A ChE GRADUATE COURSE IN MATERIALS DESIGN

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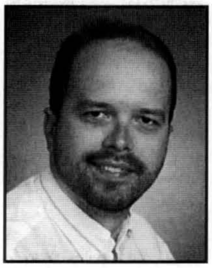
Materials science is perhaps the single largest, multidisciplinary, technological subject area, drawing together experts from such diverse backgrounds as architecture, physics, biomedical engineering, and even the arts. Chemical engineers have helped make significant advances not only in well-established "hard" materials science fields such as polymer processing and semiconductors, but they have also been at the forefront of important emerging materials science technologies such as tissue engineering (of the so-called "soft materials"), self-assembling systems, and nanostructured materials. The irony in these accomplishments is that many chemical engineering curricula neither require a materials science course nor directly prepare undergraduates for careers in these fields, much less prepare them for advanced study in materials-science-oriented research areas.

The challenge for those of us doing materials-related research in chemical engineering departments, then, is to take students who may have little or no background in materials science and prepare them to do state-of-the-art materials research. Although an undergraduate-level survey course in materials engineering and science is a good place to start, what is often needed is a second, "advanced-level survey course," if there is such a thing, to prepare graduate students to do research in a wide variety of materials-related areas.

COURSE CONTENT

Most undergraduate materials science textbooks take the survey approach; that is, a wide variety of topics are presented in relatively little depth or detail, in order to give the student at least a passing familiarity with a number of different materials-science concepts. A working knowledge of general chemistry, physics, and calculus is required, but little or no organic chemistry, physical chemistry, or differential equations are employed.



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Textbooks such as that of Callister[1] are excellent in this approach, especially since they are frequently updated and thus expose students to the latest trends in materials science. They are usually written by materials scientists, metallurgists, or ceramists, but rarely by chemical engineers. As a result, there are a number of concepts that are important to chemical engineers working in the materials field that must be taught either one-on-one with the graduate student, during group meetings, or in a narrower, graduate-level course. There are a number of excellent texts for such courses, on topics ranging from polymer rheology,[2] to ceramics processing,[3] to electrical properties of materials.[4] There is very little in between.

The undergraduate survey text is not appropriate for a graduate-level course, yet to focus on a specific topic (while it may be well-taught and of academic importance) may not provide exposure to a sufficient number of concepts to be useful to graduate students conducting widely varied materials research. Finally, and perhaps most importantly, these narrower subject courses do not address or discuss the way in which a number of important materials have been developed: through design of materials for a specific application.

The course outline for a graduate-level chemical engineering course, "Advanced Materials Design," is shown in Table 1. Four features of this course will be highlighted here: one lecture on the history of materials development; a list of selected advanced topics; a discussion of the design process; and examples of materials design projects.

HISTORY OF MATERIALS DESIGN

There are a number of truly fascinating stories related to the development of certain types and classes of materials.

For example, the work of Wallace Carothers at DuPont on the development of neoprene and nylon demonstrates not only how materials (in this case polymers) were developed as substitutes for specific, naturally occurring materials such as rubber and silk, but also how their development was spurred by historical events (World War II, in this case). This is not very technical information, of course, but students should be made aware (or at least reminded) that technological advances occur as a result of a number of different driving forces, including chance, theoretical predictions, and necessity.

There is a particularly good book by Ivan Amato called *Stuff*[5] that provides a great deal of historical information and perspective on the development of materials science as a discipline, and of specific materials. Although I stop short of making this a required text for the Advanced Materials Design course due to its lack of technical content, it is nonetheless on the "must read" list for anyone in the materials area, and it is worth recommending to all science and engineering students. It also shows how some prominent chemical engineers have played important roles in developing new materials, and how they employed design principles to accomplish their task. An excellent example is the work of Ilhan Aksay of Princeton University on biomimetic structures.

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TABLE 1
Course Outline for
Advanced Materials Design

I. Selected Advanced Topics in Materials Science
- A. The History of Materials Science
- B. Crystallography
- C. Structure of Glass
- D. Structural Imperfections
- E. Phase Equilibria
- F. Phase Transformations
- G. Advanced Characterization Techniques
- H. Mechanical Properties

II. Materials Design
- A. The Design Process
- B. Metals
- C. Inorganic Materials
  - Ceramics (low- and high-tech)
  - Glasses
  - Glass-ceramics, ceramers, and cermets
- D. Polymers
- E. Composites
- F. Case Studies, Design Projects

ADVANCED TOPICS

A graduate-level chemical engineering course should be more than a history lesson, of course. One of the primary purposes of an advanced materials course should be to teach advanced topics—those that are only introduced at the undergraduate level or that are not covered in sufficient detail. The difficult question is which topics those should be. At Tulane University, we have faculty conducting research in such areas as heterogeneous catalysis, molecular dynamics simulations of thermophysical properties in polymer single crystals, nanostructured ceramics, and tissue engineering. Some of the advanced topics we have selected to address are shown in Table 1.

Lectures on crystal structure are given at a level somewhere between the undergraduate materials science course and a semester-long course in crystallography. This topic is of use to those students who will be conducting research in practically any materials area, including polymers. In addition to reviewing the seven crystal systems, the reciprocal lattice, Miller-Bravais indices, symmetry operations, and X-ray diffraction are discussed. The advanced content comes from such exercises as calculation of single-crystal X-ray diffraction patterns from unit cell dimensions, which can be done on a spreadsheet.[6]

The lectures on the crystalline state lead naturally into lectures on the amorphous, or glassy, state. Again, discussions of radial distribution functions, the glass transition, and phase transformations are equally applicable to inorganic glasses as well as polymers. Structural defects often receive a great deal of attention in an undergraduate materials science course—deservedly so, since they directly affect many physical properties. One topic on structural defects that does not receive a great deal of attention, except in courses on ceramics, is point defect equilibrium and Kroger-Vink notation.[7] Once Kroger-Vink notation has been described, the determination of equilibrium point defect concentrations is particularly relevant for graduate-level chemical engineers, since the point defect species are treated like any other chemical species, and defect reaction equations are like any other chemical reaction.

Phase equilibria is also an area that most chemical engineers get a great deal of exposure to at the undergraduate level. Most of it deals with the liquid and vapor states, however, and is mostly applied to binary systems. Ternary, condensed-phase diagrams are described in Advanced Materials Design. Although this is not mathematically challenging material, terms and concepts such as conodes, isopleths, coprecipitational divariant equilibria lines and alkemade lines take a bit of practice to fully understand. As a final example of the advanced survey format of this course, a number of lectures are spent on advanced materials characterization. Once again, this can be a course in-and-of itself, but there are a few techniques that are of particular importance to our department and its researchers. Tulane University has a complete thermal analysis laboratory. It contains, among other things, a differential scanning calorimeter (DSC), differential thermal analyzer (DTA), thermogravimetric analyzer (TGA), dynamic mechanical analyzer (DMA), thermomechanical analyzer (TMA), dielectric analyzer (DEA), and various combinations of these instruments. A number of graduate students in the department wish to use the thermal analysis facility, and without turning a graduate-level course into a technician training session, the students are introduced to the operation of these analyzers, and the theory behind selected instruments is discussed.

THE DESIGN PROCESS

It makes sense in a course on "materials design" to discuss not only the "materials" part, but also the "design" part. The design aspect of engineering education has certainly not been lost on other parts of the chemical engineering curriculum, such as process design, and has in fact been emphasized more recently across the curriculum through emphasis of design-oriented problems at all levels and in all subject areas. The design approach has not been taken to any appreciable extent in materials science courses.

In the Advanced Materials Design course, general design methodologies such as Cross's methodology,[8] concurrent engineering,[9] and market-driven design[10] are discussed. More materials-oriented design methodologies are then described, in which Ashby's dated, yet still appropriate, text on mechanical design is used.[11] Not all materials design problems, especially newer ones, require a significant mechanical property component, so students are encouraged to use the more general design strategies to carry out materials selection and development.

An excellent text on materials design that contains a great number of case studies is by Lewis.[12] This book offers a wealth of information and emphasizes cost analysis—something that is often lost in academic environs. The remainder of the course is spent reviewing the traditional grouping of materials science topics, with an emphasis on physical properties that can be exploited from a design standpoint.

THE DESIGN PROJECT

As with many chemical engineering courses, the heart of the materials design course is the design project. The design project topics for Advanced Materials Design are gleaned from the recent literature (see Table 2 and references 13-28). The *Materials Research Society Bulletin* is a particularly useful source for these topics, as the articles in this monthly journal tend to be of intermediate technical difficulty, yet represent some of the most current, cutting-edge materials research being conducted. These articles also generally have excellent bibliographies, thus providing a good starting point for the students' literature reviews. The students get to choose

TABLE 2
Sample Design Project Topics Grouped by Traditional Subject Areas

Polymers

- Properties and applications of dendrimers[13,14]
- Graded-index optical fibers[15]
- Molecule-based magnets[16]
- Electrically-conducting polymers[17]
- Materials for flat panel displays[18,19]

Ceramics

- Ceramic thin films using self-assembled monolayers[20]
- Artificial bone[21]
- Semiconductor nanocrystals[22]
- Nanoceramics[23,24]

Composites

- Discontinuously reinforced metal-matrix composites[25]
- Biomimetic transducers[26]

Metals

- Metallic glasses[27]
- Properties of quasicrystals[28]

TABLE 3
Design Project Requirements

Objective

To develop a specific application for the material in the selected topic area. For some topics, this will be evident; for other topics, some creativity will be required.

Requirements for Minimum Grade

► *Ten-page report with at least one figure and complete bibliography that conforms to the following outline:*

☐ Abstract
☐ Keywords
☐ Introduction
☐ Background
  - Review of pertinent literature, important physical property data
☐ Proposed design
  - Design methodology
  - Material selection and justification
  - Advantages and disadvantages of selected material
  - Alternative materials
☐ Conclusion
☐ Bibliography
☐ Appendix

► *Twenty-minute presentation*

the topic, with the stipulation that it be outside of their research area. Some of the topics are very general, such as nanoceramics; others are more specific, such as discontinuously reinforced metal matrix composites. Some of the topics already have an application associated with them, such as materials for flat panel displays; others are still in search of "break-through" applications.

The project topics are selected and assigned early in the course. For the first homework assignment, the students must find three additional articles for their topic, preferably varied in scope; *e.g.,* one review article, one on molecular mechanisms, and one on processing. They must also write a brief summary of the potential significance of the topic and areas where it can be applied. The requirements for the final report are listed in Table 3.

The goal is to come up with a specific application for their material—all the way down to drawing a schematic of the apparatus or article and describing how it works. This may seem trivial for a topic like "Materials for Flat Panel Displays," but in this case the student must reverse engineer the component, determine what the specific materials constituents are, and more importantly, why they were selected.

In either scenario, the student must come up with a justification for the selected materials. In doing so, the student applies the design criteria, or sees how others applied them, uses advanced materials science concepts in the analysis of the application, and thinks practically, yet critically, about how newly developed materials can be used.

CONCLUSION

Graduate courses need not emphasize the use of elliptical integrals, nor be as narrow as the instructor's most recent grant proposal in order to be considered advanced. The three highest levels of Bloom's taxonomy of Education Objectives—analysis, synthesis, and evaluation[29]—are sufficiently challenging for graduate students, even in a survey-type course, when the technological content of the system being analyzed and evaluated is sufficiently complex. Today's materials applications certainly meet the technological requirement, and a design project for chemical engineering graduate students on advanced materials applications challenges the students to use many of the chemical engineering principles they have learned as undergraduates.

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