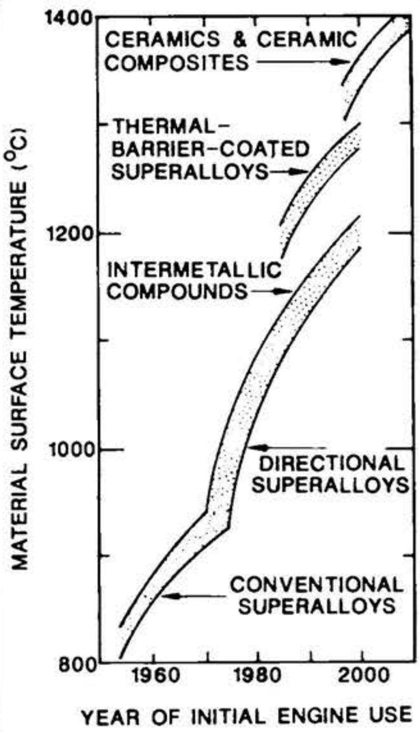


Fiber modulus of polyoxymethylene versus temperature. The experimental values (from x-ray measurements) at low temperature and high draw ratio (λ) approach the value calculated from molecular mechanics, indicating that an optimum morphology is being obtained experimentally. The goal is to be able to screen candidate materials for high modulus fibers by molecular mechanics predictions.



Calculated heat capacity of polyoxymethylene compared with experiment. The calculated values are accurate up to the onset of serious anharmonicity effects.

Ceramics Provide High–Temperature Options to Increase Efficiency . . .

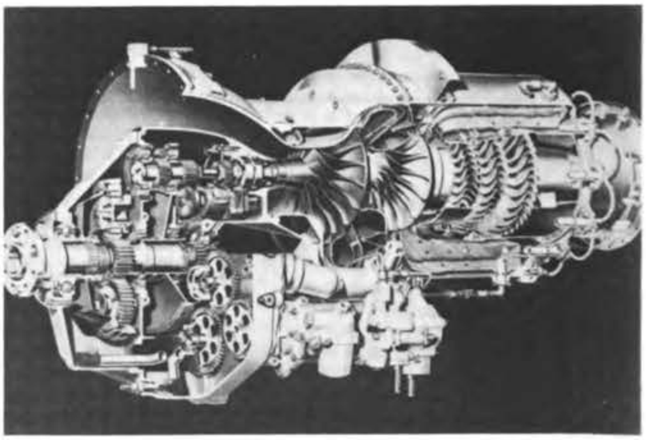


Ceramics have been traditionally thought of as materials for housewares and industrial furnace linings. In fact their high-temperature stability and strength, hardness, low thermal conductivity, and wide range of dielectric properties make them desirable for much wider structural and electronic use (see figures below). These applications have not been realized in many instances because ceramics are prone to brittle cracking and failure, especially in residual and thermal stress fields.

More recently, researchers have tried a variety of microstructural approaches to enhance the toughness of ceramics, resulting (in some instances) in order-of-magnitude improvements. Since such improvements are sensitive to microstructural details based on crack-microstructure interactions, micromechanics models that relate the fracture resistance to microstructural specifics have been the primary contributors to the development of these vastly improved ceramics.

Our understanding is now at a stage where numerical simulations for crack growth can play a major role; preliminary results are encouraging. Further numerical research should allow ceramic designers to conduct optimization studies that take into account the influence of the various known mechanisms and, more importantly, calculate the synergistic effects of multiple mechanisms.

Engine components made from ceramics have improved properties.



	T76 ENGINE	CERAMIC ENGINE GOALS
POWER OUTPUT	715 SHP (533 KW)	1000 SHP (746 KW)
SPECIFIC FUEL CONSUMPTION	0.60 LB/HP-HR (0.365 KG/KW-HR)	0.54 LB/HP-HR (0.328 KG/KW-HR)

Comparison of metal alloy and ceramic aeroengines justifies the increased interest in ceramics.

Supercomputers Are Aiding the Design and Performance of Ceramic Materials . . .

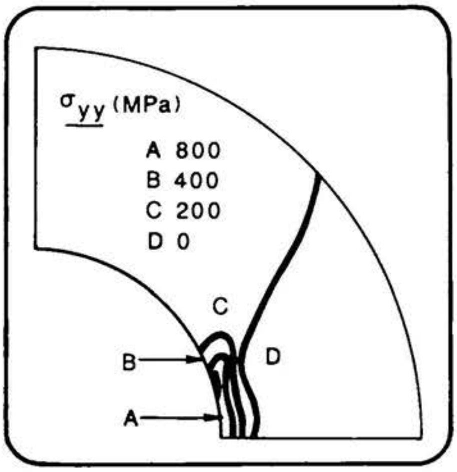
Materials scientists are simulating crack growth in ceramics and ceramic composites with theoretical models for micromechanical behavior. In materials like tetragonal zirconia, phase transformations occur near the crack due to locally high stresses. In others, such as an alumina-zirconia composite, microcracks result from stress-induced phase transformations near the macroscopic crack tip. A number of U.S. researchers have determined the extent to which the crack tip is shielded from damaging stress because of material distortion during a phase change. Others have developed models for microcracking. With these models, microfracturing around the tips of major cracks is being analyzed.

Below is a supercomputer simulation of crack growth in a *microcracking* ceramic, showing contours of microcrack density around a growing macroscopic crack. The microcrack zones shield the macroscopic crack from the applied stress, making it more difficult for the applied stresses to open the crack further. In other words, the material is tougher. Increases in toughness are calculated in these simulations and related to the material's microstructure.

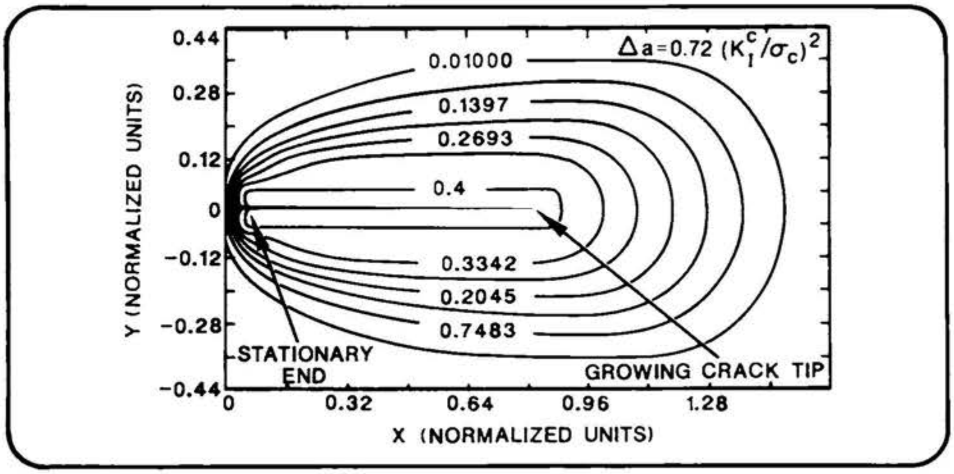
With such supercomputer simulations, ceramics designers can determine the optimum mode of toughening. Other simulations can model the effect of reinforcing fibers or whiskers, ductile particles, or microstructural bridges constraining a major crack. By modeling the complex interactions among such micromechanical features, materials scientists will be able to develop new tough ceramics.

Recently, researchers have also developed constitutive models for transformation-toughened ceramics such as zirconia partially stabilized with magnesia (Mg-PSZ). The models represent the shear strains and expansion produced by the stress-induced transformation of zirconia from a tetragonal to a monoclinic phase. Finite element analyses of fracture behavior based on these models have successfully predicted toughness enhancements and fatigue crack growth from notches subject to cyclic loading.

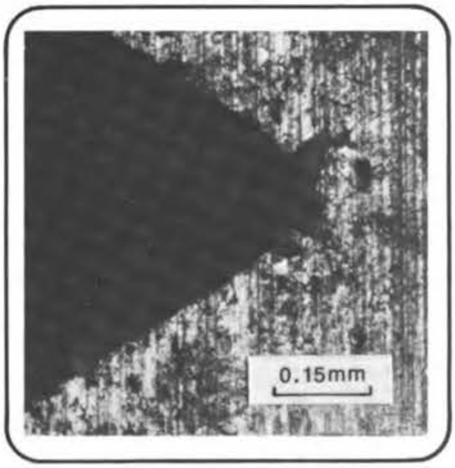
The contour map on the right is a computer simulation of residual *tensile* stresses at the tip of a notch in Mg-PSZ that was loaded and unloaded. The photograph beneath it is from a fatigue experiment on Mg-PSZ. The direction of crack growth, predicted by the maximum tensile stress contour A, was experimentally observed. These results demonstrate how computer simulations derived from physically based models of microscopic deformation can aid in understanding and predicting the macroscopic fracture behavior of ceramic materials.



Contours of a constant normal stress at the notch tip in a Mg-PSZ ceramic after complete unloading.



Contours of microcrack density near a growing crack in a ceramic composite from a supercomputer simulation. Δa is the amount of crack growth and K_I is the applied stress intensity.



Crack growth from a notch tip in a Mg-PSZ ceramic.

Materials Technology Has Always Been

While other animals have developed occasional and specialized uses of materials, man has been unique in his exploration and development of sophisticated materials and materials processes. With each successive advance in materials technology, large-scale political advantages—along with the spread and flourishing of culture, ideas, and government—have accrued to those skilled in their manufacture and use.

In the Great Lakes region of North America, in the third millennium B.C., massive deposits of pure metallic copper were available for arrow points, awls and needles, and artistic objects. Despite its plentifulness this New World copper was predominantly used for non-utilitarian, decorative objects, being too soft to supplant the existing Stone Age technology for sharp tools and weapons. Thus the lifestyle and productivity of the hunter-gatherer societies were not significantly affected by its presence.

In contrast, in the Near East the absence of large, easily obtained supplies of native copper led to the development of a new materials process, smelting, about 3500 B.C., which made it possible to produce copper in large quantities. Moreover, co-smelting with other ores produced alloys of bronze, tin bronze in particular, the first true technological metal with the strength, ductility, and formability to be vastly superior to polished and chipped stone materials, permitting the production of far more sophisticated weapons and tools, and intricate art.

The principal problem with tin bronze lies in the scarcity of tin ores, which are located in only a few parts of the world. Hence, early bronze societies became perforce trading societies, mounting expeditions and making trade contacts over long distances. An exception was the premier ancient power, Egypt, which continued to slumber along, relying on imported goods and looking inward upon itself. As a result, the center of Bronze Age political power and influence shifted to Sumeria and Babylon in the Mideast and to the seafaring nations of Crete, Troy, Greece, and Phoenicia in the Mediterranean.

In the middle of the second millennium B.C., another power shift occurred as industrial production of iron became a reality among the Hittites (southeast of the Black Sea). Iron had been produced earlier in small pieces but never utilized as a significant industrial material. The Hittite bloomery furnaces changed history as drastically as Alamagordo did in our lifetime and marked the commencement of the large-scale production of bloomery iron around 1200 B.C.

Iron was more difficult to produce and work than bronze. Iron ore, on the other hand, could be found in large quantities in bogs and outcroppings. Suddenly, metallurgy could tap a vast supply of readily obtained raw material. It allowed the large-scale production of metal tools and weapons for an entire population, not just for an elite aristocracy as was characteristic of the Bronze Age. Although early iron weapons were cruder and less efficient than their bronze counterparts, they were available in large numbers; entire armies, including peasants as well as the chariot-riding aristocracy, could be equipped with metal weapons and armor. Perhaps not surprisingly, the rise of the Iron Age was accompanied by a devastating military ascendancy and expansion of iron-producing barbaric tribes.

Iron had a dramatic effect on the history of China as well. By the second millennium B.C. the Shang and Zhou dynasties had developed a large-scale capability for making monumental bronze castings, some weighing several tons. During the Zhou dynasty, iron development took over on a massive scale. In part this can be attributed to the large blast furnaces developed for bronze castings and probably also to high-phosphorus ores in which a low-melting ledeburite cast iron formed at temperatures well within the range of the furnaces. Indeed, estimates are that by the Han dynasty, every Chinese family had in its possession some 5 to 20 kilograms of iron in agricultural implements and weapons.

The Chinese also learned that reheating chilled iron castings for an extended time converts brittle white cast iron into tough, ductile, malleable iron for high-impact uses such as plowshares, swords, and armor. They also developed composites in which high-wear-resistant surfaces (e.g., for plowshares) were made of the hard cast iron backed with a ductile iron support.

The Chinese developed monumental industrial operations that produced iron at the rate of several tons per day per furnace, dwarfing anything in the Mediterranean or Near East at the time. Their iron provided agricultural tools for producing a large food surplus that sustained a rapid growth in population. The large population and iron weapons of the Han dynasty supported armies which, for two centuries, slowly pushed the barbarians out of Central China. The disruption dislodged Turkish and barbarian tribes and forced them westward across Central Asia. Finding few resources there, these displaced tribes eventually burst into Europe and the Mideast, laying siege to the Roman Empire and ultimately overcoming it. Thus the Vandals, Goths, and Huns that descended on Rome in the 3rd and 4th centu-

at the Foundation of Thriving Civilizations . . .

ries were the direct result of the metallurgical developments of massive iron production in Zhou and Han China 200 to 400 years before.

Roman metallurgical works were also well organized and monumental, ranging from the copper mines at Rio Tinta in Spain to the ironworks through the north of the Po Valley, where adequate fuel and sophisticated mining produced large and massive quantities of iron. Perhaps one of the more spectacular finds is a Roman nail hoard at the legionary fort of Inchtuthil in Scotland, a remote outpost on the fringe of the empire and only occupied A.D. 83 to 87. Over 900,000 iron nails, some 5 tons, were found stored as the normal produce of an iron-using society. Indeed, a Roman legionnaire, with his iron-tipped javelin, iron short sword, and iron-banded armor, was invincible for close to 500 years.

In the New World, a small number of Spanish conquistadors equipped with iron armor and steel swords challenged and overcame the large native societies, which were organized in a military hierarchy but were demoralized by the seemingly invincible weapons of the Spanish. Although lacking iron weapons, the Indians did possess large quantities of gold and silver, which had great monetary value in Europe. Spain became the wealthiest nation in Europe. There was little need to develop the industries and precursors of the Industrial Revolution, which were springing to life under harsher conditions in northern Europe. The purchase of mercenary armies made it unnecessary for extensive Spanish participation or risk in the military. The Spanish Empire, owing to its easy access to valuable materials, became a society based on consumption rather than production. Spain was eventually eclipsed by the poorer but more industrial nations to the north.

Again it was iron, and the ability to produce it more efficiently and in large quantities, that provided the driving edge for Dutch, English, and British expansions. By the mid-1600s crude bloomery furnaces were giving way to blast furnaces, which produced substantial quantities of cast iron, and to the chafery refining process, which allowed the cast iron pigs to be refined into a relatively tough wrought iron. Made in extensive quantities, it not only supplied the needs of the inhabitants, but produced a substantial surplus for export. The ancient empires of Asia and the vast hinterland of Africa gave up their treasures, luxuries, and even their inhabitants for the iron and agricultural tools from Sheffield and Birmingham and the cloth from Manchester and the low countries. The possession of materials of great utility and in great demand, mass produced at a low price and made available by efficient sea transport, transformed small, poor, cold, and relatively infertile nations into world powers.

In the 20th century, it was American materials and production that dominated the world scene. Although the major wars of this century found the United States ill-prepared, the productive capacity and quantity of arms produced overcame, by sheer weight, the professional armies, military science, and tradition of Europe and Japan.

And now we are in the throes of yet another expansion, which threatens to eclipse the traditional producers of America and Europe. The Pacific Basin nations are producing high-quality materials and products, not only those of traditional technology such as steel, plastics, machines tools, cameras, and automobiles but also the newer electronic chips, electronic devices, and computers. Inexpensive, educated, and motivated labor is part of the story, but the thrust of development of new materials also appears to be passing to Japan. Engineering ceramics, advanced electronic materials, superconducting ceramics, and new chips all seem to be coming from that one nation. With the momentum of materials development and utilization, economic and technological dominance may follow.

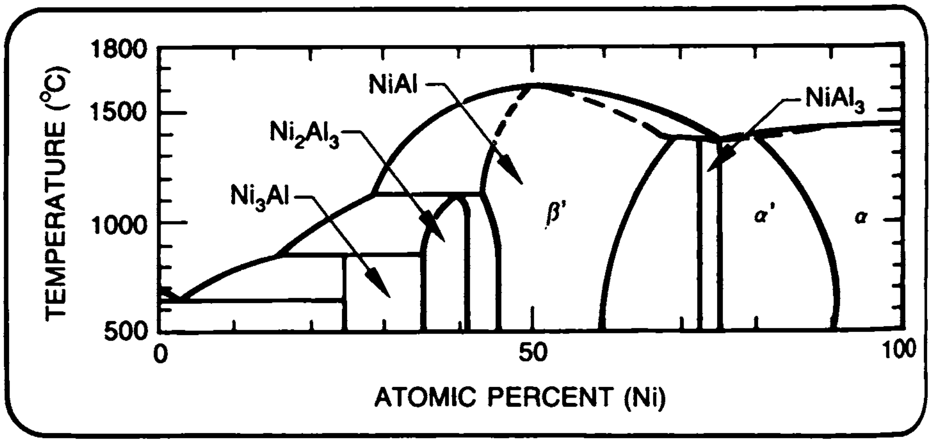
Efficient materials processing on one continent has more than once led to a civilization's downfall on another continent.

Alloy Development Is a Costly and Time–Consuming Undertaking . . .

The possibility of tailoring material properties by means of alloying stands as one of the oldest principles discovered and effectively exploited by mankind. The emergence of new technologies in, for example, the aerospace and electronic industries creates a constant need for the design of new materials that can operate in a variety of demanding environments. In some instances it is even desirable to redevelop existing alloys in order to eliminate or minimize the use of strategic materials such as cobalt and chromium. Unfortunately, redevelopment is often unattractive because the traditional approaches to alloy design are economically prohibitive. Despite its long history, the process of alloy development is still based on gradual improvement by empirically driven trial-and-error experimentation and is seldom guided from fundamental physical principles.

The starting point for alloy development is knowledge of phase diagrams, which show the composition and amounts of phases formed when elements are mixed to form an alloy. Alloy properties (mechanical, electrical, optical) depend critically on the amounts and properties of the constituent phases, among other factors like microstructure. For structural alloys the phase diagrams are usually complex. Below, for example, is the binary (two-element) nickel-aluminum diagram. Most aircraft engine turbine blades are made of nickel-based alloys. These contain aluminum and chromium for oxidation resistance and other elements such as tungsten, titanium, and carbon for strength. A typical commercial superalloy may contain five elements or more.

Binary and ternary phase diagrams are traditionally determined experimentally with great difficulty and with significant investments of time and resources. It is virtually impossible to obtain quinternary phase diagrams or to find an effective mode of representing the data. An ability to calculate such diagrams from first principles would revolutionize the design of new alloys. For example, the recent discoveries of Ni-Al intermetallic compounds (see page 34) that are ductile and refractory, and of ordered phases in semiconductor alloys such as those observed in InGaP and GaSbAs, have opened new areas for developing potentially useful materials. The challenge will be their optimization for various applications.



Nickel-aluminum phase diagram.

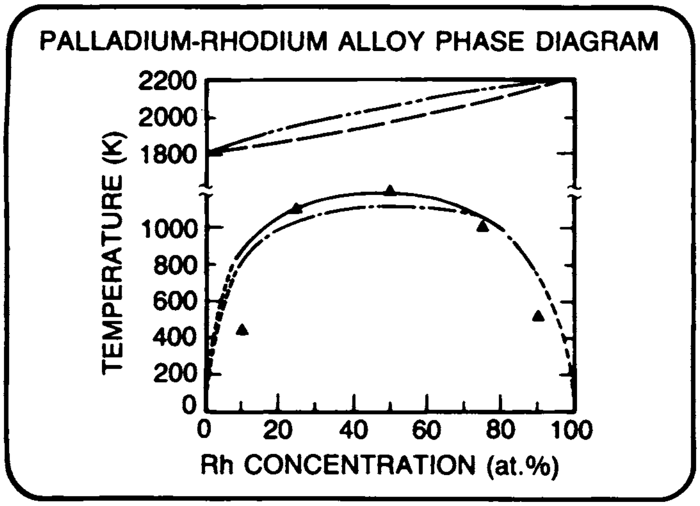
Supercomputers and Quantum Architecture May Offer a Road Map to Alloy Design . . .

The last 10 years have witnessed the emergence of powerful theoretical tools that allow the calculation, from first principles, of the total energy of complex crystalline compounds and its dependence on structural parameters. To a great extent these developments have been closely linked to the increased availability of supercomputers. It is now possible to answer, from a strictly computational approach, some of the most fundamental questions raised by alloy designers, such as those regarding the relative stability of complex phases in metallic and semiconductor compounds.

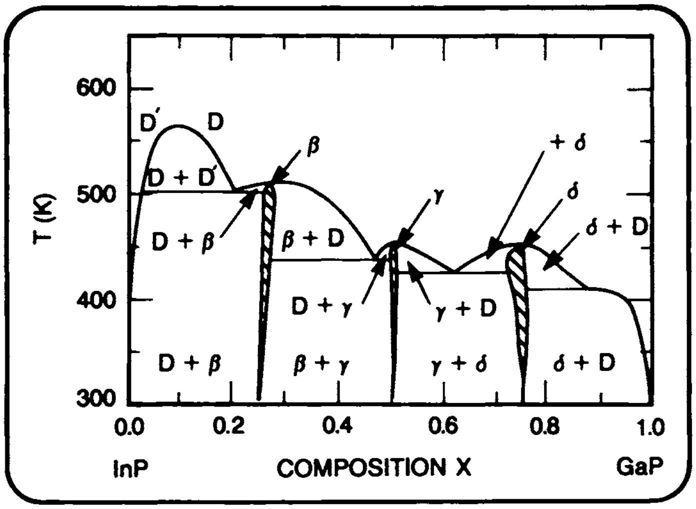
Recently, *ab initio* quantum calculations for ordered compounds have been extended to disordered alloys. With only the atomic number of the chemical species as input, researchers are studying alloy stability at finite temperatures and computing temperature–composition phase diagrams. As an example, the figure on the left below displays the experimental phase diagram and the calculated stability limit of solid-state phases for the palladium-rhodium system. The agreement between experiment and calculation (based on the Korringa-Kohn-Rostoker approach for disordered alloys) underscores the potential usefulness of quantum calculations in materials development. The challenge for the future will be to apply these algorithms to multicomponent systems and to compute similar phase diagrams for complex engineering alloys. In order to meet this challenge, and to profit from the benefits of accelerated alloy development, supercomputers are essential. For example, based on the binary phase diagram calculations, it is estimated that a ternary phase diagram would require several thousand hours of present supercomputer time.

Alternatives have also been proposed for studying alloy phase stability at finite temperatures. For instance, with the increased computational speed and memory currently available it is possible to calculate, for a given alloy system, the total energies of a large number of ordered compounds with different compositions and crystal structures. From these total energies effective atomic potentials can be obtained for the disordered alloys; and with the potentials, the temperature-composition phase diagram can be computed. An illustration is the phase diagram for the InP-GaP system, shown on the right below, which was obtained using the cluster variation method and a first-principles pseudopotential approach to calculate the total energies of five high-symmetry ordered compounds. These calculations offer convincing evidence for the existence of ordered phases in InGaP semiconductor alloys.

In the future the ability to compute phase diagrams is also likely to have considerable impact on the development of advanced materials based on metastable phases. Although metastable phases are potentially useful, they are particularly difficult to obtain with conventional experimental techniques. In fact, metastable phases are usually obtained in the laboratory only through extraordinary processing efforts, such as very rapid cooling or epitaxial growth. Supercomputers thus offer a cost-effective approach for the systematic investigation of these novel materials.

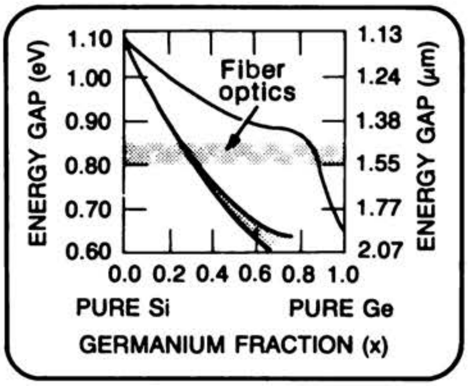


Supercomputer calculations (triangles) of the phase diagram of PdRh alloys are in excellent agreement with experiment (solid and dashed curves).



First-principles calculations of the phase diagram of InP-GaP semiconductor alloys reveal the existence of ordered phases (regions labeled β, γ, δ). These new-found phases are expected to impact the semiconductor industry significantly.

SiGe Layers Offer Alternatives with the Economic Advantages of Silicon . . .



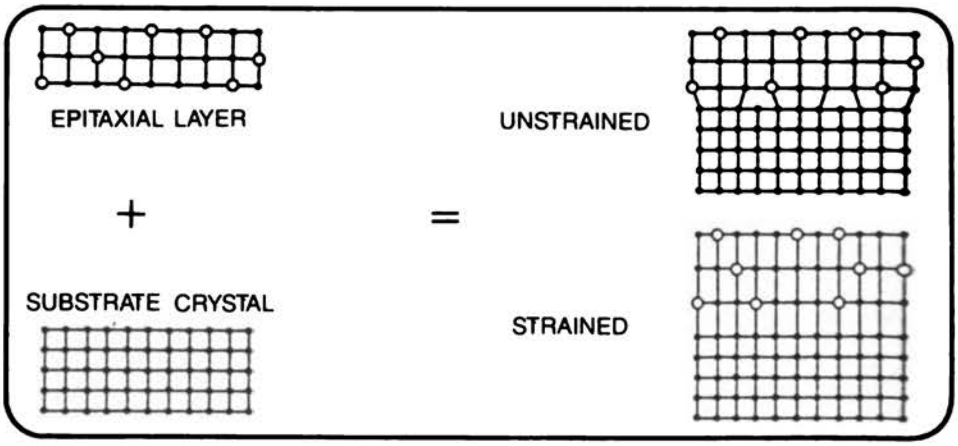
The calculated energy band gap for Ge(x)Si(1-x) semiconductor layers indicates what Ge fraction is needed for maximum optical efficiency. Upper curve: unstrained material; lower curve: strained-layer epitaxy on silicon substrates.

Although silicon is a poor light emitter because of its indirect band gap, it has definite economic advantages over other materials. This fact, together with the advantages of combining optical and electronic functions on the same chip, is currently motivating the "band-gap engineering" techniques being applied to silicon alloys. One concept that shows promise is to form an alloy of Si and Ge on the surface of a Si substrate.

For a SiGe alloy to match the minimum-loss wavelength in optical fibers, its band gap must be below about 0.85 eV. The upper curve in the figure to the left shows the variation in the band gap of pure SiGe alloys as a function of concentration. It implies concentrations of at least 50% Ge are needed. The lattice constant of Ge is 4% greater than that of silicon, however, and even in the 50% concentration range the SiGe lattice is 2% larger than silicon. When the 50-50 SiGe alloy is grown on a Si surface, this mismatch is large enough to produce an enormous number of "misfit" dislocations at the SiGe-Si interface. This phenomenon is known as incommensurate epitaxial growth. Although poorly understood, these defects are known to be catastrophic to optical processes.

Fortunately, sufficiently thin layers of SiGe can be grown on Si as a result of the natural compression of the spacing between atoms along the plane of the interface with Si, along with expansion perpendicular to the interface (see figure below). This technique produces commensurate or "strained-layer" epitaxy and eliminates the deleterious dislocations. An important question is whether this higher quality strained-layer epitaxy can be maintained for thicknesses large enough to be useful in device electronics, and if so, whether these layers remain stable over time.

In addition to eliminating misfit dislocations, strained-layer epitaxy also results in an even greater shift in the band-gap energy per Ge atom added to the SiGe alloy, as shown by lower curves in the upper figure: A 20% concentration of Ge will shift the band gap to the 0.85-eV range. The required lattice mismatch is then reduced to only 0.8%. However, to fulfill the promise of strain-layer superlattices as technologically important for future semiconductor devices, scientists need a better understanding of these materials and novel tools to model them.



When a Si(50)Ge(50) layer is ordinarily grown on a Si substrate, the mismatch in lattice constants produces undesirable misfit dislocations. The solution to this problem is strained-layer epitaxy.

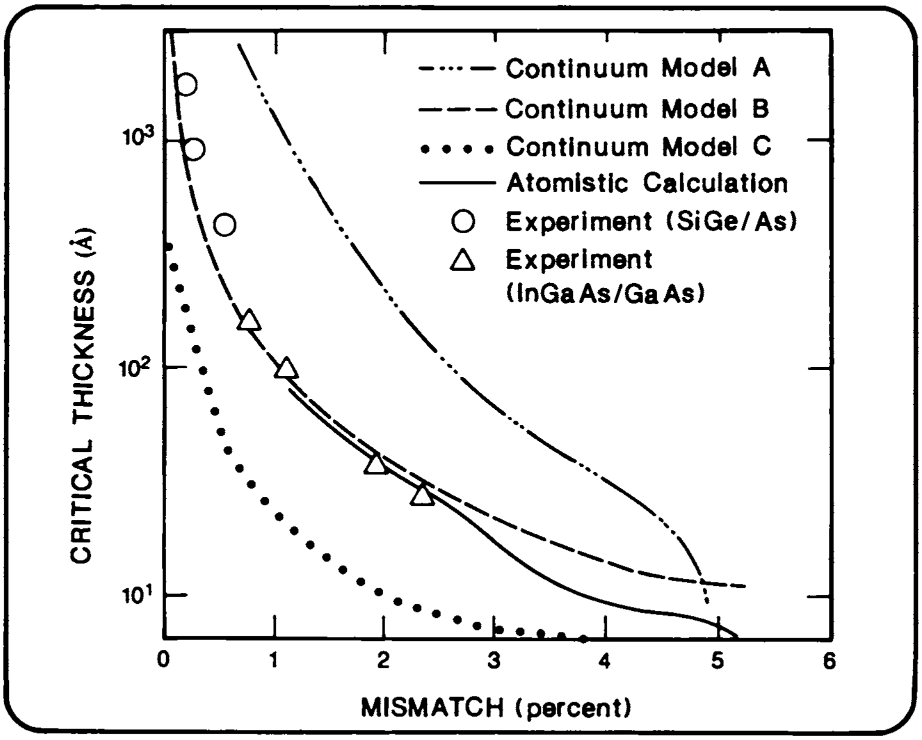
Computer Simulation of the Growth of SiGe Films Is Vital to this Technology . . .

If a thin film of SiGe is grown on a Si substrate, it begins as an epitaxial layer without misfit dislocations. With continued growth there is a critical thickness beyond which these deleterious dislocations are spontaneously generated. This thickness depends on the intrinsic lattice mismatch between the Si substrate and the alloy, and can be controlled by the alloy composition.

Various continuum models of solids and dislocations led initially to the concept that misfit dislocations are spontaneously generated whenever the energy expended in their formation equals or exceeds the liberated strain energy in the epitaxial layer. Although these continuum models appeared to provide qualitative understanding, they differed dramatically in their quantitative results. It was not clear which model should be trusted for very thin layers of atomistic dimensions, and even where one was trusted, if its prediction of absolute layer stability applied to the real strained-layer superlattice (which could be in a metastable state). Progress was made after a sufficiently large layer could be modeled on a supercomputer.

The supercomputer simulations provided two important answers. First, only one of the continuum models captures the correct physics, but its predictions become inaccurate at layer thicknesses of 2 mm and less (see figure on right). Second, epitaxial layers produced by molecular-beam epitaxy are actually metastable to much larger thicknesses than the critical thickness for absolute stability. This latter recognition has evolved to a concept of *critical thickness for metastability,* which is controlled not only by the lattice mismatch but also by the temperature that determines the thermally activated motion of dislocations from the substrate material to the epitaxial layer.

Even though the supercomputer has played a vital role in this research and development effort, further advances will likely make it an indispensable tool. Atomistic calculations of more complicated processes are being pursued with more realistic interatomic potentials, and first-principles calculations for the band-gap structure will have to be done in greater detail.



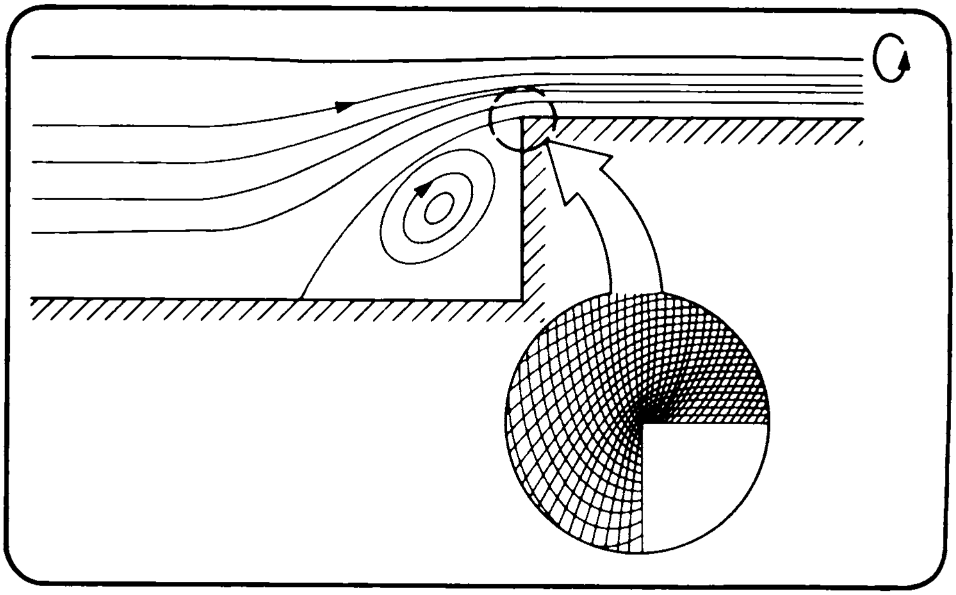
The critical thickness of a strained-layer heterostructure is the maximum overlayer thickness for which the resulting structure is thermodynamically stable. Thinner structures can be confidently assumed to be physically robust in applications, whereas long-term stability is questionable for thicker overlayers. The figure compares a recent atomistic computer calculation of the critical thickness for silicon-like strained-layer structures with experimental data and three continuum models. The atomistic calculation confirms one continuum model for large thicknesses and indicates that the structures are considerably less stable than predicted. This destabilization can be significant in considering potential applications.

The Vexing Problems with Polymeric Liquid Flows . . .

The need to produce fibers and extrude parts is found in almost every sector of the manufacturing industry. For polymers, both operations take place in the liquid state. Currently there is no reliable flow model to help design the necessary equipment.

Ordinary fluids (like water) can be described by a constant viscosity that does not depend on the fluid velocity. Such fluids are called Newtonian. Polymeric fluids are viscoelastic, which means that fluid deformation governs the local stress and viscosity. These fluids are decidedly non-Newtonian and exhibit flow phenomena strikingly different from those encountered with ordinary fluids. To predict these unusual phenomena (and thus enable the chemical engineer to control them) has so far been a most vexing problem.

There are two fundamental issues at the root of this problem. First, the constitutive law that determines the viscosity as a function of flow velocity gradients is not known *a priori* for either polymer melts or polymer solutions. Second, polymer flow problems are highly nonlinear and can only be solved by numerical approximation methods. One such approximation is based on dividing the fluid into many small but finite elements. For most finite element calculations, the finer the mesh, the more accurate the approximation. For polymer flows, however, the computed velocity fields are often uncertain, and it has not been clear whether the uncertainty is due to numerical artifacts or the fact that the constitutive law does not correctly describe the actual flow properties. Comparisons between computed and experimentally observed flow patterns have led to inconclusive results. And, as shown on the facing page, they have even led to misconceptions and erroneous beliefs. The causes are just now beginning to be unraveled.



Polymeric flow through an abrupt contraction has been difficult to model.

Benchmark Supercomputer Calculations Have Provided Unique Guidance to Polymeric Flow Theory . . .

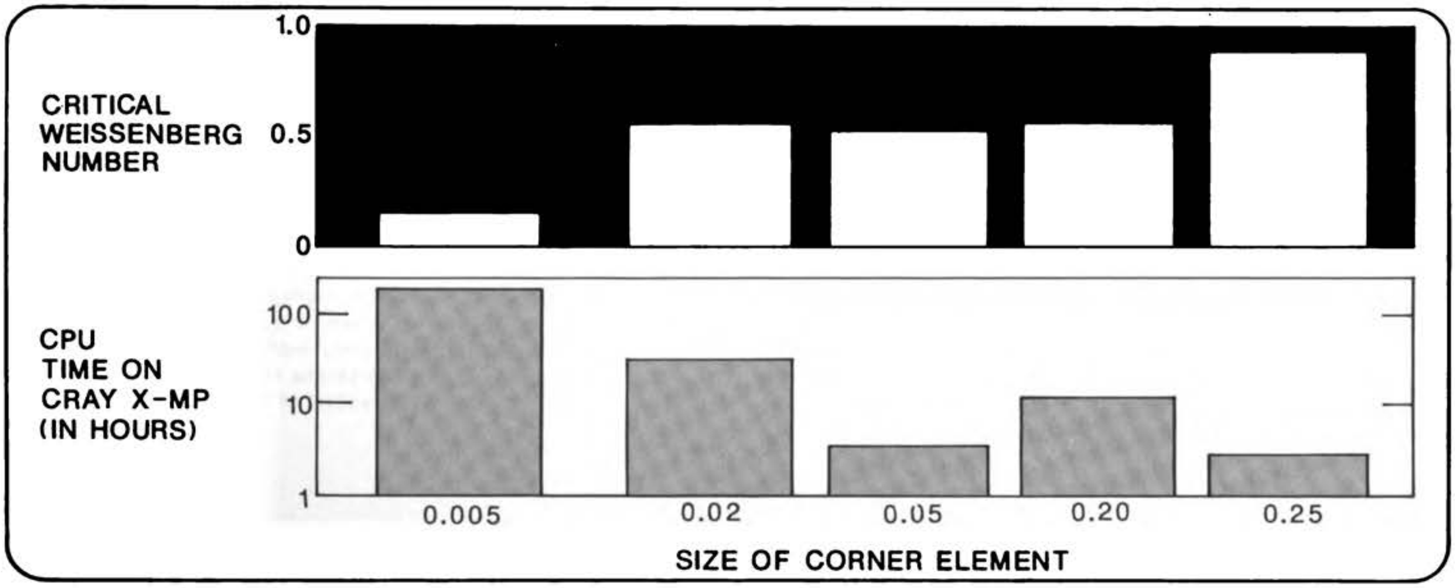
In ordinary fluid flow, an instability such as the onset of turbulence is characterized by a dimensionless number called the Reynolds number. In polymeric fluid flow there are also instabilities characterized by Reynolds numbers, but there are additional instabilities that are characterized by other critical numbers. One such instability occurs when a polymeric fluid flows through an abrupt constriction. Here the crucial quantity characterizing flow stability is called the Weissenberg number. It is a measure of (a) the rate at which stresses in a fluid build up due to flow constriction and (b) the rate by which the viscous flow relaxes these stresses. Increase in mass flow raises the Weissenberg number to a critical value, beyond which the flow becomes unstable and irregular.

When this flow problem was first solved with an intermediate finite element mesh for a polymeric fluid modeled by the simplest possible extension of Newton's flow law, the critical Weissenberg numbers approached an apparent asymptotic value between 0.5 and 0.6 (see figure below). This asymptotic value was considered to be real, in particular because it was similar to the value for a Newtonian fluid. However, using a supercomputer with a significantly refined mesh, the critical Weissenberg number was predicted to approach zero! (an unphysical result). This problem also demonstrates that ordinary computers are not only incapable of handling non-Newtonian flow, but they can even yield misleading answers and misguide research efforts.

The discovery of this breakdown of the critical Weissenberg numbers initiated much research and extensive computer calculations that were only possible with supercomputers. Researchers have concluded that the constitutive law does not adequately model the viscoelastic flow properties and the boundary slippage at sharp corners. Moreover, the apparent stabilization of the critical Weissenberg number at intermediate mesh refinements indicates that present finite element techniques are ill suited to deal with abrupt flow discontinuities.

There have been two major challenges in this relatively new field of non-Newtonian fluid flow. The first was to derive the actual form of the constitutive law from a molecular theory of the polymeric fluid. Although this has now been accomplished, the fundamental theory results in highly dimensional transport equations that require massive parallel computers for their solution. Fortunately, such computers are now becoming available.

The second challenge—the numerical solution of actual, three-dimensional flow problems—remains. New algorithms and numerical schemes are needed that go far beyond traditional methods; today's supercomputers are already taxed to their limits by two-dimensional flow problems. More powerful supercomputers are needed to solve real, three-dimensional flows encountered in polymer processing.



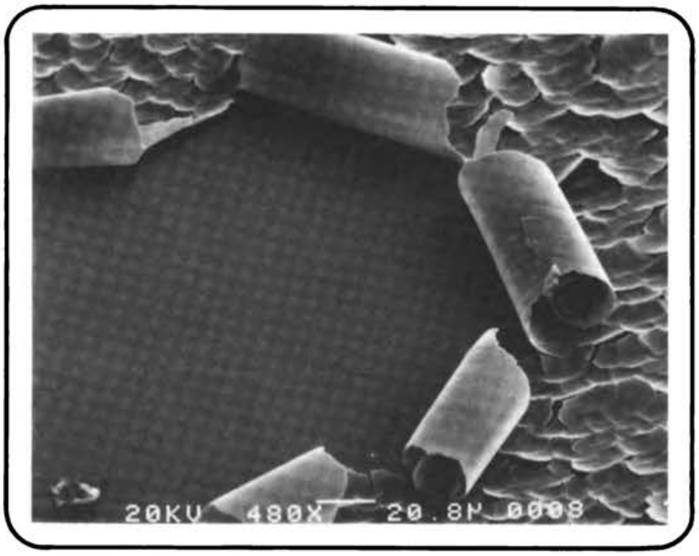
By revealing that a Newtonian polymeric fluid model yields unphysical results, supercomputer calculations have demonstrated their value as a methodology for evaluating new models in this field.

The Pervasive Nature of Adhesion. . .

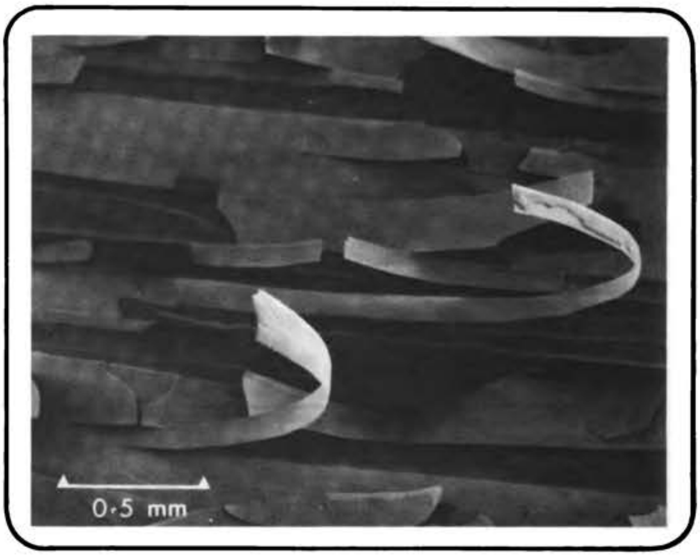
Adhesion is an integral part of diverse technologies, such as those involved with friction and wear, crack formation in materials, the performance of glues and switch contacts, and the integrity and packaging of thin-film devices like integrated circuits. The photographs below typify the adhesion problems that U.S. industry must solve regularly.

Despite the widespread character of adhesion phenomena, specific solutions are found primarily by small groups of engineers or scientists working for the industrial firms that encounter adhesive failure. Often these solutions are not recorded in the literature, and consequently the detailed mechanisms of basic adhesion are largely missing. Some examples of basic questions can be listed. Where does an interface fail, and how does this depend on the chemical structure, mechanical behavior and stress levels within the interface? How does the adhesive force depend on interfacial separation?

While encouraging progress has been made recently through new experimental probes of interfacial forces, effects such as elastic deformation and even interfacial defects are more readily included in computer simulations than isolated in experiment. Much of the future progress in adhesion research depends on advances in computer speed and new approaches to computer modeling of adhesion and its failure.



Vapor-deposited chromium films exhibit residual stresses that are compressive at the substrate and tensile at the surface. This example shows spontaneous delamination of a 400-nm chromium/50-nm copper film at the copper-glass substrate where bonding is poor. From Proc. 1987 EMSA, ©1987 San Francisco Press, Inc., by permission.



Oblique deposition results in highly anisotropic stresses in chromium films, causing them to spit and curl into hoops. Because chromium bonds very well to glass, fracture actually occurs in the glass substrate rather than at the interface. Reprinted with permission of the Materials Research Society.

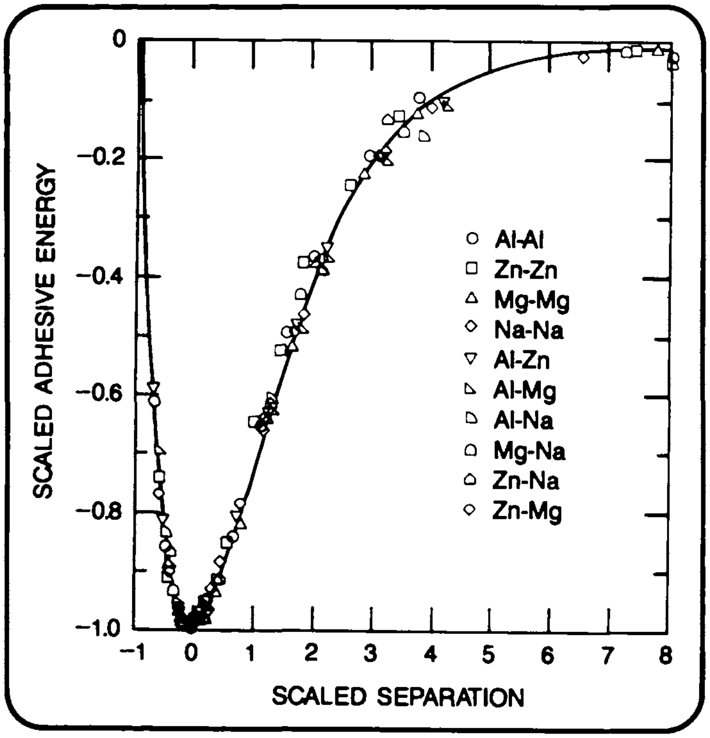
A Universal Adhesive Energy Relation Was Discovered by Supercomputing . . .

When two clean metal surfaces are brought into intimate contact, strong bimetallic interactions can occur. These interactions can be extremely strong because electrons can be exchanged between the two surfaces, forming the kinds of bonds present in bulk metals. This significant electronic rearrangement requires a fully quantum treatment of the bimetallic interface, in which the potential energy is determined by wave functions that are themselves solutions to the Schroedinger equation, i.e., the calculation must be self-consistent. That and the loss of symmetry at the interface have limited computations of adhesive interactions.

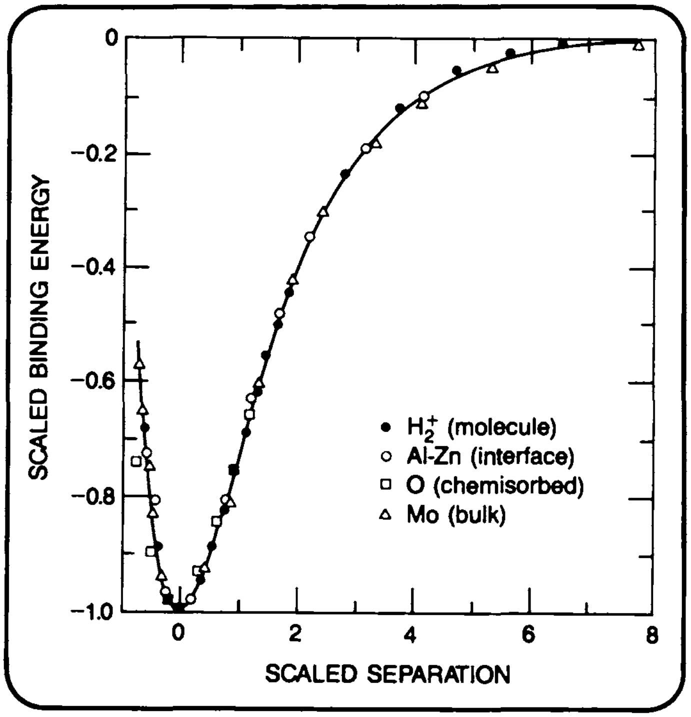
Recently, the total energy as a function of separation distance between surfaces was computed for a series of bimetallic contacts. For this calculation two (infinitely thick) solids were "brought" into intimate contact, and a fully self-consistent calculation of the electronic structure and total energy was performed for each interfacial separation of the surfaces. The range of strong adhesive forces was found to be about one interplanar spacing. In looking for trends, researchers found a simple scaling of the energy-separation curves. The energies were scaled by the energy value at the minimum of the curve (the equilibrium point), and the separation was scaled by a number such that the curvature at the minimum was the same for all scaled curves.

Results for ten bimetallic contacts are shown on the left below. The adhesive energies scale closely onto a single curve, i.e., there is a universal energy relation for adhesion. This unexpected result stimulated a search for universality in other forms of matter; typical results are seen on the right. There is a single energy relation that describes cohesion in bulk molybdenum, oxygen chemisorbed on aluminum, adhesion of the aluminum-zinc interface, and the energetics of the hydrogen molecular ion.

This discovery of an important characteristic of nature could not have been revealed without the extensive numerical computations possible on a modern supercomputer. Nonetheless, these calculations are limited to rigid adhesion in which the crystalline structure is not allowed to distort. Including distortion requires an order-of-magnitude increase in computational capability (or large blocks of time on current supercomputers); the next generation of computers will greatly simplify this task. Including impurities in the boundaries will require even greater capability although it could also be attempted with present resources. Including the effects of lubricants calls for massive computational capabilities that allow electronic structure calculations to be coupled with the molecular dynamics of polymer flow.

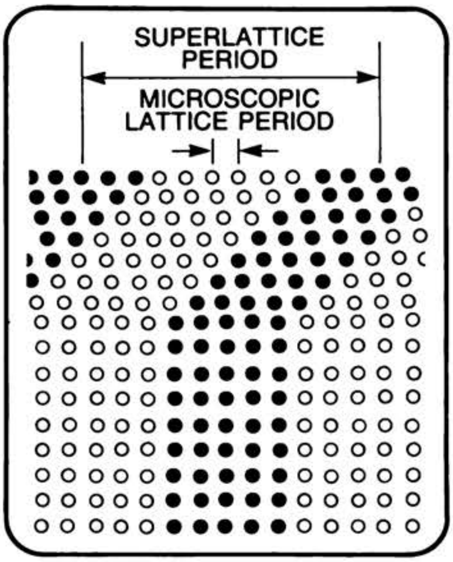


Extensive numerical computations on a supercomputer revealed a universal scaling relation for adhesion.



Additional computations revealed a universal scaling relation for molecular ion energetics, adhesion, chemisorption, and bulk cohesion.

Optoelectronic Materials Are Key Elements . . .



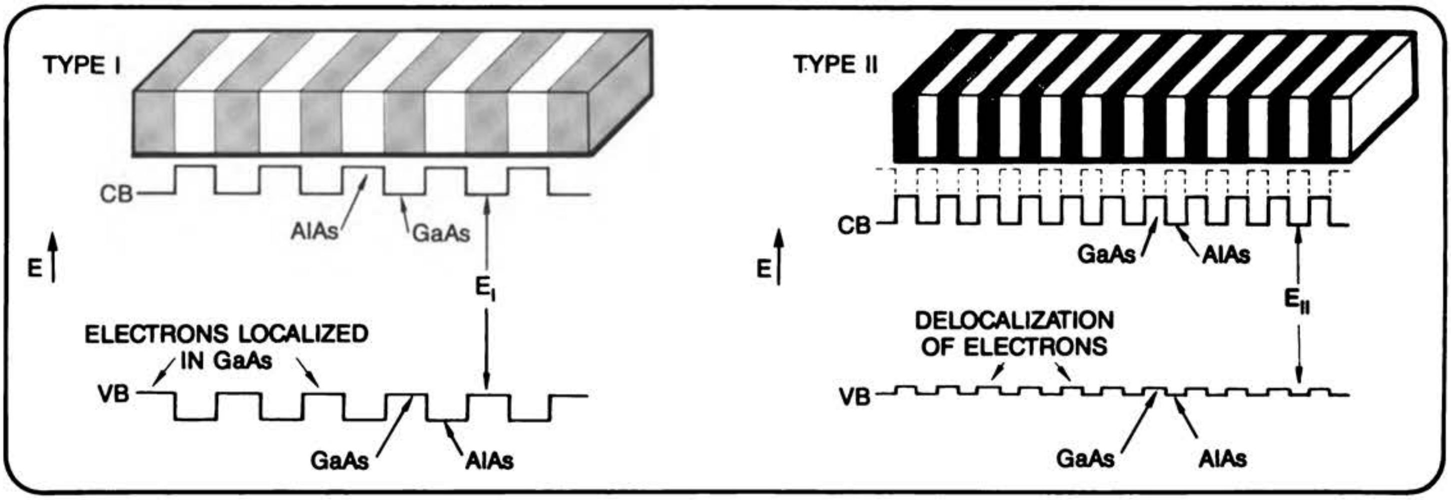
An important new material is the solid state superlattice. Consisting of alternating layers of semiconducting material, it has electronic properties different from those of either of its constituent materials.

Silicon is the mainstay of present-day semiconductor technology, but unfortunately it cannot efficiently convert electrical signals to light signals because of its indirect band gap. On the other hand, gallium arsenide (GaAs) efficiently emits coherent light at 0.88 μm (near-infrared). Although this initiated a technological revolution, 0.88 μm is not the optimum wavelength for many purposes. For example, optical fibers have their lowest loss per kilometer at 1.55 μm. New materials are being sought where band gaps are tailored to these and other needs. One way of doing "band-gap engineering" of these needed materials is through the use of superlattices.

Superlattices (see figure on left) consist of alternating layers of semiconductors with different band gaps, which split the valence band (VB) and conduction band (CB) into minibands separated by minigaps. GaAs is often chosen for one layer (because of its direct-band-gap optical properties), with AlAs or $Ga_{1-x}Al_x$ chosen for the second layer (each has a larger band gap than GaAs). The properties of the final composite heterostructure differ from those of either of the component materials. The superlattice band gap can be tailored by varying the concentration of Al and the thickness of the layers.

When the number of layers in the superlattice period is large (greater than about 10), the band gaps resemble those of the constituents, and a type I superlattice is said to have formed. When the number of layers in the superlattice period is small (less than about 10), the conduction band of the AlAs substructure is brought down below that of GaAs, and a type II superlattice forms (see figure below).

Increasingly more complicated heterostructural devices are being designed. Ultrathin layer upon ultrathin layer of materials can be formed by chemical vapor deposition or molecular beam epitaxy, making the need to understand these structures on an atomistic scale increasingly more important.



Depending on the number of layers in the superlattice period, a type I or type II superlattice forms. The band gaps of properly designed type II superlattice should make them ideal optoelectronic materials.

The Electronic Properties of a Superlattice Can Be Designed by a Supercomputer . . .

Bandstructure engineering can now be done on supercomputers. Although some of the properties of superlattices were first predicted from quantum arguments, it was impossible to compute band-gap alignment between two semiconducting atomic layers before very large-scale computers became available. Only recently has the full power of quantum theory been applied to the design of these novel materials.

Self-consistent calculations (based on local density theory) are being used to study GaAs$_n$AlAs$_n$ superlattices. The calculations are performed as a function of n, the number of atomic layers in each minilayer of the superlattice. The lattice mismatch between GaAs and AlAs is known to be only 0.5%, thus eliminating interfacial defects from the calculation (see discussion of Si-Ge layers on pages 18–19).

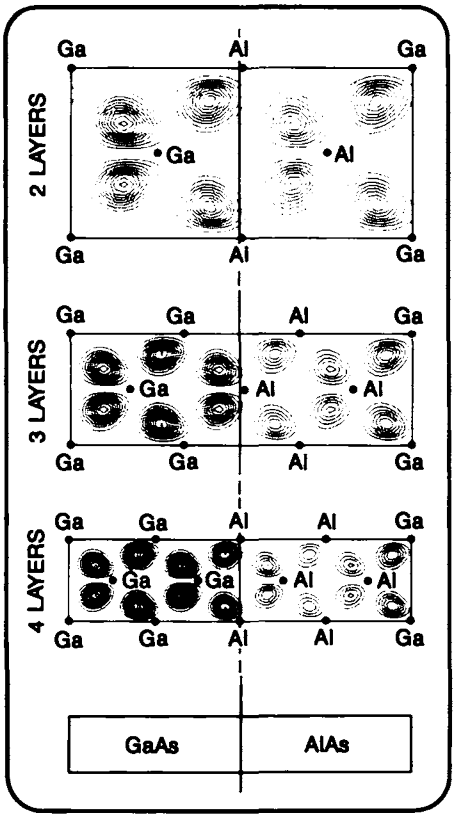
The calculations predict that the qualitative features of the localization of the valence band to the GaAs region are not substantially affected by the number of atomic layers in each period. However, the bottom of the conduction band (the lowest unoccupied level an electron must reach in order to conduct electricity) is quantitatively and qualitatively changed by this superlattice period. For large n (>10), the band gap lies within the GaAs substructure (just as it does for bulk lattices), as depicted by E_I in the figure at the bottom of the preceding page. The calculations also show that for $n < {\sim}10$, the conduction band of the AlAs substructure is brought down below that of GaAs, as depicted by E_{II}.

The figure to the right plots the calculated charge density associated with the highest occupied valence band state for 2, 3, and 4 atomic layer superlattices. For n = 2 there is virtually no preference for the electrons on either the GaAs or AlAs sublattice. As n increases, there is significant localization of the electron charge in the GaAs region. This localization is consistent with a barrier model for the highest valence band electrons. For large n there is a small "leakage" across the barrier from the GaAs to the AlAs region, but the leakage accounts for only a small fraction of the total thickness of the layer. For small n, the leakage is across nearly the entire sublattice and hence the localization disappears.

Similar quantum calculations on SiGe superlattices must include strain effects because of the enormous (4%) lattice mismatch. The results show that the band discontinuities depend strongly on the specific strain conditions.

The calculations have been extended to predict the phase stability to be expected when the atomic layers are formed. Molecular beam epitaxy permits the superlattice to be constructed layer by layer, but diffusion of, for example, Ga into the AlAs layer could lead to the formation of a disordered structure, Ga$_{1-x}$Al$_x$As. The interface between the two ordered structures would then be removed along with its value as a device. For x = 0.5, the calculations indicate that the ordered heterostructure is preferred by 0.06 eV.

The ability to tailor band gaps to technological need has massive economic implications. The time-consuming and costly trial-and-error approach can be replaced by supercomputer quantum theoretical calculations that guide the engineering of new materials.



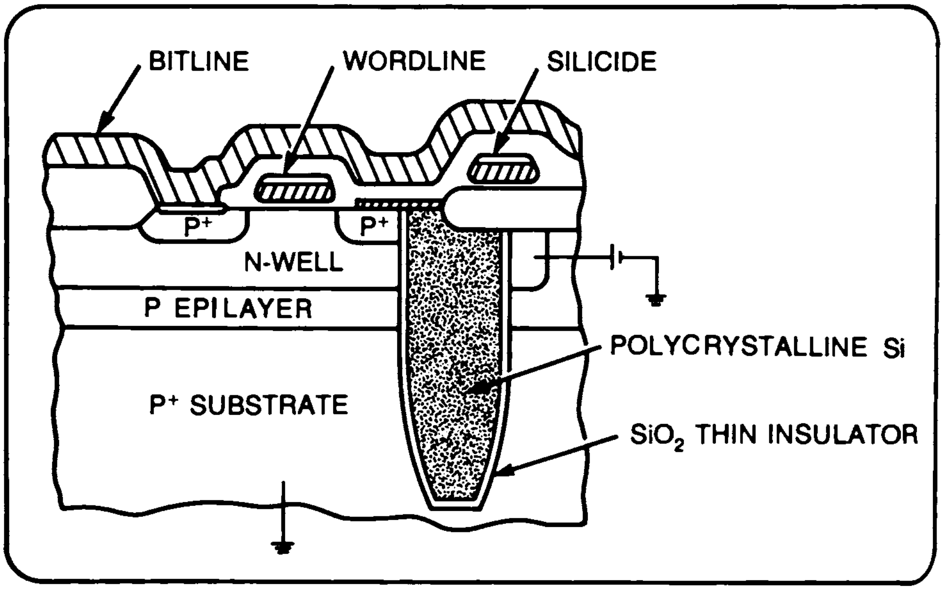
Charge density calculations for a GaAs$_n$AlAs$_n$ superlattice, as a function of the number of layers n, are leading to a new understanding of these novel materials.

Silicon Oxidation Is a Crucial Process in Advanced Microelectronics Development . . .

In comparison with other semiconductors, silicon is distinguished by the ease with which a chemically stable oxide can be grown on its surface and by the almost perfect nature of the electrical characteristics of SiO_2-Si interfaces for microelectronics applications. These characteristics have been and continue to be largely responsible for the domination of metal-oxide-semiconductor (MOS) technology in electronics. In the rapid and highly competitive world of microelectronics development, recent trends toward smaller and highly nonplanar (three-dimensional) device structures have made the oxidation of shaped silicon surfaces crucial. Many unexpected and critical phenomena have been uncovered in these new device geometries, whose precise control in the manufacturing of future microcircuits may well give U.S. industry a competitive edge.

It is now clear that the stresses produced by volume expansion during oxidation will cause viscous flow in the oxide film, influence oxidant diffusion (and thereby film growth), and affect the shape and the electrical properties of the device structure. As the SiO_2 dielectric layer in MOS structures becomes less than 50 atomic layers thick, these stress effects must be precisely predicted and controlled in every part of a microelectronic device, and this can only be accomplished with the help of supercomputers.

An example where nonplanar thin oxides are critically important is for dynamic random access memories (dRAMs). The figure below shows the cross section of one storage cell in a 1-megabit dRAM. The critical area is the corner of oxide-semiconductor interface; its properties determine to a large extent the yield and reliability of the dRAM.



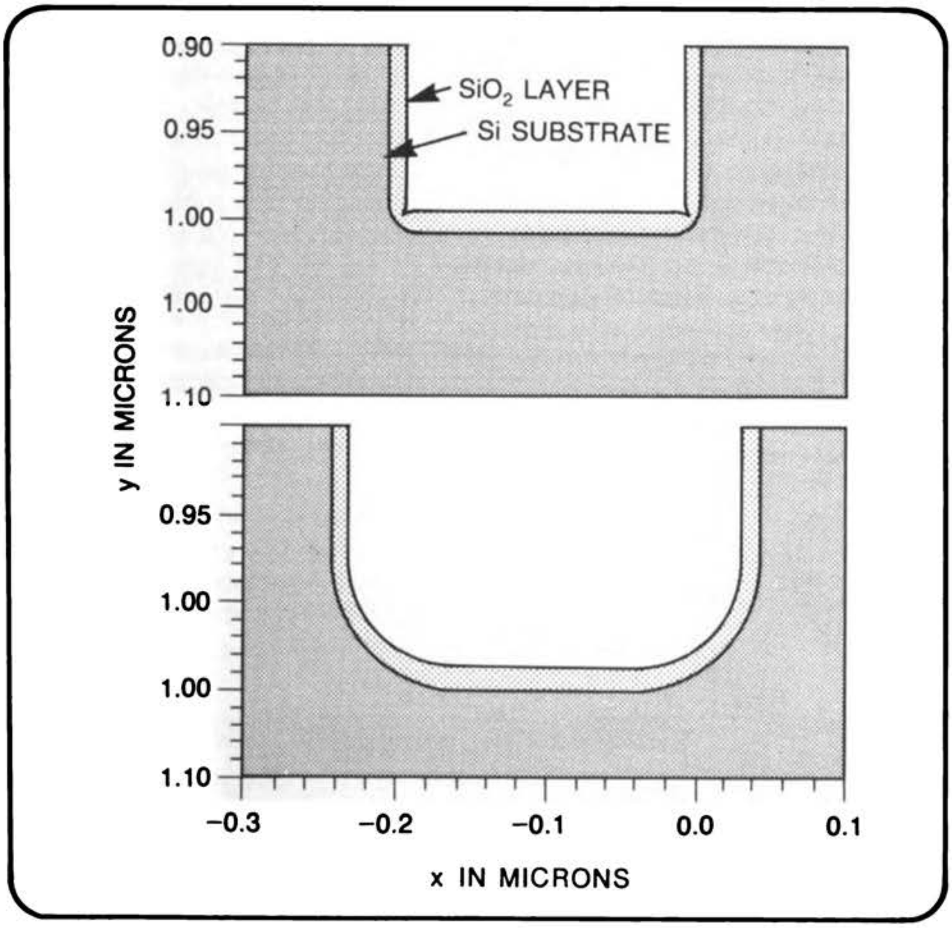
Details of a cross section of a dynamic random access memory (dRAM) showing the critical trench capacitor (dark region encased in a thin insulating layer of silicon dioxide). The stresses in this layer are critical to the performance of the device. P, P+, and N indicate the type of doping in the various semiconductor regions.

Detailed Understanding of Silicon Oxide Layer Growth Is a Highly Leveraged Opportunity for Supercomputing . . .

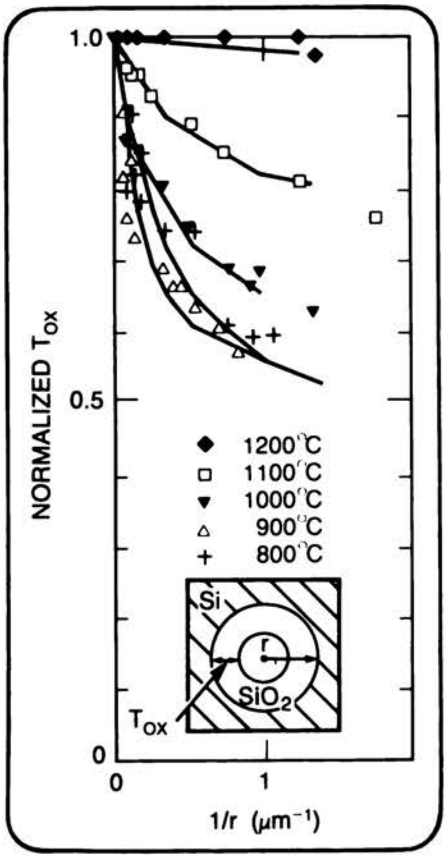
The quantitative prediction of nonplanar oxide film growth will enable us to reduce the time and cost for the design of new microcircuits and to better control the manufacturing of these circuits. Although complete modeling is beyond the capabilities of present supercomputers, software development is already under way.

To illustrate the power of present two-dimensional models the figures on the left below show computer simulations for two different fabrication sequences. The top figure is for a single-step oxidation process, which results in a thinner corner region with an undesirable high electric field strength of 1200 V/cm. In contrast, a two-step oxidation process produces a more uniform oxide layer, as shown by the bottom figure, with a dramatically reduced electric field strength of only 400 V/cm.

Two-dimensional calculations such as these are assisting in the design of isolated structures in present microcircuits. These models are not, however, comprehensive enough for computer-assisted design of entire dRAM cells and the processing steps for their manufacture. For this to be accomplished, more detailed physical models are required for stress-assisted oxide film growth in three dimensions, including such phenomena as oxidation-enhanced diffusion and the redistribution of defects and doping atoms. Supercomputers will become an indispensable tool in this endeavor.

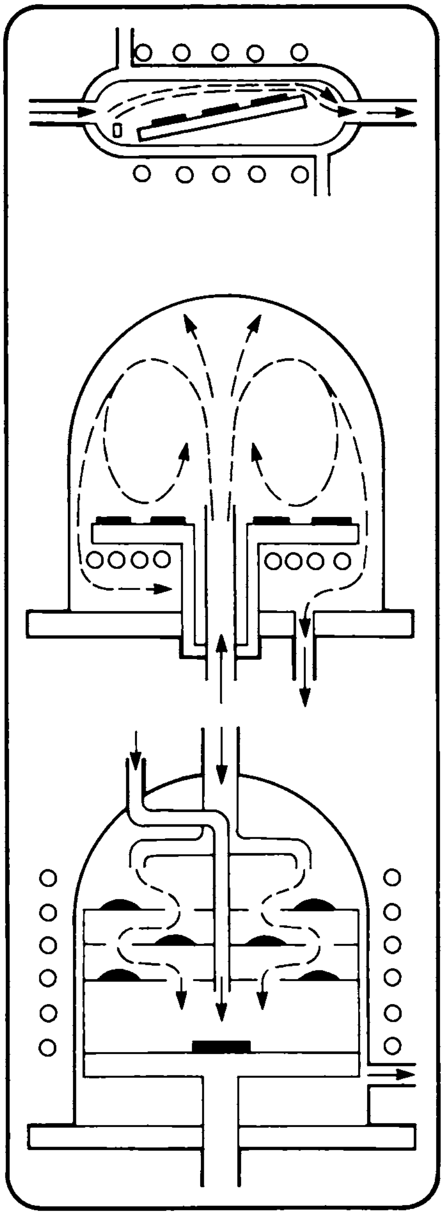


Results of computer simulations of the thin silicon dioxide insulator layer in a trench capacitor for a dRAM.



Wet oxide thickness grown on a cylindrical silicon structure, normalized to the oxide thickness grown on flat (110) surface (about 0.5 μm), versus the final curvature of silicon surface. Data points are experimental results and solid curves are model fits. These results show that misfit stresses generated in the oxide layer reduce the oxidation rate at lower temperatures.

Chemical Vapor Deposition Is Critical to Semiconductor Manufacturing . . .

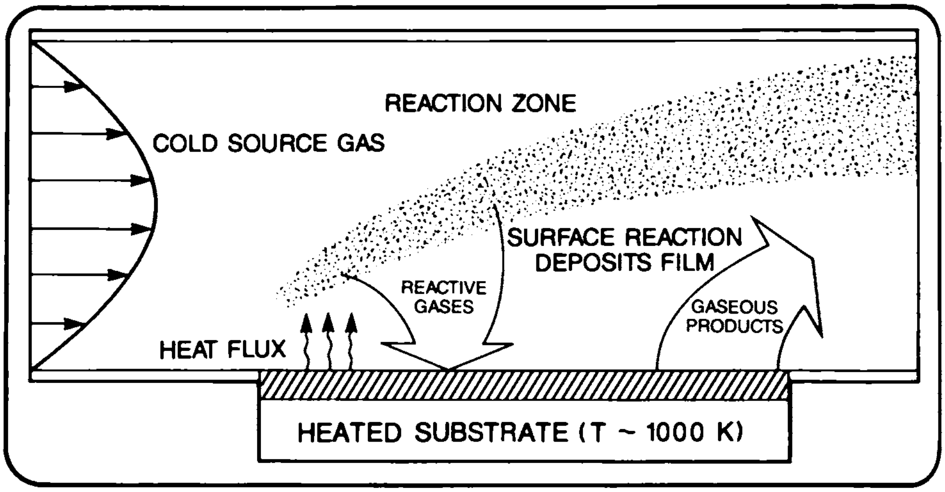


Production CVD reactors come in many geometrical designs.

Chemical vapor deposition (CVD) is an increasingly important process in the United States and other countries for fabricating electronic components. Much of the emphasis on CVD in the microelectronics industry stems from the fact that it is well suited to producing silicon films, which are essential in high-performance chips.

The process begins by passing an active gas, such as silane (SiH_4), over a substrate maintained at a temperature on the order of 1000 K. As the heat is transported away from the substrate by convection, diffusion, and radiation, the active gas chemically decomposes to form species that are very reactive on the substrate itself. Upon reaction at the substrate, a solid (for example, silicon) is deposited and a volatile product (e.g., H_2) is released back into the gas. Although this process is employed in semiconductor production today, the understanding of the process is still incomplete. Many reactors are designed by empirical rules and, as a result, are notoriously unreliable.

Important issues in the fabrication of semiconductors with CVD are deposition rate, deposition uniformity, and sharpness of interfaces between adjacent layers in compound semiconductors. A designer can control the reactor geometry, the flow rates of gases through the reactor, the flow rate distributions at the inlet of the reactor, the rotation rate of the heated substrate in the case of a rotating disk reactor, the thermal boundary conditions on the walls of the reactor, the temperature of the substrate, and the reactant gas mixture and pressure. Production reactors employ a variety of geometrical designs (as illustrated on the left and below), further complicating attempts at understanding this important materials process.



In this schematic of a horizontal channel CVD reactor, a cold inlet gas (such as SiH_4) reacts in the zone above a heated inert material (referred to in industry as the *susceptor*). Surface reactions result in the deposition of silicon and the production of volatile gases, which exit to the right.

Computer Simulation Is Guiding Chemical Vapor Deposition Reactor Design . . .

A multidisciplinary effort involving quantum chemistry, chemical kinetics, heat transfer, fluid dynamics, numerical analysis, and computer science is focusing on chemical vapor deposition. The effort is an outgrowth of research on combustion chemistry in which flow reactors, premixed flames, and diffusion flames are simulated. Common to all of these are large systems of gas-phase chemical reactions and complex molecular transport.

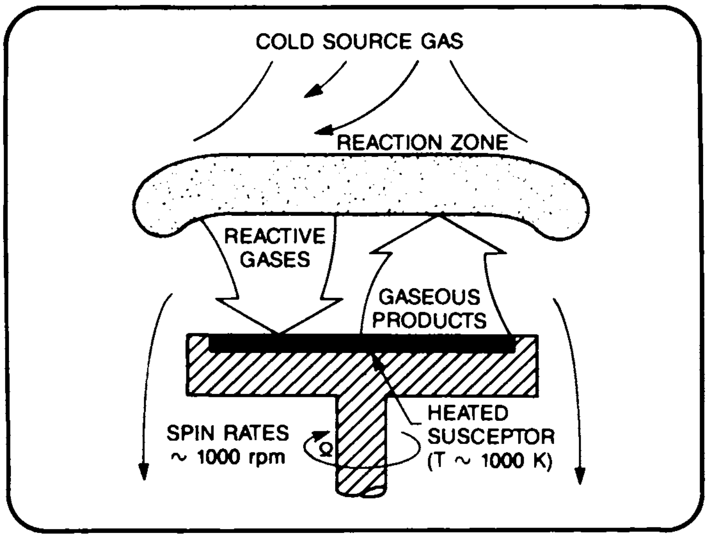
The simulation requires, as input, detailed thermodynamic properties for all the reacting species, including the source gases and all intermediate and product gases. Often the thermodynamic properties are not accessible by experiment, but state-of-the-art quantum chemical computational techniques can determine properties accurately. Rate expressions are also needed for all reaction paths, in the gas phase as well as on the surface. Although the most important rate constants must be measured experimentally, rate determinations can often be difficult. Fortunately, statistical reaction rate theory provides the tools to make accurate estimates.

Once the chemical reaction mechanism is established, conservation principles are used to derive equations that describe the complex interplay of fluid and heat transport with the chemical processes. The exact form of these large systems of partial differential equations depends on the particular reactor configuration. Typically, the system of equations is "stiff" (meaning that some of the chemical reactions are very rapid, while others are very slow). Such a system requires sophisticated mathematical techniques for its solution.

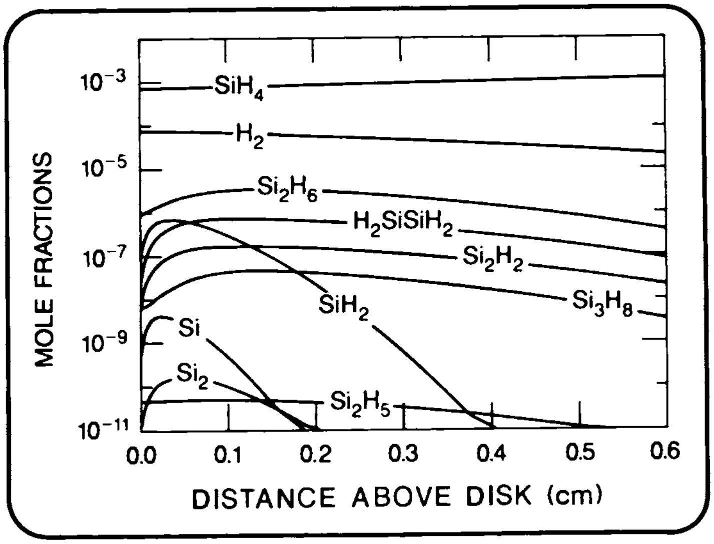
Initially this elaborate simulation was applied to the horizontal channel reactor (previous page) where the importance of gas-phase chemistry was first demonstrated and later confirmed by experiment. More recently a rotating-disk reactor was modeled (see below). The heated substrate rotates at 1000 rpm in a cylindrical shroud through which the reactive gases flow. The advantage is that the species and temperature gradients normal to the disk can be made to yield a highly uniform deposition. The simulations show that, at low temperatures, the rate of deposition of Si from SiH_4 is determined by the rate of reaction of SiH_4 on the rotating surface. At intermediate temperatures the rate-limiting step is the gas-phase chemical kinetics, and at high temperatures it is diffusion. The effect of disk rotation on the rate of deposition was shown to depend on the process controlling the deposition.

These simulations have had a substantial impact on commercial reactor design through industrial interactions. The simulations are being used to guide the choice of temperature, total flow, pressure, and rotation speed in a production reactor. They would not be possible without a large number of supercomputer calculations, ranging from the solution of basic quantum phenomena to the detailed solution of macroscopic transport.

In the future, greater supercomputer capabilities will permit the chemistry and fluid flow to be even more closely coupled in CVD simulations. Other semiconductor materials processes, such as plasma etching, will also be simulated; and other processing concerns, such as the flow of particulate contaminants, will be accessible to simulation through hierarchical modeling.



The fluid flow and heat transfer in a rotating disk CVD reactor have been simulated and used by industry to guide growth conditions and reactor design.



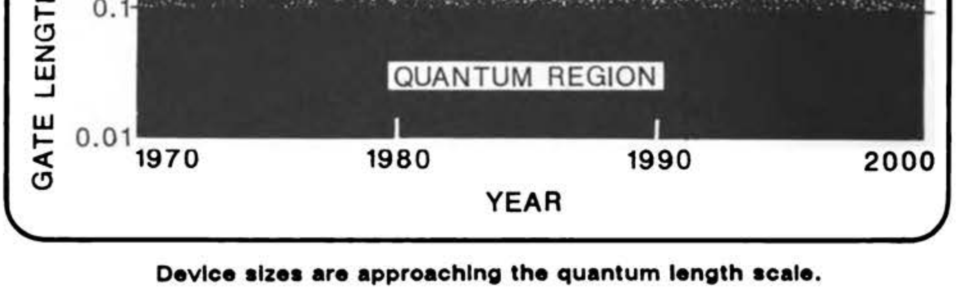
Predicted density profiles of various chemical species as functions of height above the spinning disk.

Increased Complexity Is Driving Device Physics Toward Supercomputing . . .

The continued growth of the electronics industry depends on a continued increase in packing density (number of components on a chip) so that electrons can travel over shorter and shorter distances. This trend in device miniaturization leads to inherently three-dimensional characteristics and to quantum behavior of electron transport in semiconductor materials. The development of a new semiconductor chip is greatly complicated by these effects; each design iteration can cost hundreds of thousands of dollars and take months for engineers to learn the effect of design parameter variations.

Fortunately, electron transport calculations in semiconductors have evolved to a level of sophistication sufficient to be of value to the device engineer. The area of transport analysis has been greatly affected by the numerical techniques of modern physics. Modern Monte Carlo simulations now incorporate realistic descriptions of the relationship between an electron's energy and its momentum (the "band structure" of the solid) instead of resorting to adjustable parameters to calculate electron transport properties in bulk materials. Furthermore, the scattering (deflection) of an electron by the vibrating atoms of the solid (phonons) and the ionized impurities in the solid can be meaningfully included. The results of these simulations are in excellent agreement with experiment and have been useful in understanding the physics of fast electrons in semiconductors (hot carriers). More recently, Monte Carlo techniques have been used in the area of real space electron transfer in order to model a number of electronic devices (see example on next page).

Today, supercomputer simulation can make a major economic impact on semiconductor device design. As the scale of device structures decreases, however, the physical methodology must include a more quantum description of the electron transport. Current studies are limited to quantum calculations on simplified model systems. The inclusion of fully quantum techniques in a device modeling code will require not only an increase in computer power but also improvements in the basic physics of time-dependent phenomena.



Device sizes are approaching the quantum length scale.

Revolutionary Devices Can Be Realistically Modeled . . .

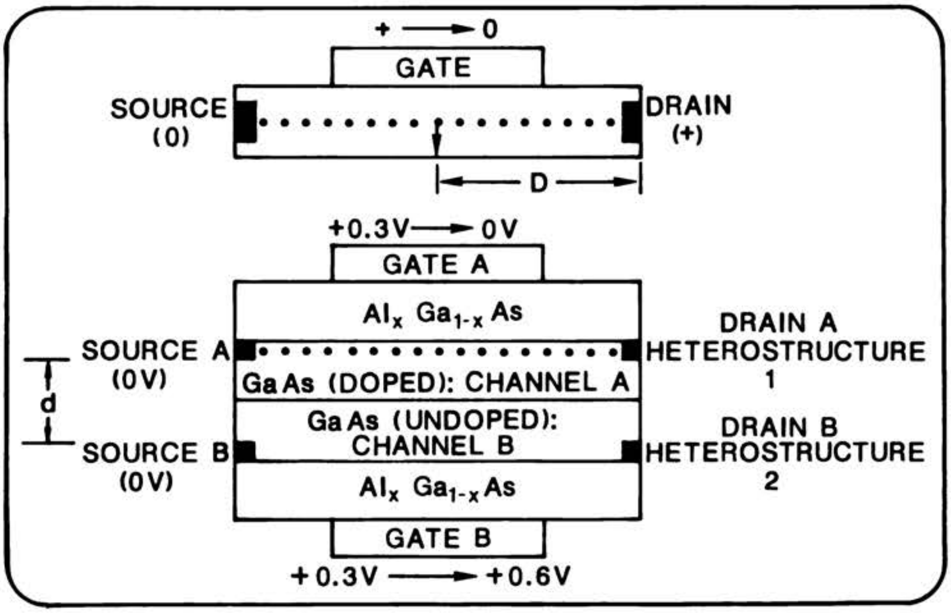
With recent advances in semiconductor device simulation it is now possible to assess the advantages of novel device structures before incurring hardware development time and costs. The *velocity-modulated transistor* concept provides an example.

In a typical semiconductor switch, electrons flow from the source (at zero potential) to the drain (biased positive) while the gate is biased positive (see figure below). When the gate is switched to zero, electrons no longer flow; the characteristic switching time is that required for the electrons under the gate to travel a distance of order D (0.5 μm) to the drain. Device designers requiring ultrafast switching times have proposed a velocity-modulated transistor (VMT), which capitalizes on the extremely short perpendicular transit times between two adjacent channels separated by a much shorter distance, d.

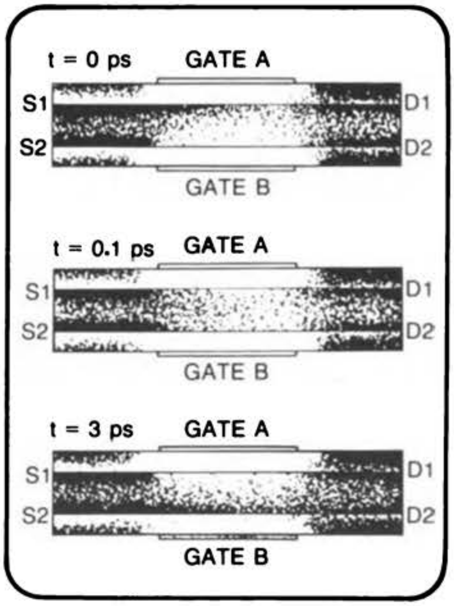
The VMT concept involves switching from a state with both sources at 0 V, both drains at +0.3 V, and both gates at +0.8 V. At t = 0, gate A is switched to 0 and gate B to 0.6 V. Electrons flowing in channel A (GaAs, doped region) are suddenly accelerated to gate B, an order-of-magnitude smaller distance than that for a traditional transistor switch. Such a design involves optimizing such parameters as the $Al_xGa_{1-x}As$ alloy composition, degree of doping of the GaAs channel A, heterostructural thicknesses, geometry, and operating temperature.

The results of the Monte Carlo simulation of this device are shown to the right. The simulation includes complete band structures for the GaAs and AlGaAs regions and the effects of all physically important scattering mechanisms (i.e., polar optical phonon scattering, equivalent and nonequivalent intervalley scattering, ionized impurity scattering, and impact ionization). The dark areas show how the electron density changes with time following switching. It was found that indeed there is a fast (roughly 0.2 picosec) electron transfer between channels A and B but a much slower (roughly 3 picosec) redistribution of electrons between the channels that dominate the switching process. This redistribution depends on the impurity concentrations in the channel regions. The switching times for the VMT were 2.0 to 3.0 picosec at 300 K and about 2.4 picosec at 77 K, significantly shorter than for a more conventional high-electron mobility transistor (over 3.5 picosec at 300 K and about 3.2 picosec at 77 K).

Future semiconductor device modeling will rely even more heavily on supercomputing as shorter length scales involve quantum effects not dominant in today's devices. The reduction in the time and cost between concept and finished product will be a driving force.



Electrons in a traditional transistor (top) must travel a distance D to turn the device off, whereas in a VMT, electrons need only travel a much shorter distance d.

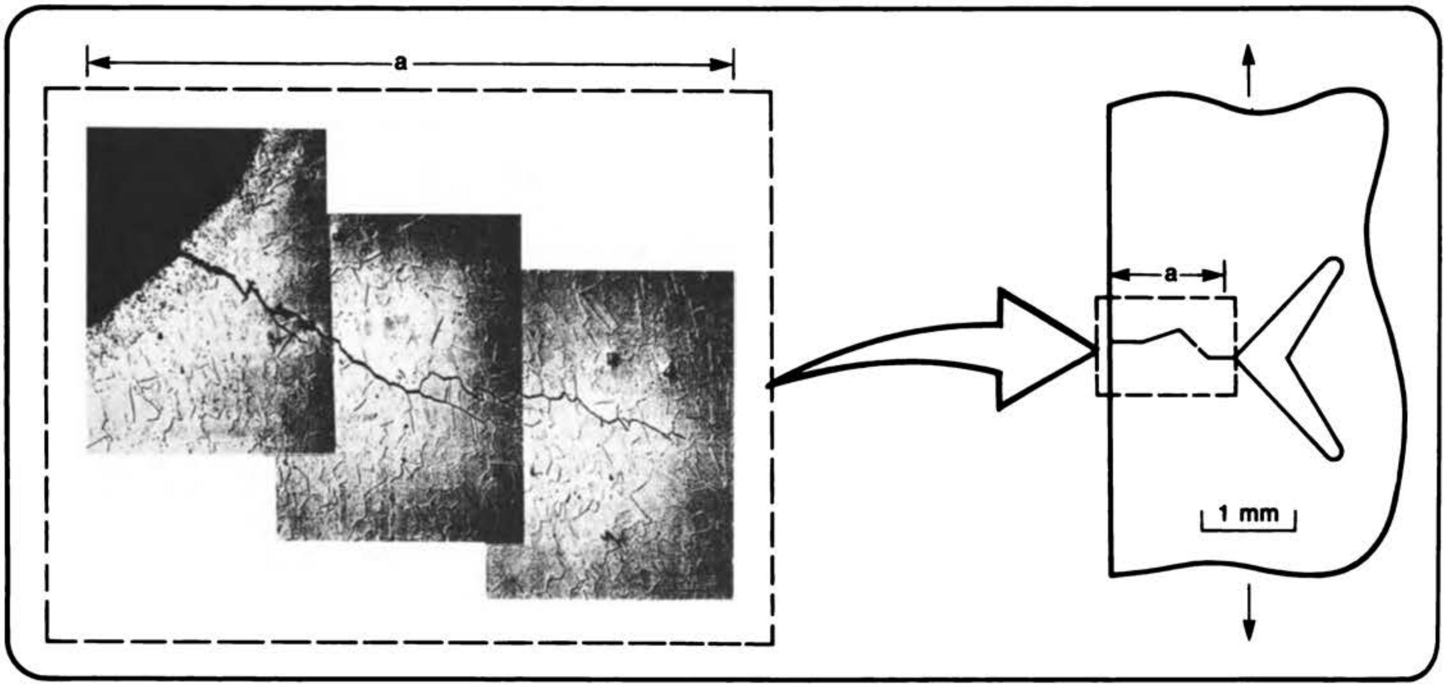


Electron transfer from channel A to B in a VMT from 0 to 3 picosec. Electron density is indicated by the degree of darkness in each plot.

Prevention of Fracture Requires a Detailed Understanding of Materials at All Levels . . .

It is inconceivable to imagine our technological society functioning without metallic materials. Their greatest attribute is that they can be fashioned to have great strength and at the same time an unmatched capacity to resist fracture. The latter property, the fracture toughness, must be carefully balanced against the yield strength, which determines the beginning of plastic deformation. Many improvements and advances in the design of parts for the automobile and aircraft industries originated from the improved understanding of the mechanics and physics of fracture and its relationship to the microscopic details of complex alloys. Dramatic improvements in this class of materials are still to be expected, provided we can bridge the gap between macroscopic fracture mechanics and the atomistic theory of cohesion in solids.

Ongoing research and progress in metal plasticity and atomistic fracture physics, made possible by supercomputers, provide clear evidence that this gap is closing rapidly and that the improved understanding of all aspects of the fracture of metallic materials will be of great technological significance. For a typical surface crack, shown below in the micrograph and schematically in the adjacent drawing, finite element calculations now routinely give the stress intensity factor, which is used in engineering design. Only recently, however, have computations of the plastic zone emanating from the crack tip become possible. Similarly, atomistic computer simulations at the very tip of a crack are only now becoming a reality. The ability to study all aspects of metal fracture simultaneously awaits a more powerful generation of supercomputers.



Left: Micrograph of a typical surface flaw in stainless steel. Right: Schematic of the plastic zone at the tip of the flaw. The nature and extent of the plastic zone determines a material's fracture resistance.

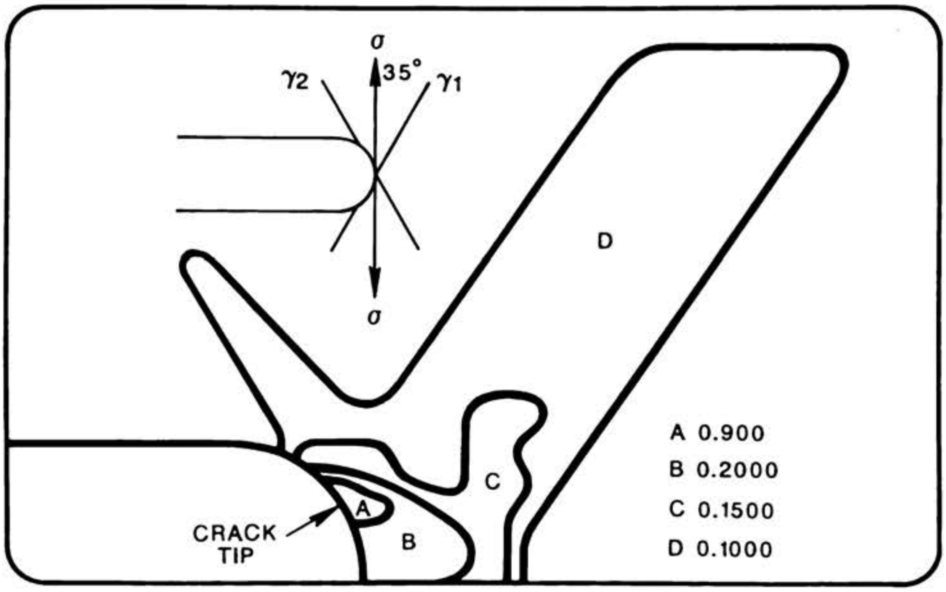
Micromechanical and Atomistic Fracture Calculations Will Lead to Improved Materials Performance . . .

What distinguishes ductile from brittle or cleavage failure at the most fundamental level is the generation of dislocations and plastic deformation at the crack tip. Plasticity on a small scale accompanies even intergranular failures caused by grain boundary embrittlement and other environmentally induced failures. At this small scale, the plasticity near the crack tip is greatly affected by the discrete slip planes of the crystal lattice structure as well as by the rearrangement of the atoms when individual dislocations emanate from the crack tip.

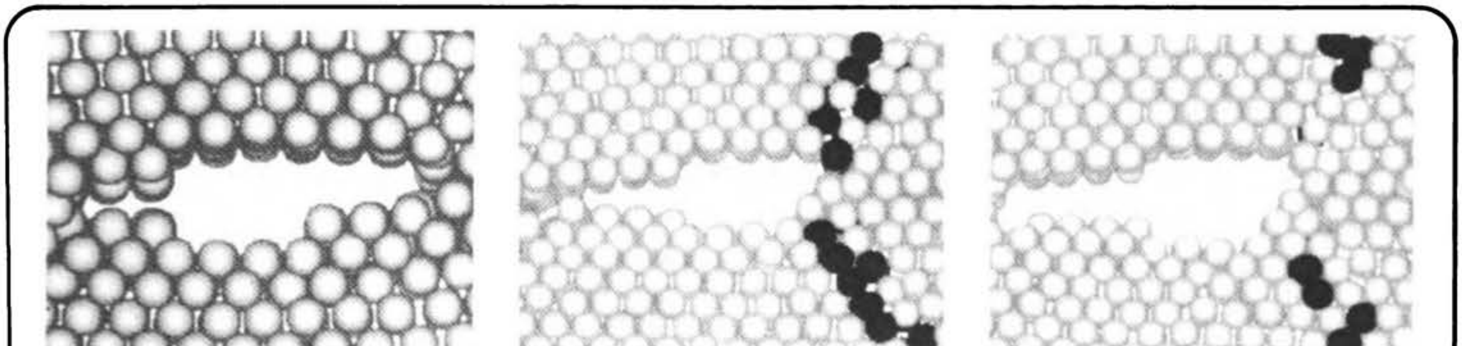
These two aspects can now be investigated in detail with the help of supercomputers. The upper figure shows the plastic zone at the crack tip in the crystal lattice of a body-centered-cubic metal. In these calculations, plasticity is described with the actual discrete slip systems and in accordance with nonlinear, finite deformation theory.

At a more fundamental level, the atomistic scale, interatomic cohesion in metals can now be described by formulations such as the embedded atom method, which is firmly based on density functional theory. With this method, molecular dynamics simulations are being carried out on disordered systems containing many atoms and subjected to external loads. The panel of three figures below, a simulation of dislocation emission from a crack, illustrates the capabilities of this method. Atoms associated with the cores of dislocations are shaded for easy visualization. The figures represent a small selection of the sequence of events that accompany the crack growth during plastic tearing.

These two examples represent a hierarchical approach to achieving a more fundamental understanding of fracture. This is clearly an area that will benefit directly from more capable computers. The ability to handle orders of magnitude more atoms is central to the understanding of macroscopic plasticity effects.



Contours of plastic slip strain at the tip of a crack in a crystalline metal. The lines at 35 deg to the axis of loading are traces of crystallographic slip systems.



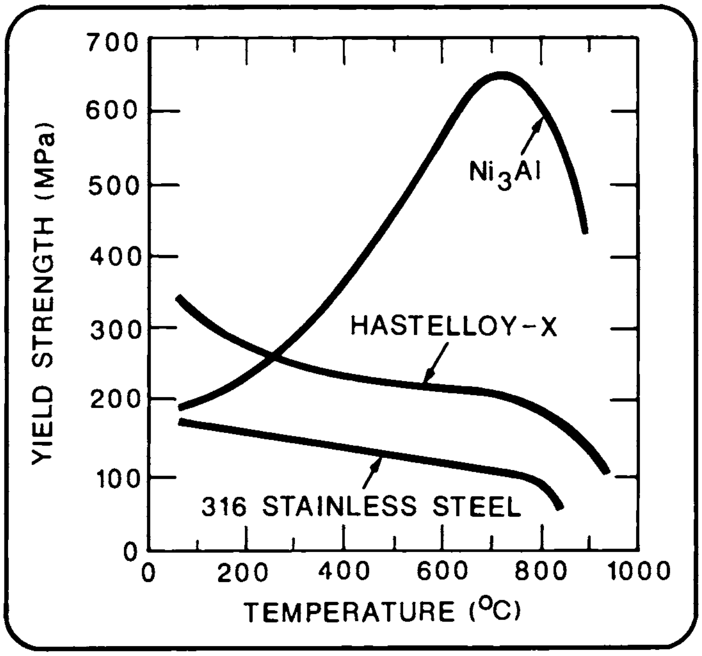
Simulation of a dislocation (dark circles) created at a crack tip (time increases from left to right).

Intermetallic Alloys Show Considerable Promise as High–Temperature Materials . . .

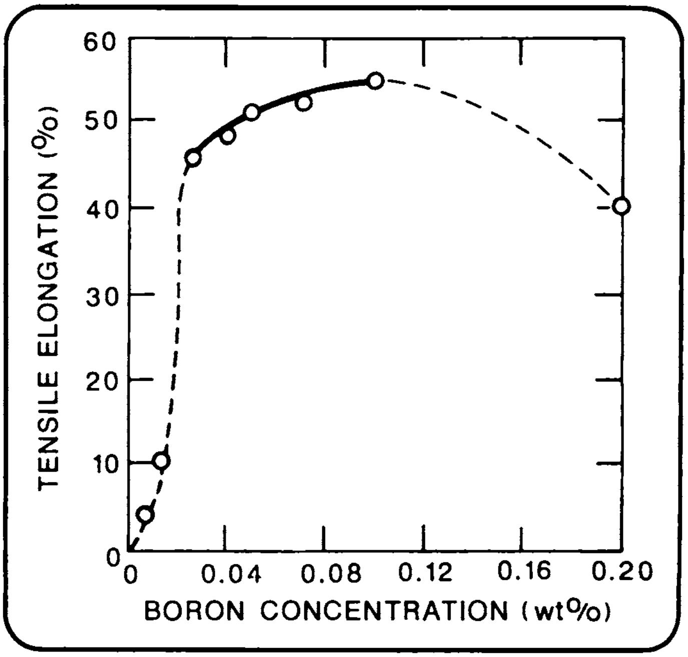
State-of-the-art jet engines require materials with considerable strength at elevated temperatures. Intermetallic alloys, in contrast to conventional commercial alloys like stainless steel, often exhibit yield strengths that increase with temperature and hence are prime candidates for such applications. In addition, intermetallic alloys have good creep resistance (resistance to long-time, high-temperature exposure), oxidation resistance, and corrosion resistance. Unfortunately, such materials tend to be brittle.

The intermetallic alloy Ni_3Al is particularly promising since it displays substantial ductility in its single crystal form. Such ductility is important in order to form the material into useful shapes and to decrease the chance of fracture in service.

Although Ni_3Al is intrinsically ductile, in polycrystalline form it is extremely brittle, which suggests that the grain boundaries are unusually weak. Empirical studies have shown that small additions of elements like boron and beryllium restore the material's ductility. While ternary elements such as boron greatly improve the grain boundary properties, there is essentially no understanding of how or why it works. Until recently, the only viable method of identifying such powerful grain boundary strengtheners (which can be different for each alloy) was the Edisonian approach of doping the alloy with every possible impurity and then measuring its properties. In addition to being time-consuming and expensive, this approach offers relatively little hope of finding those strengtheners that work only over a relatively small composition range or when other elements need to be included.



Unlike most metals, including stainless steel and Hastelloy-X (a nickel-based superalloy), intermetallic Ni_3Al has a yield strength that increases with increasing temperature.



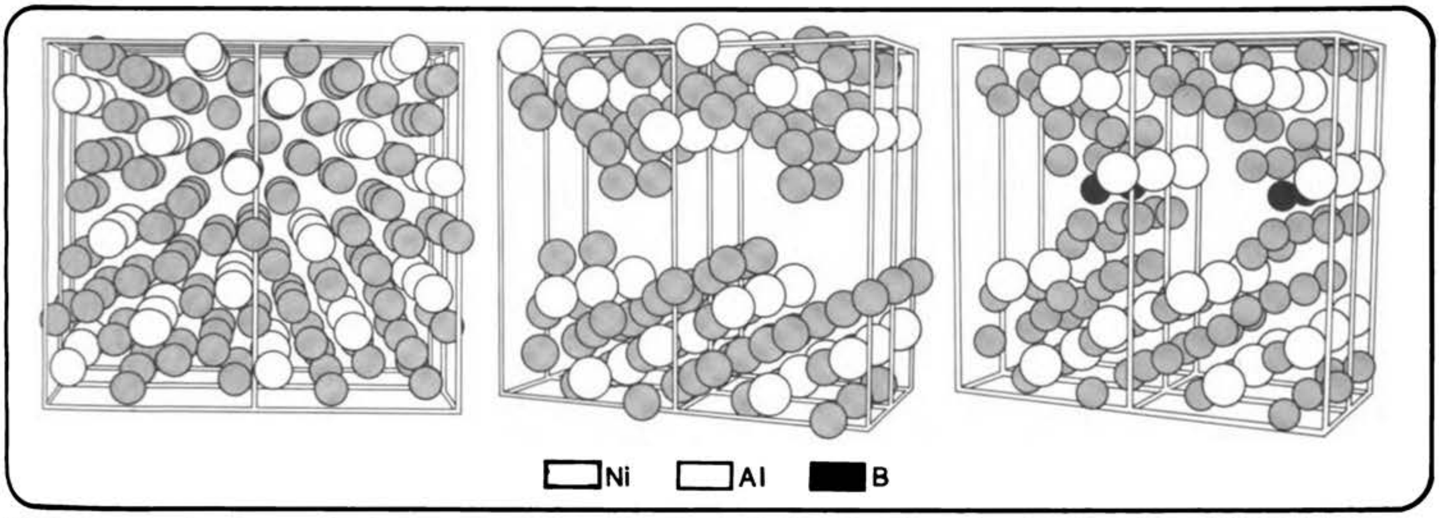
With the addition of only minute quantities of boron, polycrystalline Ni_3Al changes from a brittle material to one that is more ductile than steel.

A Hierarchy of Simulation Techniques Aids Our Understanding of Dopant Effects on Alloy Brittleness . . .

In order to understand a phenomenon as complex as the effect of impurities on fracture in ordered alloys like Ni_3Al, no single simulation technique or type of theoretical analysis is sufficient. The inherent difficulty is related to the necessity of treating simultaneously the quantum mechanical interaction between dissimilar atoms, the properties and atomistic structure of defects containing these atoms, and the influence of these defects on the macroscopic fracture behavior of the material. A hierarchical approach combining all of these factors has proved important in understanding the role boron plays in increasing the ductility of Ni_3Al.

In this approach, quantum mechanical supercomputer calculations provide a wide range of data, which are then employed to develop descriptions of atomic interactions suitable for large-scale atomic simulations. These supercomputer simulations yield information on the change in the cohesive energy of grain boundaries in Ni_3Al following addition of boron. Finally, these results are employed in a continuum description of the fracture process. *In toto*, this body of computer simulation and theory demonstrates that boron increases the cohesive strength of grain boundaries in Ni_3Al by virtue of its strong bonding to nickel atoms and its relatively small size, which allows it to fit into grain boundary interstices with little or no distortion of the grain boundary structure.

Not only is this simulation approach readily applicable to other types of impurity and interface problems, but it also provides qualitative understanding that will aid alloy designers in choosing appropriate microalloying elements.

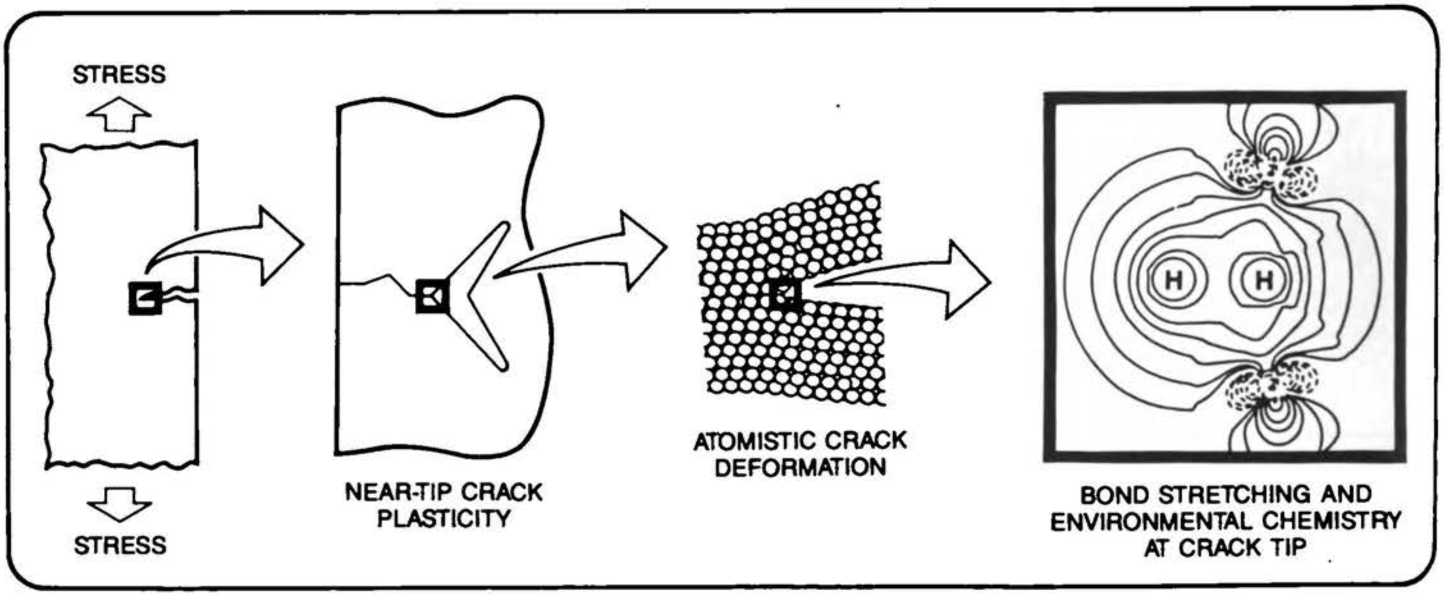


The left frame shows the calculated atomistic structure of a grain boundary in undoped and unstrained Ni_3Al. The same grain boundary opens when strained along the vertical axis (center frame). Intergranular fracture occurs; the polycrystal is said to be brittle. The same grain boundary under the same strain does not fracture when small amounts of boron are added (right frame). Supercomputer calculations reveal that the boron increases the cohesive energy of grain boundaries.

Stress–Corrosion Cracking: A Never–Ending Cause of Equipment Failures in the Chemical and Power Industries . . .

Stress-corrosion cracking (SCC) is a major and often catastophic failure mode in key engineering systems of modern society, such as in energy and chemical plants. SCC costs the United States hundreds of millions of dollars annually, as well as the loss of essential services and products, and occasionally even lives. It is a particularly insidious phenomenon that is caused by a combination of chemical environments and applied mechanical load, neither of which alone will cause failure. This phenomenon includes hydrogen embrittlement, caustic cracking, and corrosion fatigue.

SCC has been documented in almost all classes of structural solids: metals, polymers, ceramics, and composites. Methods of SCC prevention have largely been empirical since the problem is extremely complex and seems to defy complete physical understanding. In metals, SCC involves elastic and plastic deformation in a near-surface region consisting of an oxide film, an interface layer, and the substrate metal. Both layers contain a high concentration of defects. Additional complications arise because several SCC mechanisms exist and often occur simultaneously. A comprehensive model of SCC for metallic materials is not yet possible, but recent modeling of SCC in ceramics and glasses (where plastic deformation and defective surface films are absent) is providing important insights.



Stress-corrosion cracking requires a hierarchical model for complete understanding.

Quantum Chemistry Calculations Unlock the Secrets of Slow Crack Growth in Glass . . .

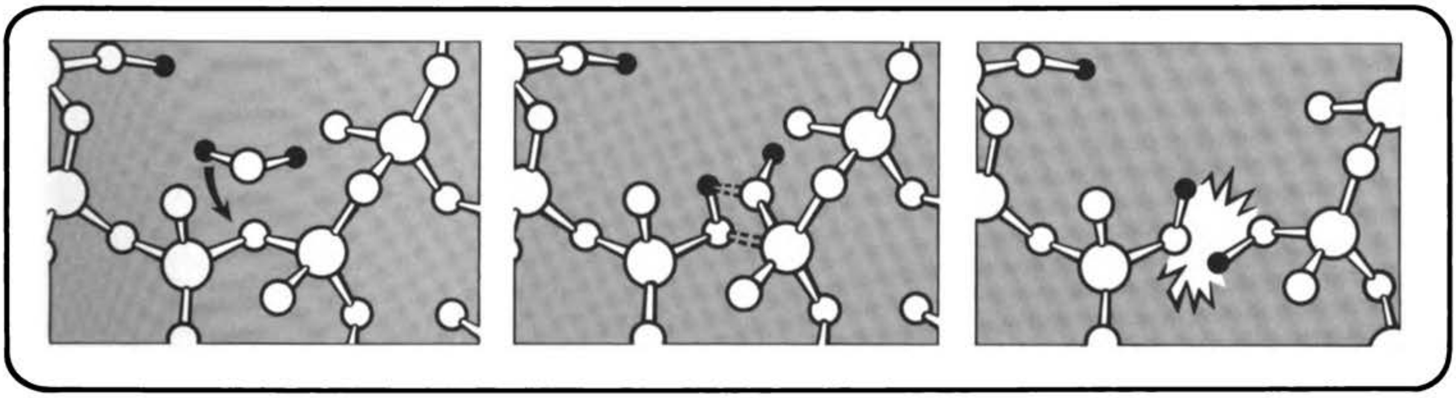
Glass and ceramic oxide materials are playing key roles in the emerging technologies of fiber optic networks and ceramic heat engines. In many of these new applications, such as optical communication lines across ocean floors, a long service lifetime is required. Engineers must contend with slow crack growth in glass and ceramic materials, which is exacerbated by mechanical loads and an aqueous environment.

In a concerted research effort, combined experimental investigations and quantum-chemical bond rupture calculations have revealed the causes of slow growth. These computations, performed on supercomputers, indicate that a distorted bond at the crack tip greatly enhances the likelihood that water molecules will bond chemically and break, and this dramatically reduces the force required to break the silicon-oxygen bond. The crack advances then by the diameter of the broken silicate ring.

These computations can also predict the effects of molecules other than water. For example, silicon atoms in the strained ring at the crack tip are calculated to be much more acidic than those in the unstressed rings. Hence all basic chemical species that the strained ring can bond to chemically will enhance crack growth, assuming the site of the reactive molecule fits into the crack tip opening (whose magnitude is load-dependent).

By taking into account the rate of molecular diffusion into the crack tip region and the rate of bond breaking, it is now possible to predict relative rates of crack growth in silica glass exposed to different chemical environments.

This fundamental understanding of stress-corrosion cracking in glass lays the groundwork for predicting fracture in other materials after long exposure. In metals, for example, the local straining and surface chemistry at the crack tip are also affected by near-crack-tip plasticity; supercomputing techniques are currently being developed to handle these additional complexities.



Water can react with glass, allowing it to crack more easily. Here a water molecule enters a crack (left panel) and is adsorbed (middle panel). The molecule causes a chemical reaction (right panel) which cleaves a silicon-oxygen bond at the crack tip as well as an oxygen-hydrogen bond in the water molecule, producing two silanol groups (hydroxyl groups attached to silicon). As a result the length of the crack increases by one bond rupture.·

Using Supercomputers, Theoretical

In 1926 Erwin Schroedinger wrote down his famous equation, $H\Psi = E\Psi$, for which he won the Nobel Prize in 1933. The equation describes the fundamental behavior of electrons in molecules and solids and is considered one of the crowning achievements of the twentieth century. In 1929 P. A. M. Dirac, another Nobel laureate (for the relativistic equivalent of the Schroedinger equation), commented:

> The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known ... and the difficulty is only that the application of these laws leads to equations much too complicated to be soluble.

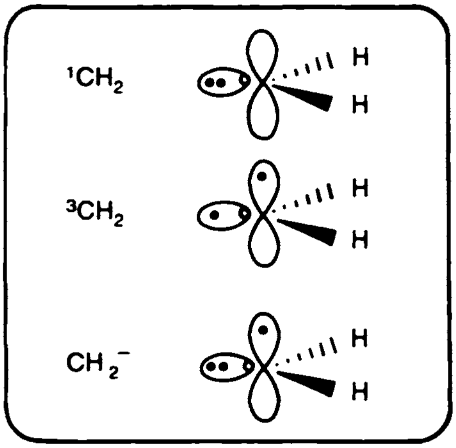
In the Schroedinger equation the H, known as the "Hamiltonian," consists of a potential energy term (for example, that due to the electrostatic interaction between electrons and protons in a molecule) and a kinetic energy term. The Ψ is the "wavefunction," the fundamental solution, and E is the total energy of the system. The equation can only be solved exactly for the simplest of molecules, the hydrogen atom, which has only one electron and one proton. Simplifications and approximations were and are therefore required if this fundamental equation is to be solved.

Theoretical physicists and chemists have approached the solution from different points of view: Physicists have tended to approximate the Hamiltonian by proposing models of the true system, which are then soluble either analytically or by computer. For example, a metal can be viewed as a "gas" of electrons in a box, a highly successful model that allows insight and intuition to guide progress. Quantum chemists, on the other hand, have taken a very different point of view: The Hamiltonian is held sacred, and any approximations must be made to the wavefunction. They made use of a theorem that allows expansion of the wavefunction in a series of well-chosen functions, called basis functions. The theorem says they will ultimately get the right answer if they make the series big enough, that is, if they include enough basis functions. The answer is exact for a complete set—an infinite number—of these basis functions.

In the past, since it was easy to get the wrong answer by not including a large enough set of functions, experimentalists could confidently claim the correctness of their results when disputed by calculation, and theorists had a rug to hide under when their results were disproved. No one was disturbed philosophically; after all, Francis Bacon taught us all to believe experiments.

Then in 1960, J. M. Foster and S. F. Boys published a calculation that predicted, in the absence of any experiments, that the CH_2 (methylene) molecule is bent by 128 degrees. Experimentalists, measuring the electronic spectrum of the molecule, concluded it was linear, not bent. Others contended that if such theoretical methods were inadequate for such a small molecule, they were useless indeed. Theorists were cowed into submission. Even when subsequent calculations in 1966 and 1969 substantiated the bent molecule result, theorists themselves blamed weaknesses in the calculation for the discrepancy with experiment. Theory was at a low ebb.

Chemistry Is Outrunning Experiment . . .



The structure of the methylene molecule has been the focus of a scientific controversy.

Theoretical chemistry came alive when, in 1970, C. M. Bender and H. F. Schaefer went after the CH_2 molecule with theoretical techniques previously reserved for diatomic molecules. They used a "double-zeta" basis set and performed a self-consistent-field calculation followed by what is known as "configuration interaction," a method used to include electron correlation effects. They found the CH_2 molecule to be bent at an angle of 135.10 degrees! They concluded that no higher level of theory would change the essential result.

New experiment after new experiment began to agree. Electron spin measurements first gave 136 degrees; somewhat later, 137.7 degrees. State-of-the-art theory had challenged experiment and had been vindicated.

A similar problem arose with the energy difference between the two lowest lying states of the same molecule. Carbon has four valence electrons, two of which it shares in covalent bonds with the hydrogens in CH_2. The two nonbonding electrons can have opposite spins, to form a singlet state, or have the same spin, forming a triplet state. Everyone agreed that the triplet state was the lower of the two in energy, and the calculations gave the difference as 11.5 kilocalories per mole (a Cal Tech group) or 13 kilocalories per mole (a Berkeley group) while the best pre-1976 experiments indirectly gave 8 kilocalories per mole, in reasonable agreement.

But then, in 1976, experimentalists formed a beam of CH_2 and photodetached the extra electron with a laser, allowing direct observation of singlet as well as triplet states. They measured 19.4 kilocalories per mole, seriously outside the widest limits set by theory. The "battle lines" were drawn, with several bottles of expensive French champagne at stake. In 1978, theorists calculated the vibrational spectra of the molecule and used the results to reinterpret the measurements themselves. It was not until 1984 that the new direct measurements gave 9.0 kilocalories per mole, and the French champagne exchanged hands.

There are numerous other examples in the literature of successes with quantum chemical methods. The approach was able to take extensive advantage of the revolution in supercomputer power over the last two decades and emerge as an equal with experiment, in many cases providing the more accurate result. It has the further advantage of being able to calculate species that are extremely inaccessible to experiment, such as intermediate states that form during a chemical reaction.

We have been discussing chemistry here, but it should be recognized that these same techniques are being employed in materials and materials processing studies. The silane (SiH_4) reaction rates required for chemical-vapor-deposition calculations, described elsewhere in this report, were obtained with these techniques. The calculations of pharmaceuticals discussed in this report also applied these methods, and researchers are hoping to achieve a breakthrough in understanding high-temperature superconductivity (discussed in brief later in this report) with similar techniques.

Developing New Anticancer Drugs Has Been a Hit-and-Miss Operation . . .

General Sequence for New Drug Development

Production, Formulation, and Toxicology: Acquisition, Screening, and Phase I Clinical Trials

Clinical Trials: Phase I - Phase IV

Acquisition
- **Marine & Plant Life**

Screening
- **Test-Tube Cultures**
- **Mice**
- **Dogs**

Phase I
- **Human Testing**
- **Eight NCI Centers**

Phase II
- **Specific Tumors (Lung, Breast, Colon)**

Phase III
- **Comparison to Standard Theory**
- **Statistics**

Phase IV
- **Same as III but with Surgical Procedures Included**

The development of more effective drugs for the treatment of cancer and AIDS is a painstaking process, which has evolved to its present state only in the last 5 years. The figure on the left outlines the current development sequence. In the acquisition phase, tens of thousands of natural products are gathered from a variety of plant and animal life from all over the world. Special submarines seek deep-sea marine life, and plankton is harvested from the oceans. These products are transformed (crushed, fermented, etc.) into a material suitable for screening. Next, in preclinical screening, the collected biological products are tested for their killing effect on a cancerous tumor, e.g., an L1210/leukemia. This screening phase, which culls potentially efficacious drugs, represents a major recent advancement in the history of drug development.

Substances showing biological activity are tested in living organisms such as rodents to evaluate their activity against a variety of tumors with uniform size and predictable biologic behavior. Since rodents tend to exhibit few "side effects," promising nontoxic (to rodents) substances are tested in larger animals. Only 1 in 4000 of the screened compounds demonstrates acceptable degrees of antitumor activity and safety to justify entry into human testing in a Phase I trial.

There are eight Phase I centers in the United States, which are supported by the National Cancer Institute (NCI). In this phase the toxicity and maximum tolerated dose are determined in human patients; some antitumor response may be observed. Careful statistical studies involving at least 16 patients are performed (a response in one of the 16 implies that 20% of the general population should have a similar response). In Phase II trials, compounds with acceptable toxicity are evaluated for their effect on specific tumors (lung, breast, colon, etc.). In each study there are a great many pharmacological parameters to be varied, not the least of which are the dose and dose rate of administration. By trial and error it is determined whether treatment once a day, once a week, or continuously is preferred and in what amount. The cost for preclinical development through Phase II testing for each individual agent is more than one hundred million dollars per drug.

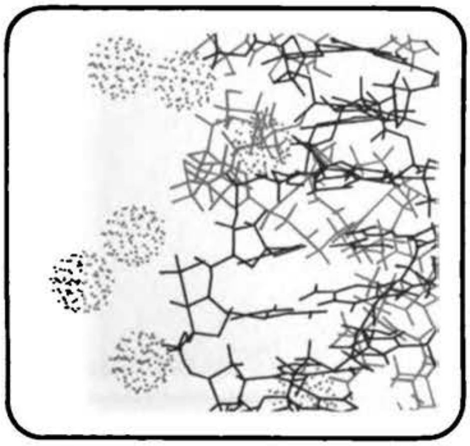
Phase III trials are randomized, controlled studies aimed at learning whether a new drug candidate is statistically better than standard therapy for cure and survival against the disease. In Phase IV, surgical procedures are added to Phase III studies.

Currently, only 1 in 40,000 screened compounds demonstrates clinical utility! Since with current intensive efforts it is estimated that about 10,000 natural products (NCI figures) can be screened per year, only one new cancer drug can be developed every 4 years by this painstaking procedure.

Computer–Designed Pharmaceuticals Are Now Possible . . .

There are some 40 clinically useful anticancer drugs presently available. Among these are several agents that have demonstrated curative potential for a variety of malignancies. The ultimate mechanism(s) responsible for the beneficial and toxic effects for any one agent requires fundamental knowledge of the specific atomic and molecular interactions between the anticancer agent and the tumor. It is becoming increasingly apparent that supercomputers can facilitate the descriptive study of larger molecular systems such as DNA or proteins, including the surrounding cellular environment.

The study of lambda-dimer protein binding to the DNA molecule involves interactions pertaining to fundamental aspects of cancer and AIDS. A supercomputer simulation of the binding of this large repressor protein to a 28-base-pair region of DNA (total 15,000 atoms) is depicted below. A hierarchy of quantum chemical techniques, from first principles to semi-empirical, was employed, allowing complex, minimum-energy molecular rearrangements to be calculated. High-resolution three-dimensional graphics helped unravel the detailed results.



Molecular mechanical simulation of the lambda dimer (blue) binding to DNA (black). Sodium counterions are shown as blue spheres.

An important amino acid–DNA interaction, missed by experimentalists working for years on this fundamental process, was also discovered by supercomputer simulation. The calculations demonstrated several molecular interactions that prompted the consideration of previously unrecognized elements of biological significance.

Supercomputers are thus providing the key to the development of an exciting new approach to cancer therapy. The goal is to design agents that selectively inhibit targets controlling regulated cellular functions in the tumor cell. A tumor-specific "homing device" is sought that should, therefore, produce no side effects. Researchers can now derive computer-projected physical properties of specific atomic modifications made to nucleic acid bases—furanose and phosphate groups. These properties are coupled with chemical properties of molecular fragments from antitumor drugs with established clinical efficacy. Specific drugs are then designed based on this information and experimentally verified.

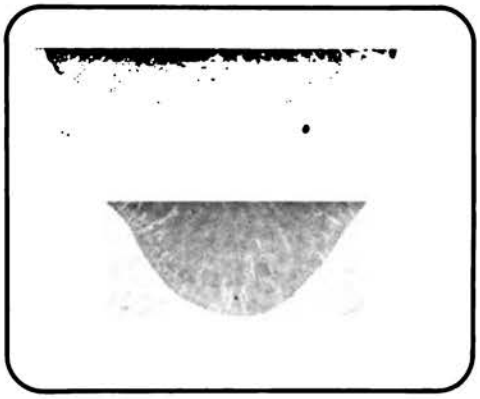
The figure on the right shows the results of a supercomputer simulated interaction between a modified nucleotide strand (part of a typical anticancer drug) binding to a complementary segment of DNA, as would be found in a human cancer gene.

Many fundamental chemical properties of DNA are retained in these molecules (i.e., the complementary segment); uptake and genomic incorporation of these agents is allowed by the tumor cells, resulting in interference with gene function or production of essential proteins unique to tumor cells (the fundamental genetic problem of cancer). The calculated structure assumes a helical conformation similar to that of native DNA, confirming the essential predictions of the simulation.

One of the most important elements in future drug design will be the integration of supercomputers and advanced molecular computational methods with prospective experimental efforts. In this way research efforts will develop more focused multidisciplinary experimental approaches based on computer-projected physical properties of molecular systems. As computational methods and the tight coupling of theory with experimental approaches improve, reduction in time and resources in future development of more effective agents should be expected. Commensurate with these developments will be gains in the understanding of atomic and molecular processes critical to normal and abnormal cellular function, along with a broadened perspective. The ultimate benefit of such efforts will be improved medical therapy, resulting in reduced mortality and morbidity from diseases such as cancer and AIDS, that will likely impact virtually all other areas of medicine.

Simulation showing the reactive fragment of an anticancer or AIDS drug forming a stable bond between the two strands of the abnormal DNA, preventing their replication. Normal cells are not affected since they lack the abnormal DNA sequence. This is the essence of "targeted drugs."

Welding Procedures Are Still Being Determined Largely by Trial and Error . . .

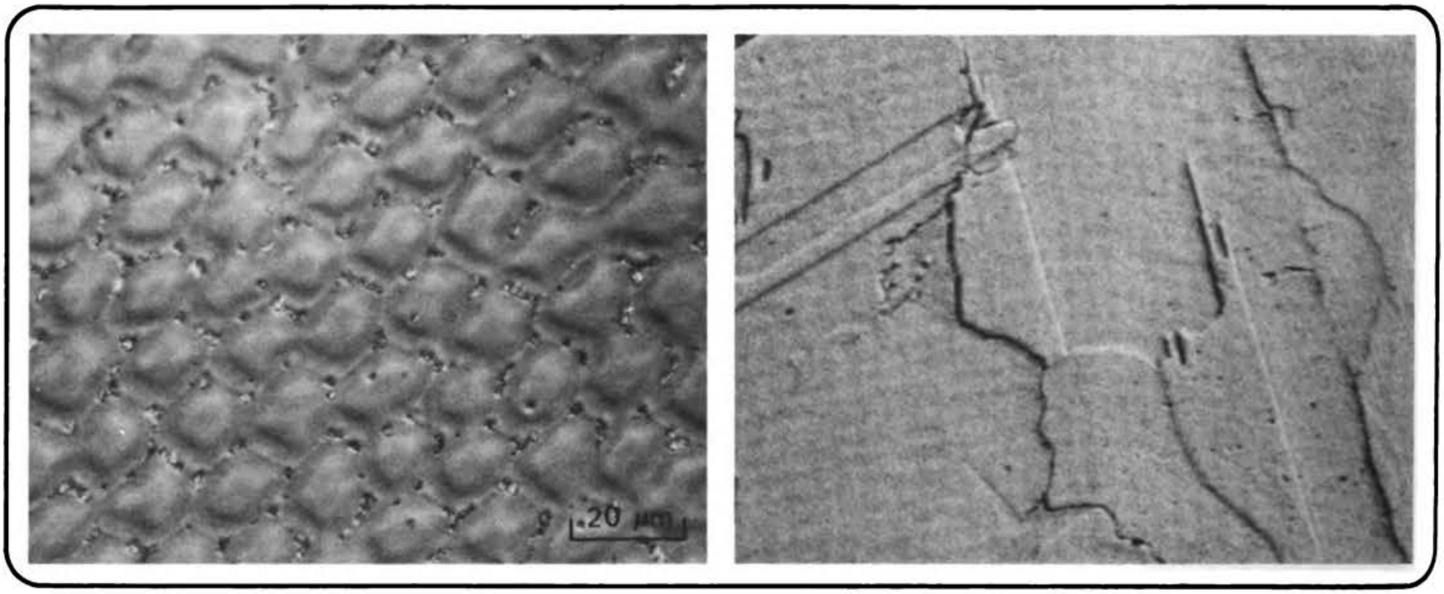


Cross sections of welds in 304 stainless steel made with identical weld parameters but differing sulfur content: top, 30 ppm; bottom, 150 ppm.

Welding is one of the most widely used industrial techniques for joining metal parts, but it involves so many complex macrostructural and microstructural variables that it remains more of an art than a science. Optimum welding parameters for critical welding applications are often difficult to determine, particularly when the parts to be joined have complex shapes and the weld is susceptible to cracking. The welding designer has a number of choices, such as (for fusion welding) a variety of arc welding processes as well as laser and electron beam welding. Once this choice is made, variables such as the voltage, current, weld speed, fixturing, surface preparation, and material composition must be optimized for a given weld. These are determined by trial and error—that is, empirically—at enormous expense.

The figures on the left show one of the sensitivities facing the welding engineer. The two welds shown are in ostensibly the same material, 304 stainless steel, but differ in sulfur content by 120 parts per million (ppm). A broad, shallow weld-pool region (poor penetration) is obtained for the 30-ppm sample while a deeper, narrower weld zone (higher penetration) occurs for the 150-ppm steel. Without an understanding of such macroscopic phenomena one cannot hope to predict weld penetration depths.

There are subtle microscopic effects also. The figures below show, on the left, a high degree of elemental segregation that occurred during cellular solidification of a 14%Ni-21%Cr austenitic (fcc Fe) alloy of similar composition. The partitioning of alloying elements between the solid and liquid during solidification is a natural occurrence in welds and often outlines the cellular pattern created during solidification. Because macroscopic weld properties depend on these effects, it is important to be able to understand their causes.



Metallurgically prepared micrographs of welds: left, a 14%Ni-21%Cr austenitic (fcc Fe) alloy, showing a high degree of elemental segregation; right, a ferritic (bcc Fe) alloy of similar, but slightly different composition, showing no segregation. The small change in composition is responsible for the large change in elemental segregation.

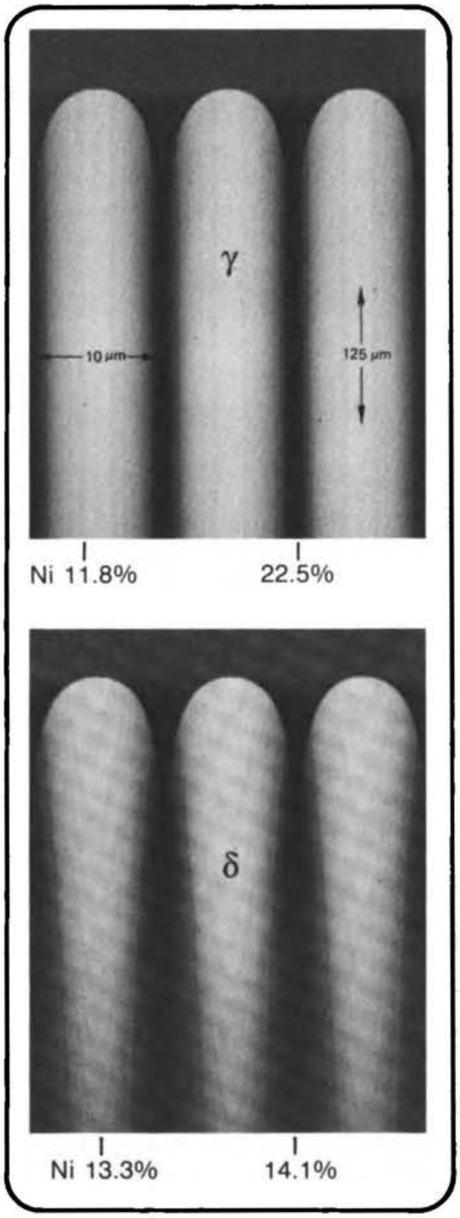
Calculational Methods Can Help in All Stages of Weld Development . . .

Welding phenomena are difficult to study experimentally because the details of what is happening in and near the weld zone are physically inaccessible, occur at high temperatures, and change quickly. Even attempts at measuring these phenomena can interfere with them, often invalidating the results. Numerical modeling is providing the tool needed to understand and control these processes.

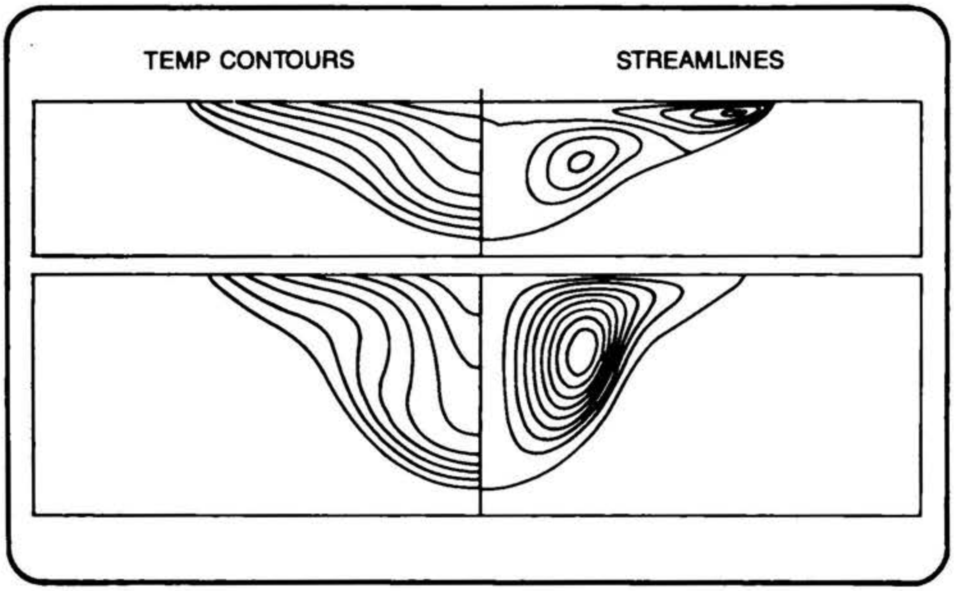
Macroscopic calculations can now include heat conduction and fluid convection in two dimensions; it is only the limitations of today's computers that prevent full three-dimensional calculations from being done. The figures on the left below show two weld pools calculated using different values of surface tension to simulate the effects of sulfur on weld penetration (see previous page). The results clearly show that a deeply penetrated weld occurs in the material in which the surface tension increases with increasing temperature (high sulfur content), in agreement with experiment.

Calculations are also capable of including microscopic effects such as diffusion during solidification and cooling. The figures on the right are simulations of the cellular solidification discussed on the previous page (these figures are longitudinal views of the weld, whereas the micrographs on the previous page are transverse views). Nickel is forced into the liquid and is eventually trapped during the final stages of solidification. In the top simulation, an fcc system, solid-state diffusion is negligible and the cellular pattern is retained in the weld. In the bottom simulation, a bcc system, diffusion in the solid is much more rapid and eliminates the high degree of segregation.

Simulations such as these are leading to more accurate models of welding phenomena and a better understanding of how to optimize weld properties. Further refinements will be possible as supercomputer capabilities increase.



Simulations of cellular solidification in Ni-Cr alloys. The shading graphically represents the nickel concentration. Top (fcc system): negligible solid state diffusion has led to a high degree of segregation; bottom (bcc system): solid state diffusion has eliminated the segregation.



Weld pool simulations show that deeper weld penetration (bottom illustration) occurs when the surface tension increases with increasing temperature.

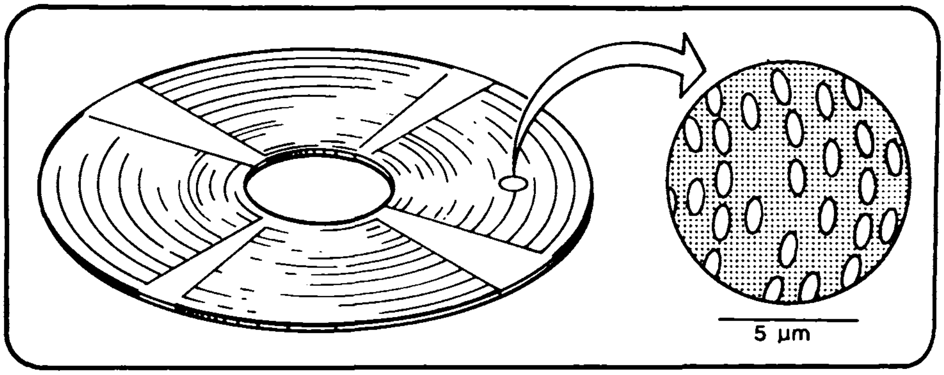
Forming of Plastics—The Challenging Search for the Constitutive Law for Polymeric Fluids . . .

Plastics, fibers, synthetic rubbers, coatings, and adhesives are among the class of materials known as polymers, which are long-chain organic substances that have become a common part of our lives since about 1920. They are commonly formed or processed by heating to the liquid state and cooling in the desired form (see figure below). In the liquid state, polymers are both viscous (syrupy or "thick") and elastic (returning to their initial shape after being deformed). Furthermore, the properties associated with their viscoelasticity are anisotropic (different in different directions) and dependent on the flow history (the polymer fluid "remembers" the way it was treated and flowed in the past).

These complications make it difficult to measure and formulate a constitutive law, a law that would describe its flow, for example, as it fills a die to form a plastic part or is extruded into pipe. In particular, a constitutive law relates the stress to the rate of deformation and is analogous to the stress-strain or Hooke's Law relation so important to solid mechanics. Given the constitutive law, the same calculations done for metal forming could be done for polymer forming, thus revolutionizing an industry that designs dies by the "cut and try" method.

The determination of this law is also complicated by the fact that the viscosity of a polymeric melt rises extremely rapidly with its molecular weight (with the 3.4th power in fact). Although in general the higher the molecular weight, the better the mechanical properties of the finished product, manufacturability usually forces designers to choose lower viscosity materials. Consequently, tailoring polymers according to desirable flow properties for processing represents an important activity of the chemical industry.

The search for a constitutive law is proceeding through the rigorous formulation of a new kinetic theory of polymeric fluids (see page 25), which has led to a system of fundamental equations soluble only by a supercomputer. Some researchers are using direct supercomputer simulation to elucidate the fundamental molecular mechanisms underlying such complex phenomena. On the facing page we describe simulations of "reptation," the slithering motion of a polymeric chain through the surrounding "jungle" formed by the other molecules.



Compact and optical discs are examples of modern sophisticated plastics thermoforming. Molten plastic (a polycarbonate) is forced under high pressure into a mold containing a plate inscribed with digital information. The melt must then cool in a stress-free condition to avoid birefringence.

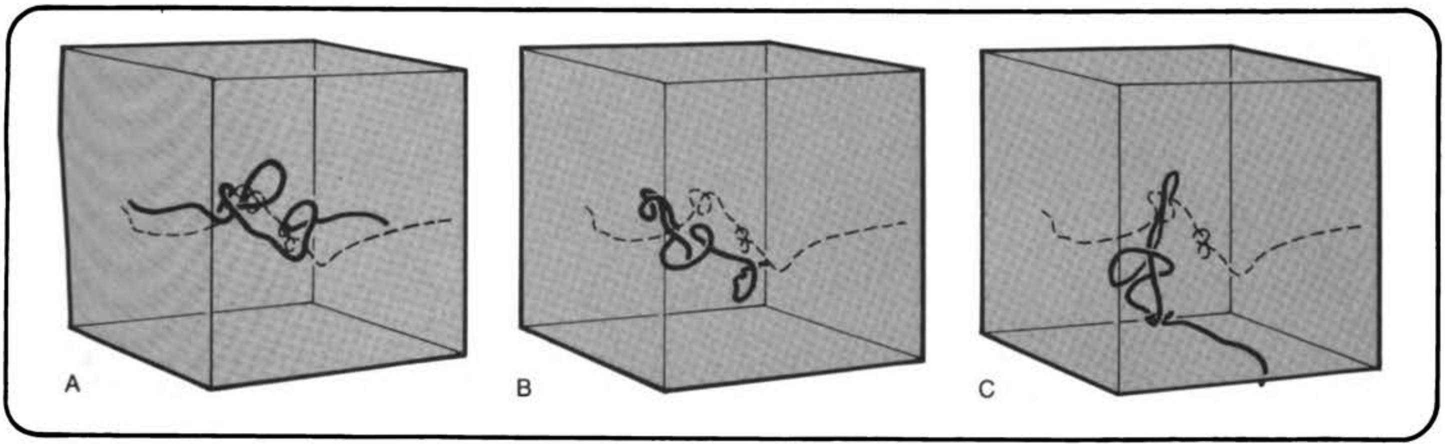
Visualizing the Molecular Motion in a Polymeric Fluid by Computer Simulation . . .

The observation of the Brownian motion of liquid droplets suspended in air provided a powerful impetus for the formulation of the statistical kinetic theory of gases. Similarly, the concept of "reptation" of a polymer chain in its melt has served an important role in the formulation of simple models of polymeric fluids. Yet, in contrast to Brownian motion, no direct observation exists to affirm the validity of this concept. Fortunately, computer simulations have recently offered an alternative for visualizing and validating reptation.

Although a complete molecular dynamics simulation of a dense system of entangled polymer chains is still beyond the capabilities of present-day supercomputers, lattice models of densely packed and entangled polymeric chains have been analyzed by dynamic Monte Carlo methods. The motion of one particular chain is illustrated below in the sequence of three snapshots. The initial position and configuration of the one chain is indicated by a dashed line, and its subsequent positions by a solid line. For clarity the surrounding polymer chains are not shown.

These simulations suggest that "tubes" formed by surrounding chains do not really exist, and that the mental picture of "reptation" is not entirely adequate. Significant motion occurs perpendicular to the chain sections, with surrounding chains passing over or under to occupy the space made available. The computer-simulated visualization predicts a cooperative interchange of relative positions of neighboring chains such that the polymeric fluid density remains as uniform as possible. In addition to allowing visualization of polymer motion, this type of computer simulation also provides scaling relationships for the dependence of the self-diffusion coefficient and the shear viscosity on the molecular weight of the polymer molecule.

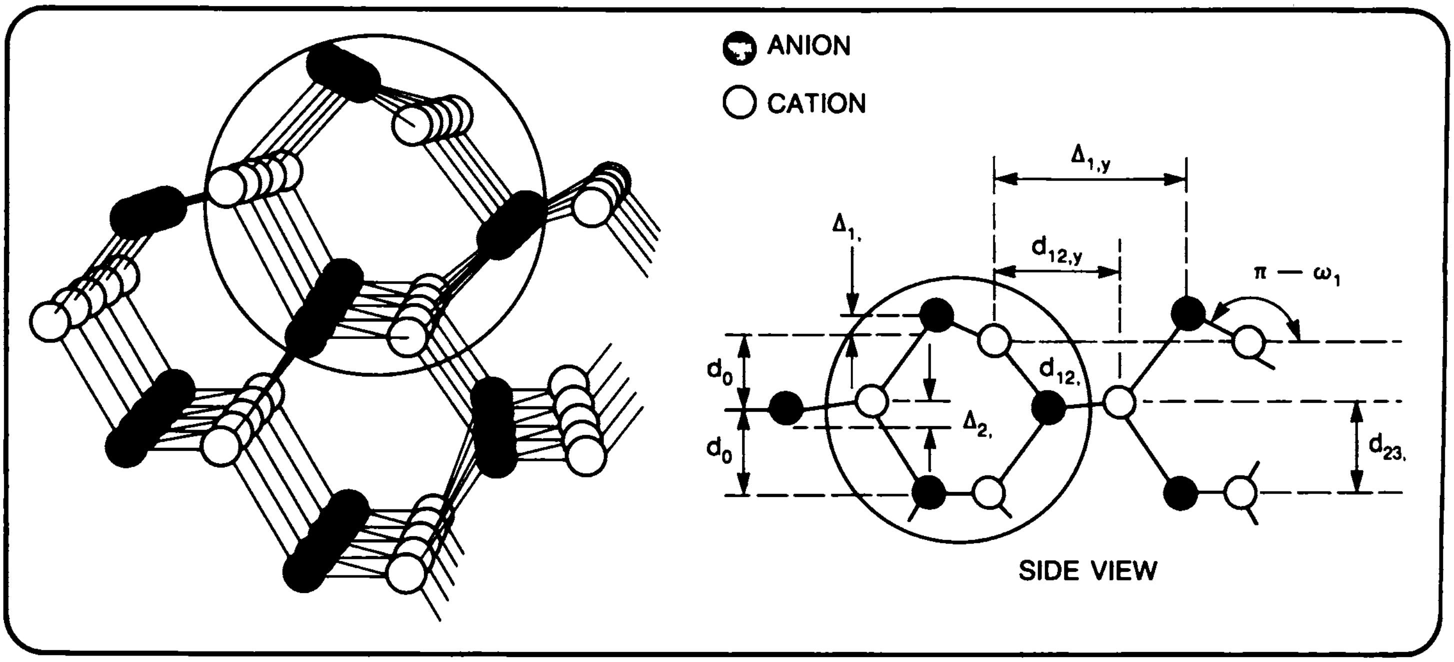
Present simulations represent a new method for evaluating novel concepts for more concise mathematical descriptions of complex collective motions of polymers. Such simplified models would provide a computationally simpler approach than complete molecular dynamics simulations or multidimensional transport equations. More powerful supercomputers will let us add increasing levels of sophistication to these models.



Computer simulation of chain motion in a concentrated polymer solution. Shown are three snapshots of one chain position (solid lines) at consecutive times (from left to right), compared with the original chain position (dashed lines). Extensive analysis has shown no evidence for the existence of "tubes" through which the chain moves by reptation.

Semiconductor Interfaces Are Critical to Device Performance . . .

The behavior and growth of modern semiconductor devices depend on atomic-scale properties. For example, in the layer-by-layer growth of semiconductor interfaces, the quality of the junction is determined by the resulting atomic geometries in the interface (see figure below). Also, the alignment of the electronic energy levels between the two semiconductors, known to be critical to device performance, is thought to depend on electron density rearrangement in the interface. The understanding and modeling of these kinds of phenomena are at the forefront of current calculational capabilities. Yet it is not unrealistic to propose, for multilayer adsorbate systems of interest in microelectronic and optoelectronic device fabrication, processing studies in which atomic geometries and electronic structures would be computed as a function of process parameters. Although such a program would require the availability of considerable computer resources, it would provide a predictive capability for the semiconductor industry. This program could also aid the semiconductor research community by giving experimentalists an on-line analysis "tool box."

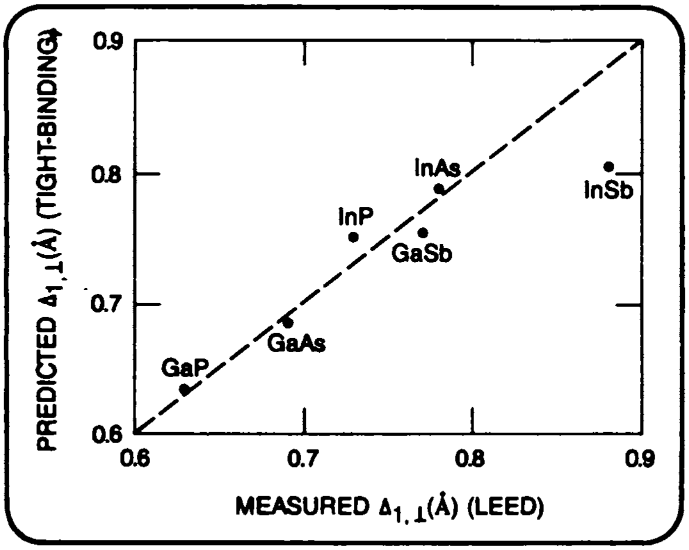


Zincblende (110) structure.

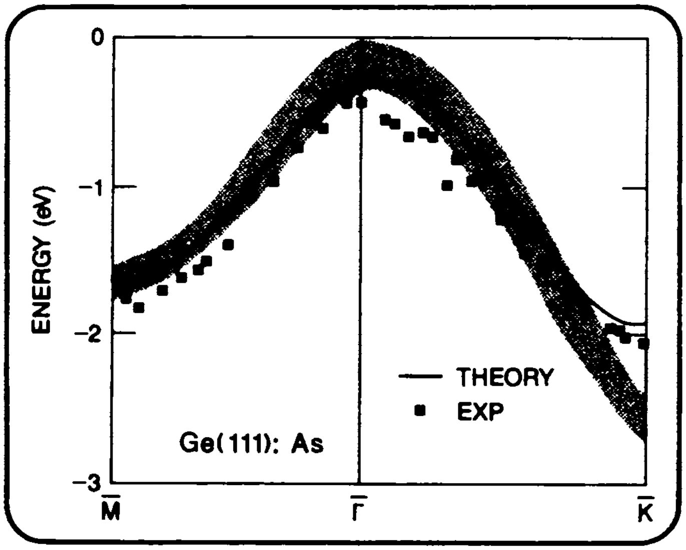
Atomic Geometry and Electronic Structure Predictions Are nearly within our Grasp . . .

Aided by a supercomputer, we can now determine surface atomic geometries for a number of semiconductor surfaces. This involves, for example, determining all of the geometric properties labeled on the zincblende structure shown on the preceding page. The figure on the left below shows the results for one of these properties. Obtaining these results consists of performing low-energy electron diffraction (LEED) experiments followed by a major computer effort in the form of a multiple scattering intensity analysis. For example, computing a LEED intensity profile (14 beams at 100 energy points) for a single atomic configuration of the zincblende (110) structure requires 5 to 15 minutes of central processing unit time on a supercomputer. As the figure shows, the semi-empirical tight-binding theory predictions compare well with the measured values across the zincblende series.

The calculation of semiconductor electronic structure has been evolving rapidly in the last few years because of the realization that methods typically used with reasonable success for metals fail to give accurate electron excitation energies, such as band gaps, for semiconductors. It has been found necessary to include the electron self-energy operator, which complicates the calculation. However, these calculations can be done, giving accurate band gaps and surface-state energies as shown in the figure on the right below. Shown there is the energy dispersion of a surface state band for a Ge(111) surface with an As overlayer. This is of interest for studies of growth of GaAs on Ge. Projected bulk energy bands are shaded for reference. These results suggest that methods may be in hand for a predictive capability for semiconductor device design: Given sufficient computer capabilities we would be able to predict semiconductor heterojunction energy levels and potentials, quantities that control device behavior.



Geometric properties of semiconductors can now be determined with supercomputers.



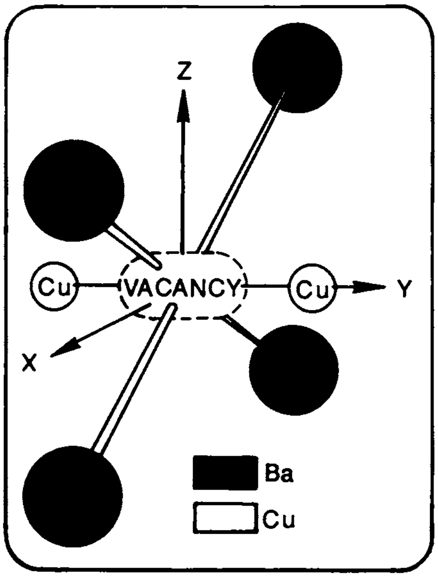
Electronic structure calculations of semiconductors are evolving rapidly because supercomputers allow greater physical detail to be included.

There Are a Great Number of Examples

The committee found the field known as materials science to be so vast that, given finite time and resources, it could not hope to properly give an account of all the outstanding computational research and engineering going on in the United States. No group should feel excluded by our not having incorporated its work here; we found ourselves reducing the number of examples for purely practical, time-driven reasons. Notable among the omissions are entire areas such as catalysis, beam processing, and superconductivity.

Superconductivity—the flow of electrical current in a material with no resistance losses—is one of the most fascinating displays of many-body effects in solids. Exciting experimental discoveries little more than a year old changed this effect from a laboratory curiosity applicable to only a few special alloys to a major technological possibility. Efficient superconducting motors could replace conventional units. Lossless underground power-transmission lines could transport electrical power from economical sources to distant users. Larger superconducting magnets could confine plasmas in fusion reactors. With dense superconducting circuitry that would reduce signal transit times, one could build computers 1000 times faster than today's.

The economic and technological importance of high-temperature superconducting materials, and the need to develop new material processes in order to utilize this discovery, warrant an all-encompassing effort to understand how superconductivity originates in these materials. Elaborate quantum mechanical calculations are in progress to try to unravel some of these mysteries. Quantum chemists (see pages 38-39) are applying *ab initio* techniques to understand the role of oxygen content: In $YBa_2Cu_3O_x$ the highest transition temperature occurs for $x = 6.8$ for reasons as yet unexplained. Solid-state theorists are using local density techniques in similar pursuits. So far, the calculations have led to a possible model—a suggestion—for how the electrons might pair to produce the superconducting effect. (The Nobel Prize–winning Bardeen-Cooper-Schrieffer theory invokes the pairing of electrons through interactions with lattice vibrations to explain superconductivity.) In the figure below there is a line of Cu atoms along the Y axis with a vacancy at the origin and four Ba atoms in the X-Z plane. The model suggests a binding energy for electrons to the vacant site that leads to Cooper-pair formation.



Models of superconductors, such as this one, are being explored vigorously with supercomputing.

Supercomputing provides a means of obtaining insight into these materials, particularly where experimentation is hindered by difficulties in growing single crystals. The field is now moving so rapidly that anything we say today may be invalidated tomorrow.

Surface science is ripe for supercomputing. The equations are known, the calculational methods are sophisticated, and the corroborative experiments are under way using single crystals and ultrahigh-vacuum systems. The system of gas-phase molecular interactions with surface-state electrons is highly complex, however, and large computational resources will be required for their solution. With so many fundamental parameters to vary in the costly process of designing a catalyst, supercomputers promise to make a major technological impact. Catalytic reactions such as the methanation of hydrogen and carbon monoxide are vital to the production of synthetic natural gas from coal. The formation of liquid fuels such as benzene (by, for example, the dehydrogenation of cyclohexane) depends on catalysts (such as copper-ruthenium) and is only beginning to be understood.

There are other areas we were unable to include. **Beam processing** techniques are central to integrated-circuit device fabrication. Ion implantation for introducing dopants into devices and plasma processing for etching and film deposition are excellent examples. To date, Monte Carlo and Boltzmann transport codes have been used successfully to model range and damage distributions for implantation as well as complex plasma kinetic effects. Yet these particle simulations represent only portions of the problem. More complete thermal and kinetic models are needed to model a host of beam processing phenomena.

For example, in ion implantation, the formation, diffusion, and nucleation of end-of-range defects is a critical and unsolved problem. Such computations would be of potential importance for implantation in compound semiconductors where defect formation is a major

We Were Unable to Include . . .

device limitation. Plasma deposition and etching techniques involve complex physical and chemical processes. Simulating the processes presents a significant challenge, but the payoff could be large in selecting the optimum conditions for damage-free removal or deposition of a wide variety of materials.

In addition to extended defect modeling, the thermal effects involved in beam processing offer exceptional opportunities for supercomputing. Beam technologies such as implantation produce damage. The damage or defects are removed by an annealing process that must be compatible with the integrity of the other materials in the structure. Different annealing strategies (e.g., rapid thermal annealing) are now being used as structures become smaller and more complex. Simulation of the annealing process, from the atomistic level to basic heat flow, should be possible with supercomputers.

At the forefront of the fabrication equipment evolution, photon-assisted processes offer revolutionary potential. Yet these processes quantitatively and qualitatively change the nature of the surface reactions: The number of reaction species *and* their energetics of reaction change. Supercomputing offers the only practical means to quantify the complex kinetics so that the processes can be harnessed to create manufacturing equipment.

Nonetheless, the reward for this effort is tremendous. The harnessing of such maskless processes could dramatically reduce the need for other more complex pattern transfer equipment and hence reduce overall fabrication cost.

Ten VAXes Do Not

There is a great deal of confusion concerning the definition of a supercomputer and, more importantly, concerning the use of large and expensive Cray-like machines if reasonably powerful machines such as VAXes can do the computation at a fraction of the cost. A VAX-8800, for example, costs under $1M, while a Cray costs $25M. Why not buy 10 VAXes and save all that money?

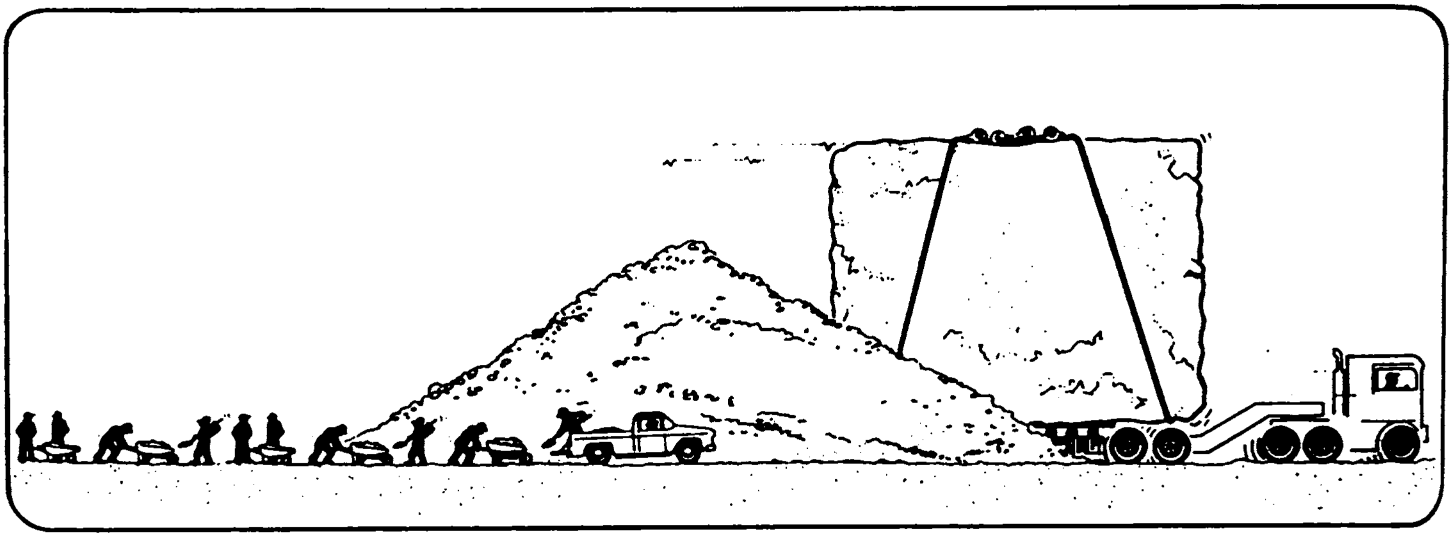
The answer seriously depends on the computational requirements and, more specifically, on the degree to which the problem can be solved by independent computers working on pieces of the problem and communicating their results at the end of the calculation. Many important scientific and engineering problems can be broken up in this way, and under these conditions, adding multiple independent processors is possible and economically desirable. Other problems require the fastest mainframe with the largest memory.

A useful analogy is found in moving gravel or stones from one place to another: Many small wheelbarrows will do the job, and adding more wheelbarrows (increasing *capacity)* will help, within limits. If, however, there is a requirement to move one large rock, a large truck (increasing *capability)* is called for, and no number of wheelbarrows will do. (Of course, there is research going on in the computer science community to tie wheelbarrows together to make an inexpensive truck; others are working to break up the rock.)

Thus, to suppose that one can always apply more VAXes to a problem (that is, multiply the power of one VAX by the number of VAXes one wishes to use) is to forget that these are *separate* machines that do not act upon the problem like a single Cray would. Consider, for example, the series of problems illustrated on the facing page. In problem A, four independent processors only need to communicate their results at the end of the calculation. A simple physical example might be the calculation of the pressure on the walls of a box containing an ideal gas such as helium. Each molecule (helium atom) creates a force on the wall independently of the others, the presumption being that the individual gas molecules do not interact with one another. Problem B is typified by parallelism with some degree of communication during the calculation. This might physically be indicative of the helium atoms in the box being allowed to interact via short-range forces between nearest neighbors.

To generalize, there is certainly a (small) class of problems that specially configured machines can be dedicated to in order to avoid acquiring more expensive Cray-like technology. There are even examples where special machines outperform supercomputers. On the other hand, dedicated machines are less flexible than supercomputers and may inhibit the testing of new ideas. Furthermore, economy is lost if each scientific problem requires a machine with a different architecture.

Adding more VAX-like computers to an existing facility will allow more researchers to use that facility (i.e., its *capacity* will be increased) but will not address a given problem any better, unless that problem can be broken into small

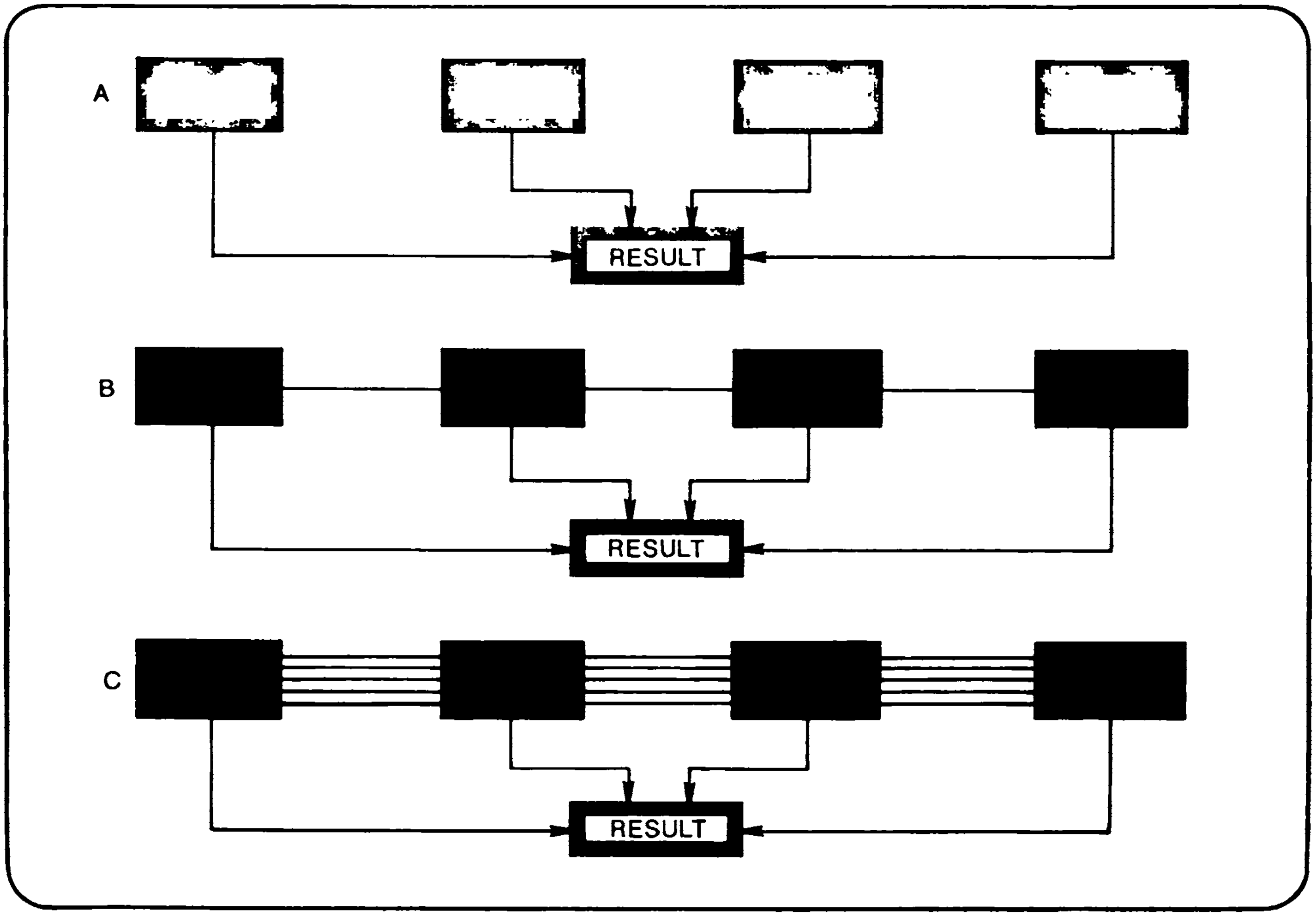


You cannot always do the job by adding more wheelbarrows: sometimes you need a large truck.

pieces that need to communicate infrequently during execution and the means of interconnecting and synchronizing the machines is in hand. (There is only one demonstrated method of interlinking such machines for a limited class of problems at the time of this writing.) The *capability* of the facility is therefore not improved by increasing the number of VAXes and the solution to the complex problem for which the additional VAX was obtained is no closer. A tacit, but important, assumption here is that if a simulation takes more than 10 hours to run on a given computer, it will not generally be considered a research-and-development tool. If there is less than one run per day, projects could take years to complete since many tens and even hundreds of iterations are generally needed. Also, engineers and scientists prefer to concentrate on a few problems and iterate as fast as they can analyze the results.

It is, of course, easier to increase the capacity of a facility by acquiring more of the same equipment, and the great majority of researchers tend to support this because it gives everyone a little. For the problems addressed here, it is the capability of the facility that needs upgrading; we need to give a lot to a few.

Several of the calculations described in this document were initially set up on smaller machines and trial subsets of the calculations actually needed were performed. **But for each of these calculations, as well as all of the other examples in the document, the magnitude of the problems soon outran the capability of the machines, and the need for a supercomputer became clear for real progress to be made.**



Whether or not a problem can be solved in a timely fashion by linked VAXes depends on the communication requirements when the problem is divided into parallel subproblems (indicated schematically by boxes). In A, each processor can work independently, with results being communicated only at the end. In B, some communication between processcrs is required, and independent processors may be hard pressed to compete with a supercomputer. In C, massive communication is required, and the supercomputer becomes the tool of choice.

Computers with Greater than 10 Times

Since the early 1960s, scientists and engineers have enjoyed an explosion of supercomputer power: The capability of supercomputers has been increasing and is expected to continue to increase by approximately an order of magnitude every 5 to 10 years. A computer with 10 times the capability of today's fastest machine is less than a year away.

In the early 1960s the workhorse of the day was the IBM, which could integrate a simple differential equation over the weekend; others took many weeks. Then came Control Data Corporation's 3600 and 6600, which changed our lives by enabling us to simulate, for example, radiation damage in metals and to determine the ground state of the hydrogen molecule from first principles. Seymour Cray, who invented the CDC 6600, introduced the Cray-1 in 1976; with its enlarged memory and speed, this supercomputer gave us the order of magnitude needed to calculate more complex molecules and to enter the two-dimensional world of modeling. Today, supercomputers are enabling us to attack previously intractable problems, a sampling of which are described in this report. Moreover, calculations can be performed in minutes that only 20 years ago took 100 hours on the supercomputer of that time; and because of the increased performance of semiconductor chips and the introduction of large-scale integration, the cost of the state-of-the-art mainframes has remained about constant.

The Cray-1 seems to have brought us within an order of magnitude of the maximum capability we can expect from a single-processor machine. But, there is no need to compute one process at a time if parts of a problem can be computed independently in parallel. The concept of computing several components of a total calculation in parallel is not new—the early ENIAC machine (1946) and the ILLIAC (mid-1970s) were based on that principle. At that time, however, there were too many other improvements that could be made by less expensive means. Now, as single processors approach limits set by electron speed and heat dissipation, parallel processing again becomes a viable option. The Cray XMP-2x series can calculate two processes at a time; the XMP-4x series, four processes at a time; and the recently released XMP-8x series, eight processes at a time. Hence, theoretically, nearly an order of magnitude increase in computing power can be gained without improving single processor speed at all.

What all this means to the materials science and engineering community is that enormous advances in an already powerful tool are not only inevitable, they are just around the corner. The Cray-3 with 16 processors should be available for benchmarking during the first quarter of 1989. The new ETA-10 features up to eight processors, new chip designs, a very large memory, and faster operation due to immersion in liquid nitrogen. IBM has recently announced a six-processor system. IBM is also funding Steve Chen in a large-scale parallel-processing initiative (Chen designed the XMP while at Cray), and has a separate supercomputer project in progress; from these initiatives a 64-processor machine is to emerge in the early 1990s. Japanese manufacturers (NEC, Fujitsu, Hitachi) are providing further options: For example, NEC has an SX2 single processor today that is 5 times faster than the XMP processor, and the Fujitsu VP200 is close behind the SX2. The Japanese also intend to incorporate parallel processing and will offer a machine in serious competition with Cray Research by the early 1990s.

No one denies that parallel processing works, but several unsettled questions remain: What is the optimum number of processors, is there even an optimum, and what is the best architecture (shared versus distributed memory)? Several manufacturers are building massively parallel machines which, at the very least, will provide supercomputer-like performance for specialized dedicated projects. It is entirely possible that these massively parallel machines will outrun few-processor architectures in raw performance. For some applications these new architectures can provide a cost-effective way to compute if the problem is properly matched to the capability. The Connection Machine made by Thinking Machines Corporation is such a massively parallel machine; it has 65,000 processors, each processing one bit of information at a time. It is clear that the quality of each processor can be enhanced as well as the number of processors, so that the gains are endless.

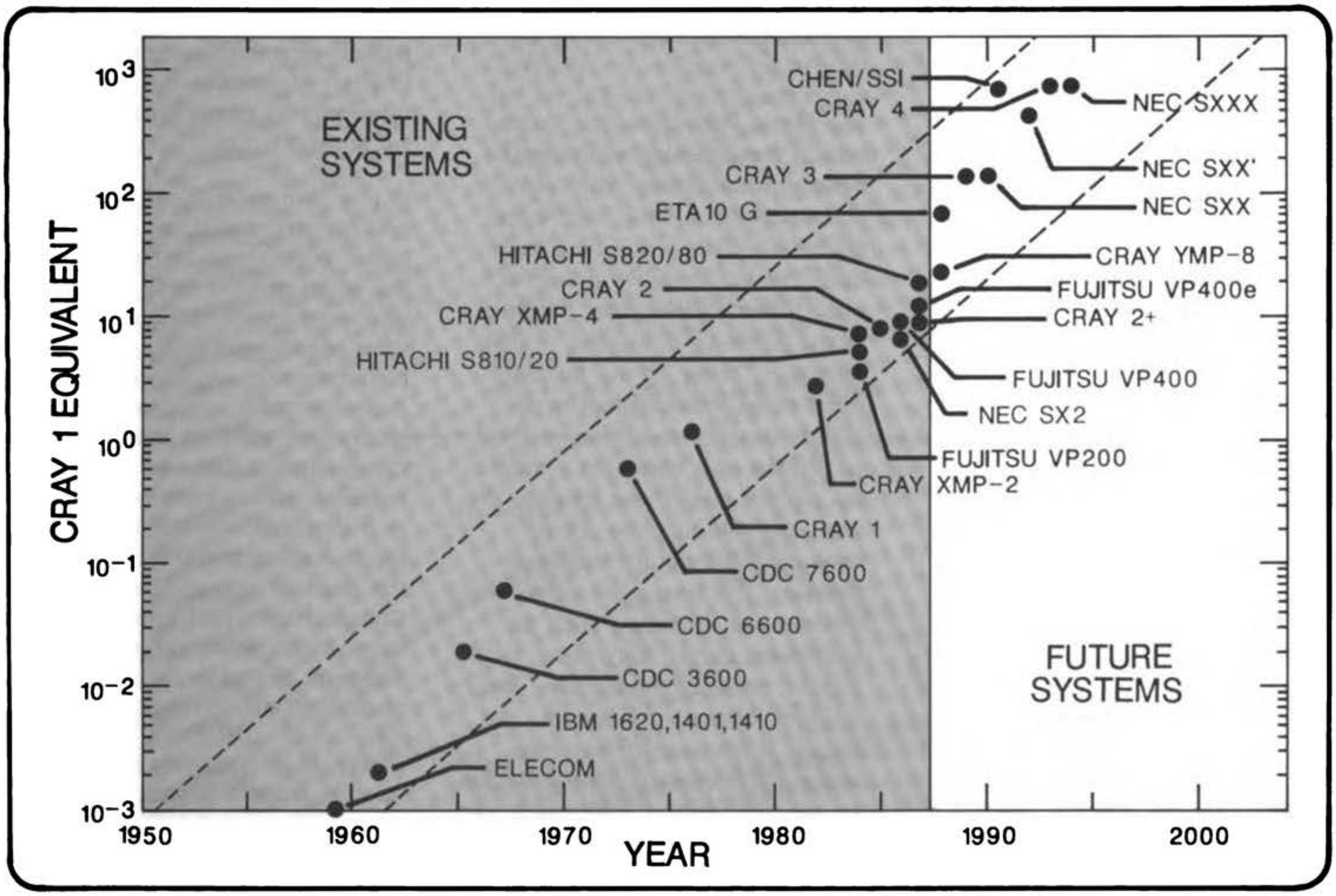
It is not only large-scale computing that has undergone a technological revolution. Minicomputers, minisupercomputers, personal computers, and workstations are growing in power at an enormous rate. Today a Vaxstation 2000 or Sun-3, rich in graphics software to permit easy manipulation of input and output information, puts the power of a VAX 11/780 on a desk. Such workstations relieve supercomputers of tasks they may not be designed for and create a user-friendly environment captive to the individual. These stations allow a user to submit jobs to a remote supercomputer, do stand-alone processing while waiting for a job, and finally post-process the results. It is important that supercomputers be employed in this way, doing

Today's Capability Are 1 Year Away . . .

what they are better at (number crunching) and letting more cost-effective tools be employed for other tasks. Ideally, supercomputers would always be interconnected with a host of smaller processors in a fast, efficient network.

By pushing the limits of gate-array technology, using high-electron-mobility GaAs instead of Si, cooling with liquid nitrogen to increase electron mobility, cleverly engineering network architectures, and adding more processors per system, we can expect the performance of supercomputers to continue its colossal increases. The demand for more detailed simulations and analyses of complex phenomena is driving this technology. As it matures, it will become available to other facets of computing so that ultimately all computer users will benefit.

It is impossible to imagine an end to gains in supercomputing performance. Never before has there been such a powerful tool to enable us to understand material processes and help the United States regain a competitive advantage.



Supercomputing capabilities are increasing by an order of magnitude every 5 to 10 years.

Centers of Multidisciplinary Research

The Birth of the Modern R&D Laboratory

The value of a multidisciplinary environment to materials research and development has been proved in a number of distinguished instances. The first dates to the late 1870s, after Thomas A. Edison purchased several acres in Menlo Park, New Jersey, for a laboratory complex. Edison signed a 5-year-contract with Western Union, which agreed to pay "laboratory expenses incurred in perfecting inventions applicable to land lines of telegraph or cables within the United States." This innocent-sounding arrangement established a significant precedent in the support of technological research and development. An independent inventor was not being paid for a new device, nor was he being asked to make specific improvements on a company's apparatus; instead, a laboratory was funded for research in a general field.

Edison's early track record stimulated this new direction in corporate strategy for managing technological development. As a professional inventor under contract, Edison worked on storage and retrieval of telegraph messages and acoustic telegraphy (which used multiple tones sent over one wire to transmit several messages simultaneously). Serendipitously, this research stimulated Edison's development of the phonograph and his contributions to the telephone.

A number of Western Union's major stockholders and officers, having seen the value of supporting technological innovation in telegraphy and then observing Edison's remarkable development of the phonograph, soon committed themselves to even more extensive support for Edison and his laboratory, in particular to pursue incandescent lighting. In the fall of 1878 they formed a separate research and development concern, the Edison Electric Lighting Company. With its resources Edison built an office, library, and a much larger machine shop at Menlo Park. He also expanded the laboratory staff from around a dozen to between 50 and 70 during 1880. With the extensive support of investors, Edison thus established the largest U.S. laboratory for industrial research and development at that time.

The Menlo Park laboratory gave Edison considerable advantages over other inventors. With the library, machine shop, and large team of researchers and technicians, he could attack many research and development projects at the same time. Instead of concentrating solely on the development of an incandescent lamp, Edison simultaneously researched all phases of a complete system for electric power and lighting. He was also able to carry out an exhaustive search for the lamp filament. The laboratory experimented with elements such as aluminum, boron, chromium, gold, iridium, platinum, ruthenium, silver, titanium, tungsten, tantalum, and nickel; alloys such as platinum-iridium; and organic materials such as fish line, cotton, cardboard, tar paper, celluloid, coconut hair, wood shavings, cork, and even visiting cards! Success came after the fabrication and testing of some 260 lamps.

The decisive advantage of this integrated research and development approach became apparent on New Year's Eve 1879, when Edison displayed to the public not only the new lamp but also dynamos, switches, regulators, fuses, and conductors.

The Advent of Supercomputing in Research and Development

So much has been said about the Manhattan Project—over 10,000 books and articles—that everyone recognizes the multidisciplinary effort it took to solve what still might be considered the world's most intensive *and secret* scientific challenge. Less known, perhaps, is that this project (which started what is now the Department of Energy) also led to the continued development of supercomputing as we know it today.

In Los Alamos in 1943, theorists and numerical analysts formed a group (with about 25 people, some the wives of scientists) equipped with mechanical calculators to perform calculations given them by physicists and engineers. A human supercomputer was created. It was recognized early on that a massive computational tool was necessary because experiments were difficult or impossible with the limited supply of nuclear materials and under the cloak of secrecy that prevailed. Computation would prove to have a tremendous effect on nuclear weapons design in reducing the number of experiments.

Today, U.S. National Laboratories use the world's largest supercomputers to make progress in weapons design. Great effort is expended at improving the design codes; that is, software is created that encompasses all known theoretical and experimental information. Physicists and numerical analysts improve models and algorithms; experimental data are carefully (and expensively) obtained from above- and below-ground tests and incorporated in the design codes. All of this takes place

Have Proved Their Worth . . .

at centers where the necessary disciplines are represented and the management clearly understands the mission. Cross-fertilization of disciplines is maximized and the computer is used as a tool to obtain the best design.

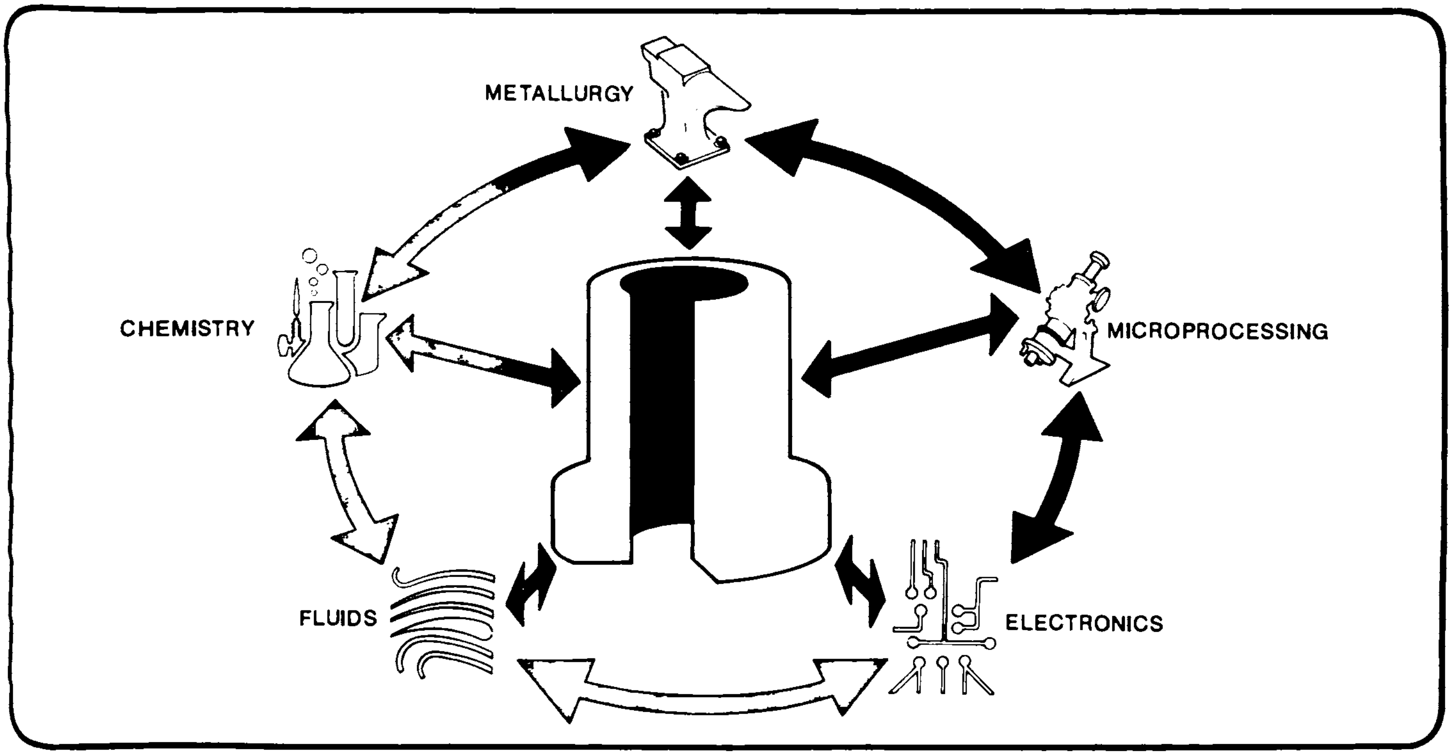
The Recognition of the Need for Supercomputing Centers Today

Outside the Department of Energy, there is increasing recognition of the value of supercomputing in a number of areas. Aircraft design, weather forecasting, oil exploration and extraction, pharmaceutical design, and automobile-fabrication tool design are among the most common. Over 200 supercomputers operate all over the world, 45% of which are outside the United States. The common thread between each of these industries is a multidisciplinary research center with the supercomputer as its most vital tool.

NASA has established in California one of the world's largest supercomputer centers for aeronautical design—the National Aeronautical Simulator. The National Center for Atmospheric Research (NCAR) in Boulder, Colorado, attracts scientists from a variety of disciplines to use their computational facilities. The reason for the success of these centers lies foremost in the cross-fertilization of ideas that comes with a multidisciplinary group.

Computer power itself, of course, can be provided by supercomputer centers like those set up by the National Science Foundation. They give isolated researchers, regardless of their location, access to the capabilities of large machines (albeit at distances that often create communications problems). Although such centers provide the necessary cycles for running powerful codes, researchers in related fields of research may not be nearby, a serious detriment when focusing on the most critical parameters of a problem. For example, improving a materials process like the chemical vapor deposition of silicon from silane gas requires detailed knowledge of the heat transfer from the substrate to the gas, the fluid flow of the gas in the particular temperature-pressure-composition range of interest, and the chemical interactions of the ionized gas with different material substrates. The velocity of the gas affects the interaction between the ionized gaseous species, which affects the rate of arrival of silicon at the surface that adsorbs different materials depending on their composition and temperature.

An interdisciplinary team of researchers familiar with each other's concerns can best search for the optimum solutions to complex real-world problems.



The supercomputer is the pivotal tool of multidisciplinary research.

We Have Come to

Because of its diversity, materials science has evolved into many subspecialties and splintered disciplines. Much progress has been made in understanding the individual aspects of materials behavior under specific environmental and manufacturing conditions. In order to optimize their usage and to exploit their potential, many of these aspects must be integrated and quantitatively described. In general this integration has rarely been achieved, and materials development and applications have been slow endeavors. In applications of materials our inability to precisely quantify materials limitations leads to overdesign, adherence to traditional materials, and "proven" methods of usage, rather than tailored and optimal designs.

1. Supercomputer simulation has a strong potential to be a powerful, cost–effective link between materials science and engineering, design, and manufacturing. The emerging advanced computers will make possible a new type of materials simulation whose key contribution will be the fostering of interdisciplinary research and development, not only within the materials fields but between these fields and other disciplines. Nowhere is this more important than establishing the bridge between materials, design, and manufacturing technologies.

These methodologies are rapidly developing toward the point where a designer can sit at a graphics terminal and watch the impact of design modifications in real time. Indeed, in some areas these capabilities have already arrived. For silicon chemical vapor deposition, an engineer or technician can continuously change the operating conditions for manufacturing using a minicomputer simulator (a tool based on physical models developed using supercomputing over nearly a decade). In the automotive industry (where design and tooling cost hundreds of millions of dollars annually) supercomputing aids the design of dies for forming sheet metal for new automobile models. The advanced computations allow physically realistic metal deformation behavior to be applied to forging large, complex parts under production conditions, significantly reducing costs.

As supercomputer and graphics hardware also evolve, we see a time just a few years away when computer simulation of materials and processes will play a key role in a majority of U.S. materials technologies.

2. New theoretical methods, algorithms, and approaches for analyzing the individual components of complex materials systems are rapidly evolving. This is enabling methodologies for computer simulation of materials and materials processing to emerge. Fundamental electronic structure calculations can predict the behavior of molecules and solids to such types of accuracies that in many cases computation has become the method of choice over experiment.

Nonetheless, it must not be forgotten that any simulation, however sophisticated, is only as good as its supporting experimental database. Even where theory has led experiment, it is experiment that proves the result. Fortunately, there is a concurrent deepening of this database as computers become more capable.

Supercomputer algorithms now allow the simultaneous solution of hundreds of equations necessary to describe a complex process. Three-dimensional solutions of heat transfer, structural, dynamical, and fluid mechanical equations are possible. These methods may be highly sophisticated, such as by including microstructural evolution during deformation of a metal. Transport calculations in semiconductors can predict electron velocity in high electric fields, properly taking account of the band structure of the solid, leading to the development of revolutionary electronic devices.

The time is ripe for these more individual efforts to be synthesized into comprehensive computer simulations of materials and materials processes.

3. To exploit opportunities in computational materials science and engineering we must invest heavily in the science underlying the methodologies, in developing software to make these useful to engineers and technicians, and in providing adequate hardware to scientists and engineers at universities and in industry. Fortunately, the supercomputer and high-performance graphics hardware needed for routine application of such simulations is continuing to become more powerful and plentiful while dropping in price. The realization of these benefits will require and stimulate the training of a new breed of scientists and engineers, who are equally at home with chemistry, physics, and materials science as well as with modeling and computational methods.

Several Conclusions . . .

The unification of materials science for the purpose of improved economic use and for new applications requires supercomputers for explorations and test simulations on shorter time scales and in more cost-effective ways than hitherto practiced. We have demonstrated by the examples in this report that supercomputers are already used for materials research, development, and processing in certain applications and branches of industry. The great economic benefits from supercomputers in materials science and technology are therefore evident but hardly exploited. This underutilization will only become more acute with the rapid advances in supercomputer development unless decisive steps are taken now.

4. For the United States to remain a leader as materials simulation moves out of the laboratory and into the industrial plant, we must act decisively now to stimulate the development of these methodologies and to develop turnkey simulation systems for industrial plants. Although the dawn of this new age for computer simulation in materials processes is just approaching, we can already see arenas where these methodologies are having a major impact.

5. Simulations can reduce design costs and the time from concept to market. We found two industries, in addition to automobile manufacturing, that are using supercomputers to save millions of dollars and months of design time. First, the polymer industry is designing dies by process simulation, resulting in enormous savings relative to the "trial-and-error" approach. Second, the semiconductor industry is turning to computation as the scale of electronic devices decreases. At present, fundamental understanding of these revolutionary devices can only be achieved through simulation. Supercomputing is also being applied to the design of the equipment with which to manufacture semiconductor devices and components.

6. Supercomputers allow us to build hierarchical design tools. The design of chemical vapor deposition equipment is but one example of the growing use of hierarchical design tools among computational scientists and engineers. The hierarchy includes equations and algorithms from different disciplines (i.e., chemistry, physics, materials science, and fluid dynamics) and processes that occur over different scales in time and space. A chemical reaction takes place because electrons that rearrange on the scale of angstroms lead to effects on a semiconductor device that may be felt on a scale of centimeters. This is the first time a tool has emerged that makes it possible to integrate complex phenomena from any number of disciplines into a useful, coherent program or code. The modules of the code can be improved as our understanding and the power of computation increase. Furthermore, the designer using the code need not be an expert in the fields of science and engineering represented.

7. Supercomputer simulation is a powerful design tool that can increase U.S. economic competitiveness today. Among the most promising areas for further progress are:

- Polymer forming and processing
- Alloy design and processing
- Ceramics design and processing
- Electronic devices
- Electronic device processing equipment

Computer hardware technology is rapidly improving; an order-of-magnitude increase in capability every 5 to 10 years continues to be the norm, with the immeasurable prospects of parallel processing on the horizon. The availability of this evolving state-of-the-art hardware to the engineering and scientific community is essential to the development and continued growth of the algorithms and methodologies that support the application of simulations to new materials technology.

We Have a Number

1. The committee recommends that focused multidisciplinary research initiatives in selected areas of materials science and engineering be started in order to integrate design and manufacturing with the underpinning research base. Supercomputer simulation of materials phenomena is at a stage where rapid new developments in science and technological applications are possible. Its early uses have been oriented toward well-defined applications and to a large extent have been possible only because of prior investment in long-term fundamental research. Opportunities now exist for simulation to address complex materials phenomena resulting from the interaction of several discrete processes, to provide information that cannot be obtained in any other manner, and to conduct benchmark computations to validate and sometimes guide theoretical modeling, experiment, and the design of new materials. Thus simulation will play a vital role as an adjunct to theory and experimentation. It is essential that suitable leadership, organization, and resources be extended to mobilize and focus our vast national talent on the challenge of designing new materials and materials processes. Some of the initiatives envisioned are:

- *Integrated alloy design and synthesis:* Simulation of materials microstructure, synthesis, and performance is an achievable objective now in some elementary cases; it is a vital long-range goal for U.S. technology to retain a forefront position in high-value-added materials and devices. One goal would be the design of new optoelectronic quantum devices, particularly involving modeling of alloy and composite semiconductor materials.
- *Materials processing and manufacturing methods:* Substantial progress has already been made in this area. Many opportunities remain to map out operating parameter regimes for producing sound versus defective materials. Areas ripe for development include semiconductor thin-film deposition and growth associated with integrated circuit technologies, joining methods for metals and ceramics, and forming operations—particularly shaping and molding complex parts.
- *Surface and interface phenomena:* Examples of promising topics include: (a) adhesion—initiation of bonding across interfaces and the effects of impurities, inelastic processes, and defects; and (b) nucleation and growth of thin films—by processes such as molecular beam epitaxy and chemical vapor deposition.
- *Atomistic simulation of microstructural evolution:* A long-range effort in this area is essential to learn how to perform simulations that involve different time or length scales. Microstructural simulations need atomic-scale information to understand the molecular and chemical structure of defects. Simultaneously, large-scale effects (e.g., millions of dislocations) require shifting attention to the dynamics of defect behavior. Simulations are a powerful means of understanding nonequilibrium effects such as metastable alloy phases and rapid chemical reactions.

2. The committee recommends the creation of a Supercomputing Center for Materials Applications (SCMA). The Center would provide a much needed means for moving the results of basic research into turnkey systems suitable for wide use in industry.

- The mission of the Center would be to provide a multidisciplinary environment in which to create software to be transferred to industry to enhance our competitiveness. This must be a "mission-oriented" facility whose management understands the role of the computer as a tool at the Center.
- The Center must be capable of handling proprietary information in order to attract industrial funding and to transfer the technology to an interested community. The Center must be able to produce software portable to U.S. industry. Smaller machines and machines with a variety of architectures must therefore be included at the Center for technological transfer purposes.
- The Center should become self-supporting after an initial, properly funded start-up phase.
- The Center should have a permanent professional staff for continuity in addition to an extensive visiting faculty program. Projects aimed at producing software for a given application could bring together a critical mass of talents from around the nation as well as from the site itself. Long- and short-term projects would both be addressed. Such a center

of Recommendations . . .

should also provide access to novel computer architectures, as required.

- The Center should be advantageously located within an existing supercomputer center. There are significant economies of scale in hardware to be gained by such a colocation.
- The Center should be advantageously located within an organization accustomed to an applications-oriented, multidisciplinary approach to supercomputing.
- The Center should be advantageously located near broadly based expertise in materials science and engineering. The daily interactions among a diverse scientific staff (including materials scientists, physicists, chemists, engineers, numerical analysts, and applied mathematicians) are of most value.

3. The committee recommends that supercomputer centers be kept at the state of the art. The momentum begun with the creation of the national supercomputer centers (for example, the NSF initiative) should be accelerated by a long-term commitment to increase the availability of computer resources to a broad scientific community. Access to state-of-the-art mainframes must be included as soon as they become available. Supercomputer technology is moving ahead at a rate that will render them obsolete in a few short years. Hence the retooling of these centers must be carefully coordinated: These are not one-time investments—they must be continually upgraded.

- The capacity of these centers needs to be expanded as well, but we again caution against the misconception that a computer center's power be measured by the total number of arithmetic operations it can perform (capacity). What really counts is how many operations can be applied to a single problem at the same time (capability), which is measured by the power of its largest (fastest) mainframe.
- The centers should provide the capability for attacking complex computational problems that cannot be solved with less powerful machines. A valuable additional function of the centers would be to make advanced-level simulation available to researchers not previously members of established simulation groups.
- The centers must include a commitment to upgrade their internal communications network as well as the network with the external user community. High-bandwidth communications are necessary for interactive usage and to take proper advantage of essential graphics.

4. The committee recommends the formation of multidisciplinary materials simulation groups (MSGs). The formation of MSGs (of several faculty spread over several departments) will create a synergy of materials scientists with computer scientists, computational mathematicians, and experts in visualization. They will generally work closely with the SCMA. New ideas in technology will require advanced computational strategies, new algorithms, and unprecedented capability to analyze and visualize results. Such groups and capabilities need to be developed and brought toward more effective solution of important scientific and technological materials research problems.

5. The committee recommends that the infrastructure of local computing associated with advanced simulation be strengthened. Solving current materials problems through simulation requires the capability of the best mainframes. Yet the trial of new algorithms, development of codes, and display of results are better accomplished in a local environment. Thus there needs to be recognition that the acquisition of advanced local computing capabilities is an important ingredient in the overall structure of advanced computation.

6. These initiatives should be implemented in a manner balanced to preserve the research strengths that are central to the success of materials engineering and processing in the future. We can today simulate several materials processes only because of the long-term fundamental research investment in the past.

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Workshop on Advanced Computation and Simulation of Complex Materials Phenomena—Technical Presentations

Topic I Thermodynamics, Structures, and Defects

M. Muthukumar *Simulation of Phase Transformations and Dynamics in Polymers*

Jeffery Skolnick *Current State of Computations in Polymer Physics*

Jorge Hirsch *Simulation of Quantum Many-Body Phenomena in Solids*

Malcolm Stocks *Ab Initio Theory of Phase Stability*

David Wood *First Principles Calculations of Alloy Phase Diagrams*

Topic II Materials Synthesis and Processing

Thomas Stoughton *Simulation of Metal Deformation by Arbitrary 3D Tool Surfaces*

Robert Brown *Large Scale Computation in Materials Processing*

Michel Dupuis *Recent Scientific and Engineering Research on the LCAP Parallel Supercomputer at IBM-Kingston*

Anthony Hopfinger *Applications of Computer-Aided Molecular Modeling and Design*

William Johnson *Amorphous Metallic Alloys and Crystal Stability*

Topic III Electronic and Transport Properties of Materials and Devices

Robert Dutton *Projections and Priorities for Topics in Electronic Transport and Materials*

Thomas McGill *Simulations and the Design of Small Structures for Applications in Electronics*

William Frensley *Numerical Modeling of Quantum Semiconductor Devices*

Steven Laux *Self-Consistent Calculation of Electron States in Narrow Channels*

John Poate *The Next Generation of Materials and Processing for Electronic and Optoelectronic Technologies: Role of Computation*

David Biegelsen *Applicability of Computational Methods to Structural, Electronic, and Transport Properties of Amorphous Semiconductors*

Topic IV Mechanical Properties and Mechanics of Materials

Owen Richmond *Dirichlet-Voroni Space Tesselations for Characterizing Polyphase and Polycrystalline Materials and Generating Finite Element Meshes for Modeling Their Behavior*

David Parks *Title Unavailable*

S. L. Phoenix *Analysis and Computation in Network Models for the Time Dependent Failure of Fibrous Materials*

Topic V Surfaces and Interfacial Phenomena

James Chelikowski *Pseudopotential Methods for the Total Energy of Surface Structures: Metals and Insulators*

Charles Duke *Prediction and Experimental Determination of Semiconductor Surface Structures*

Michael Finnis *The Tight Binding Model and Atomistic Simulation*

Murray Daw *Semi-empirical Calculations of Metal Surface and Interface Structures*

Thomas Weber *Hiking Through Phase Space*

John Smith *Total Energies and Electronic Structures of Metal Interfaces*

Topic VI Computing Aspects

Sidney Karin *Title Unavailable*

Farid Abraham *Supercomputing in Physics and Chemistry*

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Biographical Sketches of the Committee Members

WILLIAM D. WILSON earned his B.S. and M.A. degrees at Queens College in New York and his Ph.D. degree in physics at the City University of New York. He was a research physicist at Brookhaven National Laboratory until joining Sandia National Laboratories in 1969. In 1974 he became head of the Theoretical Division. Since 1984 he has been manager of the Computation Department. He is member of the American Physical Society. His research interests are in interatomic potentials, defects in solids, hydrogen and helium in metals, and diffusion.

ROBERT J. ASARO was educated at Stanford University, where he earned his B.S, M.S., and Ph.D. degrees in materials science. He held a postdoctoral fellowship in the Department of Metallurgy at Ohio State University and was a research scientist at Ford Motor Company before he joined Brown University, where he is now a professor of engineering. He is a member of ASM International. His research interests are in the plasticity and fracture of solids, metal corrosion, environmental effects on material behavior, and theoretical and experimental studies of the mechanics of crystals.

RICHARD H. BOYD received his B.Sc. in chemistry at Ohio State University and his Ph.D. in physical chemistry from Massachusetts Institute of Technology. He worked as a research chemist at DuPont from 1955 until 1962. He was professor of chemistry at Utah State University from 1962 until 1967. Currently he is professor and chairman of Materials Science and Engineering and a professor of chemical engineering at the University of Utah. He is a member of the American Chemical Society and the American Institute of Chemical Engineers, and a fellow of the American Physical Society. His research interests are in plastics, polymers and their properties, relaxation processes in crystalline polymers, and molecular mechanics simulations of organic molecules and of processes in polymers.

ROBERT W. DUTTON earned his B.S., M.S., and Ph.D. degrees in electrical engineering at the University of California, Berkeley. He was an assistant professor at Berkeley before joining the faculty at Stanford University, where he is a professor and director for design at the Center for Integrated Systems. His research interests are in process device and circuit modeling for integrated circuits, integrated circuit simulation and characterization using computers, and integrated circuit design optimization.

WILLIAM A. GODDARD III received his B.S. degree in engineering from the University of California, Los Angeles, and his Ph.D. in engineering science from the California Institute of Technology. He is currently the Charles and Mary Ferkel Professor of Chemistry and Applied Physics at Cal Tech, where he is also the project director of the Materials Research Group (NSF). He is a member of the National Academy of Sciences, a fellow of the American Physical Society, and a member of the American Chemical Society and the Materials Research Society. He has carried out research in a broad spectrum of materials, chemical, and biological areas, including catalysis, reaction mechanisms, surface chemistry, biological oxidations, superconductors, and biological and polymer simulations.

JUAN M. SANCHEZ received his B.S. degree in physics at the University of Cordoba, Argentina, and his M.S. and Ph.D. degrees in materials science at the University of California, Los Angeles. In 1981 he joined the faculty of Columbia University, where he is now professor of metallurgy and materials science in the Henry Krumb School of Mines; he is also a staff member of Columbia's Center for Strategic Materials. He is a member of The Metallurgical Society of AIME, ASM International, the Materials Research Society, and the American Physical Society. His research has been in thin film diffusion, kinetics of phase separation in solids, order–disorder theory, and statistical thermodynamics and modeling of phase diagrams; in recent years one of his major efforts has been to develop and implement theories to compute, from first principles, the phase diagrams of complex engineering materials.

JOHN R. SMITH earned his B.S. degree at Toledo University and his Ph.D. degree in physics at Ohio State University. He served in the U.S. Army at NASA's Lewis Research Center and then did postdoctoral work at the University of California, San Diego, before joining the General Motors Research Laboratories, where he is now a principal research scientist. He is a fellow of the American Physical Society, and a member of the American Vacuum Society and the Materials Research Society. His research interests are in the theory of solid surfaces, electronic and magnetic properties, and chemisorption; superlattices; adhesion; metal-contact electronic structure; and defects and universal features of bonding in solids.

DAVID J. SROLOVITZ was educated at Rutgers University, where he received his B.S. degree, and at the University of Pennsylvania, where he earned his M.S.E. and Ph.D. degrees in metallurgy and materials science. He was a postdoctoral research associate at

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WILHELM G. WOLFER received his B.S. degree in engineering physics from the Institute of Technology, Vienna, in 1961, his Diploma-Physiker from the University of Stuttgart in 1965, and his Ph.D. in nuclear engineering from the University of Florida in 1969. His professional experience includes positions as research assistant in the Plasma Diagnostics Laboratory at the University of Florida; senior engineer, Westinghouse Advanced Reactor Division; research staff member in the Metals and Ceramics Division, Oak Ridge National Laboratory; and professor in the Nuclear Engineering Department, University of Wisconsin. Since 1985 he has been a member of the technical staff at Sandia National Laboratories. He is a member of the American Physical Society. His research interests are in radiation effects, chemical reaction kinetics in condensed matter, mechanics of solids and fracture, and hydrogen and helium embrittlement.