CHEMICAL ENGINEERING

The Tailored Molecule

The secret of finding "wonder" materials for future rockets, TV sets and automobiles rests in the new science of molecular engineering.

By ALLEN LONG

SOME DAY SCIENTISTS will be able to design with engineering precision the new materials needed to perform under special sets of conditions.

When they are able to do this, the hit-or-miss approach can be abandoned and one of the biggest and most costly bottlenecks to the advancement of scientific accomplishments will have been eliminated.

This has to come, for there are no holes in the periodic table of elements. This means that the "wonder" materials for future automobiles, wall TV sets and rocket ships must be made out of the basic substances we now have at hand.

The process of designing a new material to fit a special purpose might well be called "molecular engineering." It will include manipulating the molecular structures of known substances to build in the qualities needed.

Great strides in this direction already have been made. An end-product in one case is familiar to every person who owns a pocket-sized radio. It is the transistor, the tiny, rugged, chunk of germanium that has replaced vacuum tubes in many jobs, especially in hearing aids.

Transistors work because the germanium contains a tiny amount of impurity. The impurity may be as little as a few atoms of indium in a million atoms of germanium. Other impurities such as phosphorus, arsenic and antimony can be successfully used.

Pure germanium is a poor conductor of electricity. It has no free electrons. Each germanium atom has four electrons that seek to bond other atoms to it. In pure germanium, each atom successfully makes four electrical bonds with other atoms. No electrons are left over.

If germanium is to conduct electricity, it must have some free electrons. These are made available by adding tiny amounts of such "impurities" as indium, having three electrons for bonding, or phosphorus, arsenic and antimony, having five electrons for bonding.

Thus when a germanium atom combines with one of these "impurities," either the germanium has an electron left over, as in the case of a union with indium, or the impurity has an electron left over. These left-over electrons are free to move through the substance when a voltage is applied. Thus by adding an impurity to pure germanium, scientists changed a poor electrical conductor into a good conductor. The scientists, in effect, engineered the material to get a desired result.

Before scientists can go about an orderly engineering of materials having special properties, however, an enormous amount of information must be amassed. The very first step is to learn the properties of pure materials. These properties are controlled by the crystal lattice structure, the way the atoms join to form larger units. Any imperfection in the lattice structure, or an increase in the kinds and amounts of impurities, can change the material's nature.

Then more information must be amassed as outside factors are brought to bear on the substance. These factors can be pressure, temperature, atomic radiation and the atmosphere surrounding the substance. A promising rocket material that withstands high temperatures might be found to lose this quality completely when subjected to the cosmic radiation found in space. Or perhaps the material might become even more heat resistant.

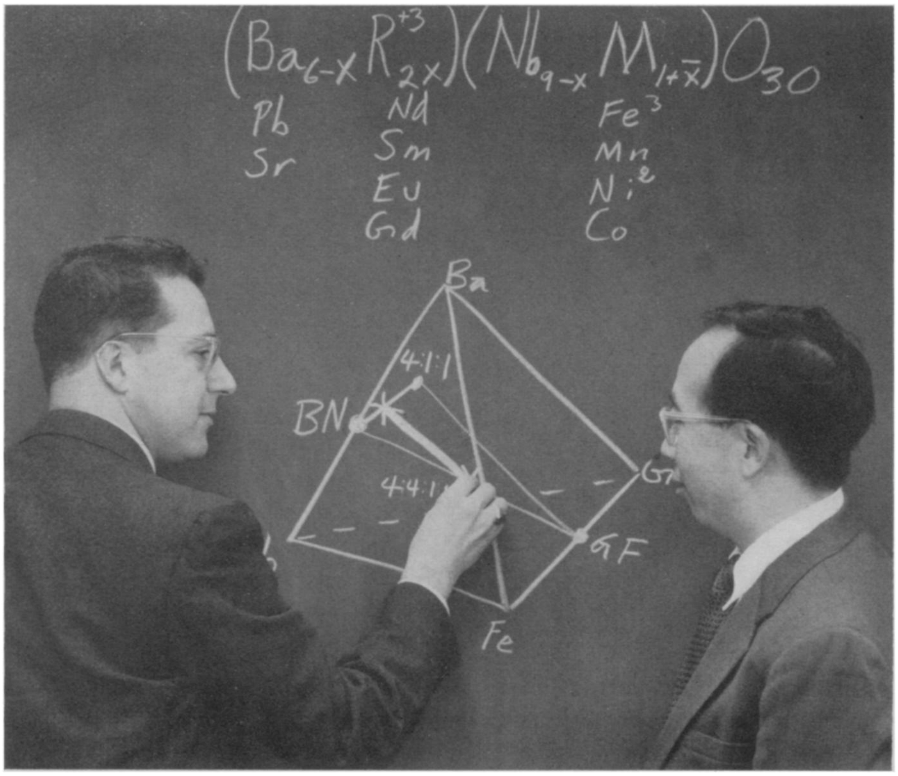
Once such information is available for a large number of chemical mixtures and compounds, scientists can take more of a slide-rule approach to the design of specific materials to meet specific needs.

One storehouse for this kind of data is at the National Bureau of Standards in Washington, D. C. Scientists there are constantly working out the factors that affect the properties and behavior of materials.

Even more-critical work at the Bureau involves the development of measuring techniques. To assure valid results, these measurement methods must be able to guarantee the scientist that he is actually measuring what he wants to measure.

To illustrate the measurement problem, Dr. Irl Schoonover, the Bureau's associate director for planning, said that when some property of a sample material is measured independently in several laboratories throughout the U. S., the results often vary widely. Before molecular engineering can get down to an exact science, all laboratories must be able to measure specific qualities and get consistent results.

Dr. Schoonover does not see the Bureau as a creative source of new, exotic materials. In advancing the art of molecular engineering, he foresees the Bureau contributing chiefly through development of "very fine methods to enable others to make the materials."



PORTRAIT OF A NEW MATERIAL—The pyramid-like blackboard drawing is a phase diagram, the portrait of a new ceramic that some day may be widely used in computers. The ceramic is a modified form of barium niobate. By substituting certain atoms for other atoms, scientists at the National Bureau of Standards have created a material that can "remember" not only by means of magnetism but also by electrical charges, combined qualities that until now have not been available in a single material.

These methods will include ways to prepare the material, to purify it, and to test its qualities through accurate measurements.

In the past, an enormous amount of work has been done in this field. Much of it, unfortunately, is of limited value.

One limitation is the temperature range at which materials were tested. Until recently, materials were studied at temperatures ranging up to about 2,700 degrees Fahrenheit. Suddenly rockets made material performance important at much higher temperatures.

Complicating the picture is the fact that composition of the materials studied was often not determined to a high accuracy.

Strange things sometimes happen under the many forces that can act upon a material, Dr. Alan D. Franklin, chief of the Bureau's mineral products division, said.

At frigid temperatures approaching absolute zero, for instance, liquid helium climbs the walls of its container. Some metals suddenly lose all electrical resistance and an electric current induced in them theoretically will circulate forever if the metal is kept that cold.

When water freezes, it becomes ice. When extreme pressures are exerted, it becomes a different type of ice. And then another type. All told, there are at least five different types of ice.

Under high pressure, new chemical compounds have been formed. Man has also been able to use pressure to produce in the laboratory things that so far have existed only in nature. For example, graphite, under pressure, can be made into diamond. Quartz, a special form of silicon dioxide (sand), can be made into Coesite.

Coesite represents an entirely new form of silicon dioxide. It is much denser than quartz. After being formed under high pressure, Coesite can be trapped in this state by releasing the pressure and cooling to room temperature.

Also at high pressures it has been found that some electrical insulators become semiconductors, and brittle substances such as bismuth and quartz become ductile. Tungsten carbide more than doubles its strength when under a pressure of 400,000 pounds per square inch. Liquid mercury freezes at 180,000 pounds per square inch.

It can be seen that a staggering panorama of material characteristics to be explored, and exploited, confronts the researcher in the molecular engineering field.

The qualities of materials are affected not only by external factors but also by their impurities, porosities, grain size, grain boundaries, lattice dislocations, strains, crystal imperfections, and ability of the surface to absorb liquids, solids and gases.

Each of these must be evaluated independently for each substance. This information is now being gathered and scientists are beginning to approach the point where "we can build in the qualities we want," Dr. Schoonover said.

Much work remains to be done before scientists will be able to engineer the materials they need. But the scope is so wide and the possible combinations of controlling factors is so astronomical that, once these are properly understood, it appears that a whole array of new and exciting materials some day can be created.

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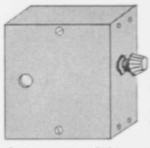

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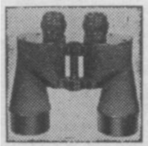

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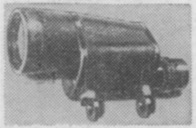

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