Molecular Engineering

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Engineering, as taught and practiced today, applies the macroscopic and statistical laws of science. Its successes are impressive, as our technical civilization testifies; but, despite displayed vigor, the leadership is slipping from the hands of the engineer, because the power of this approach becomes exhausted.

Engineering is based on the proper use of materials. At present, with rare exceptions, such materials are selected and applied by empirical methods. With concepts of the molecular properties of matter in their infancy, this procedure was the only feasible one. However, about 50 years have now passed since the inception of the quantum theory; physics and chemistry have arrived at quantitative statements about the structure of atoms and molecules and their interaction in gases, liquids, and solids. And yet, visits to engineering laboratories and discussions with contracting agencies of the Government make it obvious that very little of this knowledge is alive in the mind of most engineers. The answers to the increasingly excessive demands for materials remain empirical; they are slow in coming and are bought in uncertain approaches at an excessive cost. It is time to introduce a more fundamental foundation on which a more powerful technology can be erected.

The transition from the phenomenological approach to matter to a "molecular engineering" has to be pioneered by the universities in a new teaching and research program that forgets about boundaries between departments as well as those between schools of science and engineering. It requires the generous cooperation of industry; it requires retraining of engineers in summer courses and by postgraduate fellowships; and last, not least, it requires a modest appraisal of the present capabilities of the new methods in competition with the established ones. In cases of great complexity, empirical experimentation may frequently still reach its goal faster than scientific analysis and synthesis. But the balance of power will shift rapidly to the molecular engineer as knowledge and experience grow.

Many others in the fields of science and engineering are obviously aware of this situation, as, for example, last year's conferences at the University of Illinois and Carnegie Institute of Technology testify. The ideas expressed in this article, which are based on our experiment at Massachusetts Institute of Technology, are intended to be a modest contribution to a general discussion.

What is molecular engineering? It is a new mode of thinking about engineering problems. Instead of taking prefabricated materials and trying to devise engineering applications consistent with their macroscopic properties, one builds materials from their atoms and molecules for the purpose at hand. This approach gives the engineer a true spiritual connection with modern science, a partnership, and a new freedom of action. He can conceive devices based on ideal characteristics and then, returning to the laboratory, inquire how far such characteristics can be made to order. He can play chess with elementary particles according to prescribed rules until new engineering solutions become apparent. He can be selective by insight, foreseeing inherent limitations of materials and making use of their actual capabilities.

This solving of puzzles on the molecular scale requires the mind to develop a kind of spiritual x-ray machine that perceives behind the macroscopic boundaries of matter its elementary constituents in action. To clarify the procedure, let us assume a technical challenge and outline the response that engineering might make both in the traditional manner and according to the new mode of thinking.

Approaches to a Technical Challenge

Airplanes of the future will travel much faster and higher through the atmosphere than today; in consequence, they will heat up by friction to a very uncomfortable temperature, say 1000°F. Can the metals used in air vehicles now, the fuel serving for their propulsion, and the electric machinery developed for their control operate safely at such elevated temperatures? Obviously not. Hence a major industrial effort is required, comprising all aspects of engineering, to translate such a plane into reality.

A standard approach would be to gather the available macroscopic information on metals as to tensile strength, on fuels concerning explosion temperatures, on insulators as to electric failure, on polymers concerning plasticity and decomposition temperatures, and so forth. By analyzing such data, one would probably find that no performance characteristics have been measured at these high temperatures and under the vibration conditions of modern jet planes, that no obtainable material will qualify, but that some trends toward improved materials are discernible. In consequence, test programs evaluating high-temperature performance are initiated under Government contracts in various industries; one modification after the other is tried and found wanting; but slowly, by bulldozer tactics, the view is cleared and the goal comes in sight.

Now, if we are lost in the woods, we need not level the forest to gain a clear view, we can climb trees and take our bearings. This the molecular engineer would do. He knows of atoms and how they are bound together, from the small diatomic molecules of gases to the ring and chain molecules of chemistry and to the glasses and crystal structures of solid-state physics. He can inform himself about the strength of the bonds that hold these particles in place and thus can evaluate which types of materials might have any chance to qualify at the anticipated high-temperature level. Next, the stability of such materials in the chemical environment found at high altitudes has to be considered; the choice is narrowed step by step, as, in addition, mechanical and electric performance requirements are introduced. Thus, by thinking about the molecular structures of materials and by a few decisive experiments to provide missing data, the possible building stones can be selected from which the required materials might be made.

After this prestudy has been made, a molecular analysis is required of the macroscopic phenomena to be controlled for safe operation of the aircraft: tensile strength, explosion temperature, electric failure, plasticity, and whatever else enters. What from a macroscopic point of view appears as a simple event, measured by a simple test and described by some simple parameters, is actually the outcome of complicated molecular events

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that, depending on circumstances, may take a variety of courses. Here lies the main fallacy of macroscopic testing: the belief that a material of the same chemical composition or trade name, subjected to the same test conditions, should give the same result. It frequently does not! For example, the mechanical or electric strength of materials thus measured varies within such wide limits that only a statistical evaluation can hide the bankruptcy of this test approach.

A scatter of test data beyond the errors of our equipment is a sure indication that the phenomena under investigation contain unrecognized and, therefore, uncontrolled parameters. These parameters are generally of a molecular nature and, hence, are invisible to the classical engineer like the ghosts in Topper's television show. Let us conjure some of them for public scrutiny.

Impurities

In composing metals, plastics, glasses, and crystals, billions upon billions of identical building stones must be set by natural processes into prescribed patterns. Obviously, this requires that only these stones are at hand, but what chemist could prepare his starting materials with that purity? "Chemically pure" reagents usually contain parts per thousand of foreign matter; the starting materials of industry embody several percent of unwanted constituents; and these extraneous particles somehow have to be accommodated.

How they will be incorporated depends on the method of preparation. For example, if a rock salt crystal grows slowly over thousands of years, as it does under natural conditions, the atoms of sodium and chlorine, because they fit the lattice structure best, are selectively inserted. The foreign matter is pushed along by street-cleaner techniques and now and then discarded in pockets. This method of purification by fractional crystallization, here carried by natural processes to the extreme, produces a rock salt crystal of great apparent purity, as optical absorption measurements testify. But take the same crystal, heat it to a few hundred degrees and cool it again, and its transparency in the ultraviolet has been greatly impaired. The discard has seeped out of its pockets and the material is now inferior to any crystal grown with reasonable care in a few hours in the laboratory. This is also borne out by conductivity measurements: before heating, the crystal is a very good insulator; after heating, its conductivity increases by orders of magnitude.

Since we are bound to operate with impure materials, it depends on preparation and requirements how disturbing this fact proves to be. In table salt, impurities in the order of several percent may not matter, but even here, who actually knows? Ailments such as cancer might be induced by impurities in our food or in the air we breathe, just as a crystal can be poisoned by the atmosphere in which it grows. Through impurities and their mode of distribution, the prehistory of a material enters as an important variable in critical performance tests.

Dislocations

The influence of prehistory is not limited to the distribution of extraneous matter only. Even ideal purity could not create or maintain an ideal material. When building stones are set endlessly on building stones, mistakes are bound to occur. Suddenly, here is an extra row of atoms that has to end in a blind edge; there is a hole in the structure we forgot to fill; and over there a row of atoms must be pivoted around a corner. These mistakes, called dislocations, will become more numerous the faster nature works —that is, the higher the temperature. As the result of statistical laws, atoms will be missing from their regular lattice sites with a probability increasing exponentially with temperature, and they will be misplaced to surfaces or interstitial positions.

In consequence, a material at any temperature level can be characterized by an equilibrium of disorder; but it takes time to create a predictable amount of confusion. As the temperature is lowered, this time lengthens exponentially from seconds to minutes, days, years, and centuries. Only by creating a material at low temperature can we therefore hope to produce the improved order realizable at that temperature level. This is the secret of why "cold rubber" tires are superior to those made by the hot vulcanization process. In general, materials will contain a disorder that is "frozen in" from some higher temperature.

Use of Imperfections

If imperfections have to be taken in stride, why not use them to advantage? After all, we pay more for a hand-woven Persian carpet than for a machine-made one, because the irregularities of the former reflect the artistic sense of its maker and replace endless repetition by ingenious variation. A perfect crystal would prove similarly uninteresting. Nonmetals would not conduct or fluoresce, ferromagnetics would not show a useful magnetic response, steel could not be hardened, even trees might not grow or life originate in such flawless surroundings. To be sure, perfection has some striking advantages—the mechanical strength of metals, the electric strength of insulators, and the moral strength of human beings could be raised a hundredfold—but adventures in life and nature arise from imperfections.

Many deviations from perfection occur besides impurities and misplaced lattice points. Electrons and electron defects, for example, may enter a dielectric from the electrodes or be generated in the volume by dissociation. These electric charges, moving combined with mass particles as ions or striking out on their own with all kinds of velocities and laws of motion, are the active ingredients of our modern electronic devices and will lead to a host of others yet to be invented. They also are the key to such chemical puzzles as: why certain compounds cannot be made in stoichiometric proportions; how colors fade and photographic films operate; how certain catalysts work; and why many tricks of the organic chemist prove to be successful.

Boundaries are imperfections, providing the highways for surface conduction, diffusion, and chemical attack. Filled with intercrystalline cements, they may be the focus of embrittlement by mechanical vibration and chemical transformation; metal fatigue and catastrophic failure result. Boundaries cause heat insulation: a single crystal of quartz conducts heat like iron by passing it on through its lattice vibrations. Disorder destroys the periodicity of motion and scatters these vibrations; hence, fragmentation and glass formation lead to the silicate materials that insulate our houses. Special boundaries, the domain walls, impart usefulness to ferroelectrics and ferromagnetics. Motion of these walls caused by external fields gives us control over the stored electric and magnetic energy and leads to the memory devices on which the success of modern computing machines depends.

There is no end to the variability of the real structure of matter and to the possibilities offered by its control. We have not even mentioned how the elementary building stones themselves, the 90-odd different atoms, can enter the design patterns of materials in endless substitutions, from the homeopathic doses of parts per billion that are required for transistors to the large-scale replacements as in mixed crystals, glasses, and metal alloys. But let us return to our airplane problem and draw some conclusions from this glance into the molecular world.

Conclusions

Our faith in the beliefs and test procedures of the classical engineer has been shattered. The test data published in the literature are not binding as soon as they concern structure-sensitive properties. A material is not characterized by its chemical composition alone; its prehistory and the detailed arrangement of its building stones enter decisively. Taking apart a material by chemical analysis destroys the clues as effectively as the police would if they cleaned up a murder house with soap and water. Engineers have to become detectives who are familiar with sensitive nondestructive tools, including x-ray analysis, spectroscopy, electric and magnetic measurements of all kinds, and the new probing methods of nuclear-, para-, and ferromagnetic resonance.

Phenomena such as mechanical strength and metal fatigue, explosion hazard and electric failure, decomposition of plastics and loss of ferromagnetism, which are decisive for design considerations of the airplane of the future, are structure sensitive; only molecular analysis will bring them under control. Much of the needed information has been acquired by the scientists; much more is still missing. However, the incompleteness of the art does not give an excuse to let the engineer spend a further generation in the bleachers before he enters the arena. His game is being played now by stand-ins, the physicists and chemists. Only by enlisting him as an active partner in molecular thinking can we prevent squandering of our resources in antiquated approaches.

According to our experience, this educational problem is not solved by a few more courses in the science departments. If the physicist, for example—and I am one of them—talks to an engineering student in typical lingo and aloofness, the information generally passes straight through the skull, ear-in ear-out, without leaving any permanent impression. What we try to create as our answer to this situation are truly interdepartmental laboratories for molecular science and engineering. The strong foundation is fundamental research leading into the unknown for the sake of knowledge only. After new knowledge has been acquired, questions can legitimately be asked about its practical implications. Thus, from the first floor of the house, mainly populated by scientists, we reach the second, where one dreams of long-range applications. Finally, when the implementation stage has been reached, the problem passes to the top floor for the development of prototypes.

Such a laboratory structure challenges any kind of talent found in schools of science and engineering, from mathematician and theoretical physicist to the wizard of devices. Here the physicist cannot explain away difficulties with impunity, the engineer's prototype does not work, and a real answer is required. Here the ceramicist cannot persist in his old-established methods of handling materials. The scientist, inquiring into phenomena of a new order of complexity, sees what single crystals can accomplish and asks why ceramics cannot compete. Here is a feedback between all activities, stimulating thinking and critical appraisal. The modern research tools of science and engineering, when combined in one laboratory, allow a more searching approach from many angles, and the specialists able to handle them work as allies. There is no excuse for doctoral students to remain narrow minded; their research problem fits into a broad context and may be pursued with any promising tool of any discipline under expert guidance.

This effort can succeed only if the over-all problems attacked are broad and challenging and if the staff members have full freedom in their individual research and receive full credit for their contributions. The Laboratory for Insulation Research at Massachusetts Institute of Technology has been built up since 1937 as a pioneering test case. Its present staff consists of physicists, chemists, electrical engineers, and ceramicists; we hope to form an alliance with mechanical and chemical engineers, metallurgists, and biologists as experience and confidence grow. The name of the laboratory is somewhat misleading; it was originally chosen to emphasize a connection with the problems of the electrical engineer. However, there exists no true "insulation" either in electric equipment or in human affairs. Any material can be made to conduct electricity; and the generation, motion, and control of charge carriers in gases, liquids, and solids, with all transitions from insulators to metals, is one of our broad fields of interest. Other long-range projects concern the origin and action of electric and magnetic moments, from individual electron clouds and nuclei to the cases of extreme coupling, the ferroelectrics, and ferromagnetics. In short, we try to contribute to the fundamental understanding of the electric and magnetic properties of matter and to their circumspect application in engineering devices.

If laboratories for molecular science and engineering are established on a broader scale and their aims are supported by teaching on an interdepartmental level, does this solve the problem that Government and industry face in learning and applying with dispatch the concepts of molecular engineering? Obviously, the students thus educated will make their impact but only gradually. Summer-session courses and postgraduate fellowships have to be added to bring promising men back from industry to the universities for days or a year of unhampered study as coworkers in these challenging laboratories. Returning to their organizations, they will spread the new comradeship and understanding cooperation between science and engineering in molecular thinking. As a step in this direction, a 10-day course in molecular engineering will be offered at Massachusetts Institute of Technology in the summer session of 1956.

The experiments adduced by Dr. Franklin in support of his hypothesis were most ingeniously contrived and happily executed. A singular felicity of induction guided all his researches, and by very small means he established very grand truths. The style and manner of his publication are almost as worthy of admiration as the doctrines it contains. He has endeavoured to remove all mystery and obscurity from the subject; he has written equally for the uninitiated and for the philosopher; and he has rendered his details amusing as well as perspicuous—elegant as well as simple.—Sir Humphry Davy. Quoted by E. N. da C. Andrade, in "The scientific work of Benjamin Franklin," *Nature* **177**, 61 (1956).