MATERIALS INSTRUCTION FOR CHEMICAL ENGINEERS

What Should Be Taught By The Physical Chemist?

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In the design and development of new processes, the chemical engineer must make a choice from various possible construction materials. Twenty or thirty years ago the problem of suitable construction materials was relatively simple compared to some present day problems. The growth of our technology is continually requiring new and better construction materials, particularly in the areas of nuclear energy development, the direct conversion of heat into electrical energy, and space flight development. Where once a relatively few metals such as iron, nickel, aluminum, copper, lead, zinc and some of the noble metals were of primary commercial importance, today practically all the elements have taken on a new importance in various phases of commercial development. The chemical engineer may be concerned with processes operating at liquid helium temperatures, a reactor core which hopefully can operate at 1500° to 2800°C, the reprocessing of reactor fuels using a fused salt and liquid metal as solvents instead of the more usual aqueous and organic solvents, or processes involving ultra high vacuum or extreme pressures. Many potentially useful concepts cannot be developed because suitable container or construction materials are not available. Conversely, the availability of better construction materials can open up new fields and permit development of new and more economical processes.

The service behavior of a material involves an environment, and its serviceability will be determined by its interaction with the environment as well as its mechanical properties, both of which will depend on chemical kinetic and physical factors. From a chemical point of view, containers or construction materials are additional components in a heterogeneous system which must not take part in a deleterious way with the reactions or processes of interest. From a mechanical point of view, the construction materials are members or units of a structure or device designed to withstand various mechanical stresses and perform some useful purpose. The chemist or physical chemist is more interested in the chemistry, chemical kinetics, surface phenomena, and phase equilibria involved. The mechanical engineer is more interested in the static and dynamic characteristics of the unit, how the various pieces fit together and the elastic, creep, fatigue, wear-resistance and other properties of the construction materials. The chemical engineer should have some appreciation of both of these areas. It is in the first area that the physical chemist can contribute most to the chemical engineer's training. The wide range of available metals, alloys, refractories, cermets, composite materials, etc., and possible environments precludes emphasis of any one type of material or environment. The training program which will be most effective in preparing the chemical engineer to cope with the materials problem is, of course one which emphasizes basic scientific and engineering principles. The basic principles or theories involved cut across many branches of science or engineering. With the growing complexity of our technology, new branches are added and there is always a great deal of controversy as to what the scope of the new branch should be and whether it will grow or eventually wither away. Chemical engineering has been established for a sufficiently long period of time that it is perhaps safe to say that the primary concerns of the chemical engineer are the unit operations, chemical reactions and kinetics and the physical processes such as heat and mass transfer for the particular process to be developed. The selection of suitable construction materials, although very important, is only one of his problems. The development of new and better alloys, ceramics, refractories, semiconductors, etc., is more appropriately a problem for the metallurgist, ceramist, or the material scientist, and the development of better plastics, fluorocarbon resins such as teflon and and related materials is more appropriately a problem for the organic chemist. Nevertheless the chemical engineer should have some knowledge of the utilization and limitations of construction materials and some understanding of their service behavior.

Chemical engineering curricula require basic courses in chemistry, physical chemistry, physics, and mathematics which form a basis for understanding the behavior of matter and a background upon which a more detailed knowledge of materials can be developed. Even without exposure to materials problems in chemical engineering courses or a special course in materials the student has the background to enable him to make various broad generalizations in this area. He is well aware from his training in chemistry as well as experience that some materials react vigorously with water or air while others are relatively inert. From his study of free energy and the equilibrium constant, he is aware that the reaction of water or atmospheric oxygen with most metals, alloys, and many other materials is thermodynamically favorable. His introduction to chemical kinetics and the effect of temperature on reaction rates serves as a basis for understanding why many of these materials are stable in air at ordinary temperatures. Similarly, he can conclude that iron is able to form a suitable container for a dry alkali metal chloride since the displacement of the alkali metal by iron is thermodynamically unfavorable and the iron will remain in the reduced state. His study of heterogeneous equilibria and phase diagrams enables him to conclude that although metals A and B have the requisite strength for service at a given temperature, a structure with A and B in contact will fail if these metals form a eutectic which melts below the proposed operating temperature. Molten salts as well as molten alloys have been propsed as nuclear fuels. The selection of a suitable metallic container requires knowledge of the thermal conductivity, nuclear properties, mechanical properties, the alloying behavior and reactivity of possible metallic container materials. The same problems would have to be considered in the case of a nonmetallic container.

There is probably little or no disagreement that the material covered in the usual one-year course in basic physical chemistry is pertinent to the materials problem as well as other phases of chemical engineering. Examination of undergraduate physical chemistry texts will show that the material covered is rather extensive. In many cases, such as the text, "Physical Chemistry", by W.J. Moore, Prentice Hall, the material included in the text is admittedly more than can be profitably discussed in the usual one-year course. Incorporation of additional material would mean a less advanced or less thorough discussion of other important topics. Further training in thermodynamics, theory of rate processes, alloy theory, corrosion, etc., would certainly be desirable. If two semester courses could be devoted to this area in the undergraduate curricula, a number of possibilities exist. An additional semester devoted to basic physical chemistry, or a semester course in chemical thermodynamics, thermodynamics of solids or physics of solids followed by a one-semester course in physical metallurgy would be very helpful in strengthening the student's background.

Since metals and alloys are the most commonly used construction materials in chemical processing, an introductory course in physical metallurgy would be very worthwhile. There are various texts available that could serve as a basis for such a course. An outline of material to be covered might be as follows:

1. Electronic structure of the elements.
2. Types of bonding, ionic, covalent, metallic; introduction to the free electron theory and band theory of solids; classification of solids as conductors, semiconductors and insulators.
3. Crystalline nature of solids, crystal geometry and classification of crystals; x-ray diffraction techniques.
4. Correlation of physical properties with crystal structure and type of bonding.
5. Imperfections in crystals.
6. Diffusion in solids.
7. Interpretation of phase diagrams and their correlation with the microstructure of alloys; effects of heat treatment with special emphasis on iron-carbon alloys.
8. Work hardening and recrystallization, nucleation and growth, age hardening, martensitic transformations, brittleductile transitions, radiation hardening, dispersion hardening.
9. Introduction to theories of creep, fatigue and fracture.
10. Cermets and high temperature refractories.
11. Corrosion and corrosion mechanisms.

The degree of emphasis to be given to the various topics and the extent to which nonmetallic materials should enter into the general discussion will depend on the background of the student and the time allotted for the course. Various texts can serve as a guide to the extent of coverage and level of treatment that may be considered suitable for an advanced undergraduate course. Some texts that may be considered for this purpose are: "Elements of Physical Metallurgy", by A.G. Guy; "Physical Chemistry of Metals", by C.S. Darken and R.W. Gurry; "Physical Metallurgy", by Bruce Chalmers; "Physical Metallurgy", by C. Ernest Birchenall; "Theoretical Structural Metallurgy", by A.H. Cottrell; "Solid State Physics", by A.J. Decker; "The Solid State for Engineers", by Maurice J. Sinnott; "Elements of Material Science", by Lawrence H. Van Vlack; "Thermodynamics of Solids", by Richard A. Swalin; and "Mechanical Metallurgy", by George E. Dieter, Jr. A recent review of theories for creep, fatigue, fracture and the mechanical behavior of materials is given in "Mechanical Behavior of Materials at Elevated Temperatures", edited by John E. Dorn. Another possibility is a two-semester course based on a text such as "The Solid State For Engineers", by Maurice J. Sinnott. This text has been written for the specific purpose of introducing to the engineer the basic principles which underlie the behavior of solids.

Whether such courses are to be taught be a physical chemist, metallurgist, chemical engineer or other qualified persons is not important. The primary emphasis should be on general principles. This is not intended to imply that training in basic principles is all that is necessary for the practical application of engineering materials. As already indicated the problem is complex and it is not yet possible on the basis of first principles to predicate in detail the behavior of a material under various service conditions. Knowledge of what materials or classes of materials are available or have been used successfully for various types of service, methods of testing and evaluating materials for a specific use, and economic factors are equally important. Training in this area is more appropriately covered in engineering courses.