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An Introduction to Materials Science

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Chapter One

What Is a Material?

From a practical standpoint, we know that *material* objects are essentially all substances that a human being needs to *build things*. This definition includes solids, but also liquids (e.g., liquid crystals that create LCD displays), and even gases for more specific situations. Really, every raw material used by industry could be included in this classification, but we use the word "material" in a restricted sense: We think about materials whose properties might not be an exact image of those that their elements possess. Thus, we especially concern ourselves with how elements are structured in macroscopic bodies, with how treatments are used during the elaboration of materials, or with the physicochemical aggregation of different elements—all activities that condition the properties of the materials we generate.

The selection, modification, and elaboration of materials to satisfy our needs merge in the foundations of human culture. From the very beginnings of prehistory, humans have manipulated substances so that they would be more useful. To create more useful materials, our forebears wanted to understand and control the composition of materials, and they often succeeded in modifying a material's behavior and properties and in predicting the effects of such manipulations.

This task developed over time, beginning as a handicraft that employed empirical and speculative knowledge. The history of materials science and engineering had already begun in the Stone Age when stones, wood, clay, and leather began to be manipulated. In the Bronze Age, mankind discovered the value of temperature and used it to modify materials by thermal treatments or by adding other substances. Yet, in spite of technological improvements, materials science remained empirical until the end of the nineteenth century. Materials science, as we now understand it, began with the appearance of Mendeléev's periodic table. Since that time, some properties of elements that are related to their position in the periodic table began to be explained scientifically, and these results became incorporated in the annals of science. Since the end of the nineteenth century, the introduction of chemistry and physics, calculus, and modern experimentation have brought the use and profits of materials to a mature status. Currently, thanks to more reliable knowledge of the structure of matter, we can design new materials atom by atom, to achieve the properties we want. At last we have materials that not only satisfy our requirements, but also permit us to create new ones that were hitherto unthinkable.

Thanks to this science, we can even speculate about using new, alternative materials to solve socioeconomic problems by avoiding the decimation of natural resources or trying to reach long-range sustained economic development. Conversely, the solution of unsolved problems improves our theoretical knowledge as well as the scope of materials in science and engineering.

In this context, materials scientists must analyze how the structure and composition of materials relate to their properties, and the effect of the method of preparation of a material. Materials engineers examine the preparation, selection, and application of materials in agreement with known and desired properties. Engineers also incorporate technical and structural analysis and examine key concerns: energetic, economic, ecological, aging.

For materials science and engineering, changes in *physicochemical properties* in response to a stimulus are highly significant. These properties can be classified into groups according to the kind of stimulus: mechanical, thermal, electromagnetic (throughout the spectrum), chemical, and scattering. In brief, mechanical properties, such as deformation and fracture, among others, are responses to applied mechanical forces. Thermal properties, like thermal conductivity and heat capacity, are affected by heat fluxes or temperature changes. Electrical properties such as the dielectric constant or conductivity occur in response to electromagnetic fields. Magnetic properties, like different types of magnetism, are also a response to electromagnetic fields. In a similar sense, optical properties, such as the refractive index or absorption, among others, respond to electromagnetic fields having high frequency. Chemical properties, like the chemical affinity, are responses to the existence of reagents in the environment, and the scattering properties are responses to the impact of particles depending on the material's structure.

In thinking about properties as a response to determined stimuli, we can group materials into families that facilitate a common analysis to determine the origin of the properties. For example, materials can be classified according to their electrical properties; hence, the materials are grouped as good or poor electrical conductors. This brings us to a taxonomy that permits us to see common features between materials in a family, to understand the basis of a property, and to predict the origin of new materials.

In the selective process of materials engineering, the choice of material is limited by the required properties and by the available budget. The requisite properties are imposed by what we wish to make from the material, by environmental conditions, and by the degradation of the material. In this selection we have to take into account that the usage of materials and environmental conditions will provoke their degradation. The degradation of materials determines the required properties in an environment. When environmental conditions can be controlled, material selection is defined by its usage and the budget. That is, the economy plays a key role in materials engineering.

Materials science itself tries to analyze phenomena by the usual activities of contemporary science, and, without relying on economic aspects, to determine how structure, the presence of impurities and defects, production, purification, or mechanical transformation affects material properties.

Materials science can also do the converse: As a group of desirable properties is defined, the material that can display them, although it might not exist in nature, is designed. There are well-known examples of this: stainless steel, powders used in metallurgy, ceramic materials with a controlled coefficient of expansion (which can even be zero), conducting plastics, plastics with a high resistance to friction, such as the one used in some aircraft radomes (a word formed from radar dome), or glasses with a saturable transmission coefficient.

The continuous development of new materials has also prompted the growth of an innovative industrial sector whose products, such as microelectronics or photonics, have greatly transformed the relationship between humans and their environment. Suffice it to say that with the many appliances that are electronically controlled, with the computer industry, with the substitution of copper by optical fibers in telephone conductors, or with satellite communications, we are challenged to make sense of the socioeconomic impact that these changes imply. Countries need to modify their industrial structure so they can survive the modifications that the new materials technology generates.

1.1 CLASSIFICATIONS

The phase of a material—which defines its macroscopic presentation—characterizes the material's properties and depends on external variables like temperature and pressure. This phase can be modified when external parameters are changed. If we want to assert that a sample is of a certain type, we have to specify, apart from the material, the interval of environmental conditions in which its phase is stable. For example, we cannot say that aluminum is a conducting material without specifying the temperature at which it acts like a conductor; this is because at temperatures lower than 1.19 K aluminum reveals a superconducting phase with quite a different phenomenology from the conducting one. Often this is not enough. Metastable states appear because of a material's degradation, hence allowing a sample of a material that is stable under certain conditions to coexist with another sample in another phase under the same conditions. As an example, carbon in normal conditions can naturally coexist in allotropic forms like diamond and graphite. It is not sufficient to indicate the environmental conditions; data about the sample's *history* are also required. In this example the pressures and temperatures applied to the carbon atoms and their duration are required for unambiguous determination of the phase of a sample. Without analyzing such problems, we list below some possible classifications.

The most general materials classification consists of dividing them into *simple materials* and *composites*. Composites are formed of more than one different type of material. After this simple classification, it is common to classify materials according to their different properties; hence, for example, as follows.

- Components:
    - Simple elements: monatomic and polyatomic.
    - Compounds: diatomic, polyatomic, macromolecular (organic and inorganic).
    - Mixtures. These correspond to composites and can be of different chemical compounds or of different phases of the same compound. Blends can be either homogeneous or heterogeneous. The division of mixtures is made with reference to the following scales: atomic, microscopic, mesoscopic, macroscopic (various). For example, it is not enough to assert that a granite sample is heterogeneous; it has to be stated that it is heterogeneous at the 1 mm scale, which is homogeneous at the 1 km scale.
- Type of bond:[1]
    - Ionic (insulators, ceramics, metal-nonmetal). Bond energy 3–8 eV/atom.
    - Ionic-covalent.
    - Covalent (polymers, ceramics, and so on).
    - Metallic (metallic materials). Bond energy from 0.7 (Hg) to 8.8 eV/atom (W).
    - van der Waals: fluctuating induced dipole (H_2, Cl_2, and so on) with bond energy of 0.1 eV/atom, induced dipole-polar molecule (e.g., HCl) with bond energy of 0.1 eV/atom, permanent dipole or hydrogen bond (e.g., H_2O, NH_3) with bond energy of 0.5 eV/atom.
    - Pseudobond or physical bond (*sticky* materials).

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[1] We will deal with this classification at the beginning of chapter 2.

- Electrical properties:[2]
    - Metallic or conducting, including principally metals and metallic alloys. In conductors the electrical resistance R is low but increases as the temperature rises.
    - Semimetallic. In these, the electrical resistance R is appreciable, but there are 10^{-4} fewer electrons than in the metallic materials. Again, the resistance R grows as the temperature increases.
    - Semiconducting. They have an appreciable electrical resistance R that diminishes if the temperature rises.
    - Insulating or dielectrics. They have a high electrical resistance R.
    - Superconducting. Their electrical resistance is $R \approx 0$.
- Arrangement of components:[3]
    - Monocrystalline.
    - Polycrystalline.
    - Glassy materials, which present short-range order.
    - Quasicrystalline.
    - Semicrystalline.
    - Partial order. For example, the material may have positional order (the mass centers of the components have an ordered disposition) but not orientational order (the components, necessarily anisotropic here, do not have an ordered orientation).
    - Amorphous.
    - Composite (see the classification according to the components).

Because of the existence of many such nonequivalent classifications and of intermediate materials, the classifications above are of limited value. We assume, usually, the following classification, but for our convenience and for didactic reasons sometimes we will use either one or another of the preceding classifications.

1.2 FUNDAMENTAL PROPERTIES OF DIFFERENT KINDS OF MATERIALS

Although the properties of the materials in each category can sometimes vary, properties broadly accepted as defining the categories are the following:

- Metallic materials:
    - They are built up of metallic elements or of compounds of metallic elements.
    - They have many unlocalized electrons in the so-called conduction band.
    - They are good thermal and electrical conductors. They are opaque to visible light.
    - They are usually strong and plastic.

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[2] We will use this classification in sections 2.5 and 6.5 and in chapters 4 and 7.

[3] We will use this classification in sections 12.2 and 10.3 and in chapters 2, 3, and 9.

- Ceramic materials:
    - They are chemical compounds of the type metal + nonmetal.
    - They are generally good electrical and thermal insulators.
    - They are stronger than metallic and polymeric materials at high temperatures and in chemically aggressive environments.
    - They are hard and brittle.
- Polymeric materials:
    - They are compounds, generally organic, in the form of long chains.
    - They have low density.
    - They are flexible or elastic or both.
- Semiconductor materials:
    - They have properties intermediate between conductors and insulators.
    - They have properties that are extremely sensitive to impurities and to temperature.
- Composites:
    - They are composed of more than one type of material.
    - They are designed to obtain better properties or combinations of properties. For example, glass fiber is as resistant as glass filament and as flexible as the polymer that forms it. Another example is adobe. Adobe, a mixture of clay and straw (up to 30%), has been employed in making bricks and in primitive buildings. Composites also serve as new materials in the aerospace industry. Together, these are the two technological ends of composites.
    - They are designed by taking into account typical targets of materials engineering. As an example, the aims of the aerospace industry are first to reduce operating costs (i.e., to reduce the mass of structures to increase the payload); and second to raise the fatigue limit, stiffness, toughness, and thermal shock resistance. It is almost impossible to attain both aims with simple materials, so one must take into account composites like graphite-epoxy, among others.