

# SCIENCE of MATERIALS



Witold Brostow

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WITOLD BROSTOW

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# Preface

Before embarking on a study of a scientific discipline, one usually asks questions such as: "How large is the field covered by this discipline?" "Is it important?" "How long has it existed?" "Where does it come from?" In the case of the science of materials, answers to such questions are quite extraordinary.

The science of materials covers all materials known to men, both natural and man-made (or modified by humans). Thus, even in gross understatement, it is very important indeed. Other disciplines of comparable importance are known to have existed for two thousand years or more, yet the science of materials has received recognition only in the second half of the twentieth century.

The answer to the last question posed above is perhaps even more unexpected. Many new fields of study appear because of the natural branching process of science. Some of them are prompted by technological needs, by wars, and in a few cases by economic needs. I believe that (contrary to some laws of biology) the science of materials has three parents: economics, technology, and pure science.

The reason *economics* features here is in fact quite natural. For thousands of years, consumers of all kinds have been asking the question, "What can I get?" Recently, however, some people assumed that everything was possible; a new generation of consumers said, "I need this and this, I don't care whether it has been invented yet." Thus, in the market place dominated originally by proprietors of raw materials, the end-use industries became important. Given all kinds of possible and impossible demands, the end-use industries could not tolerate the separate developments of metallurgy, ceramics, polymer science, and so forth, and these disciplines began to melt together into what we now call the science of materials. Some signs of this phenomenon were already noted

in 1967 by the editors of *Scientific American* in a special issue, reproduced subsequently in book form, with the title "Materials." They observed that more and more materials scientists work "back from end-use specifications to the choice, adaption and invention of materials."

*Technology* contributed to create the science of materials, partly by itself and partly with science; this accords with what A. G. Chynoweth calls "the science-engineering coupling." Prompted by technological needs, the science of materials first appeared as a descriptive discipline. It supplied lists of industrially important materials, with properties or characteristic parameters attached to each material. When a new material with certain desired properties was needed, it was obtained by a trial-and-error procedure; the number of attempts before the successful one depended mainly on luck. But we have to realize that there are, in general, three stages: *description*, which materials science already had; *explanation* of what we have observed, which was lacking; *prediction* of new properties, which was the aim sought. Thus the coupling with *science* began to function, and materials scientists started to dig deeply into physics and chemistry. And now we see a new part of materials science emerging. It is based mainly on molecular physics and physical chemistry. Some like to call it molecular engineering. The name was apparently coined by Arthur R. Von Hippel and his colleagues at the Massachusetts Institute of Technology. With foresight, Von Hippel in 1959 defined molecular engineering as the building of materials to order.

When I started to teach a course in materials science a few years ago, I wanted to make my life easy and to adopt one of the existing textbooks as a basis. I found that none of them corresponded to my view of what should be taught. Many books were still confined to the descriptive side. On the opposite side of the gap, there were books on solid state and theoretical physics—excellent in themselves, but containing only few bridges toward practical problems. There were books devoted mainly to metallurgy that contained not enough on polymers, and vice versa. There were also books that discussed various classes of solid materials on a comparable footing, but the hundreds of pages were too many for me and my students to chew. In most cases liquid phases were treated inadequately, while gaseous materials were hardly mentioned at all.

Under the circumstances, I decided then to develop a new course from the beginning. What you are reading now represents the expansion of notes for a one-semester course. It has the following characteristic features:

1. For the first time, materials that under normal conditions occur as liquids or gases are treated with the same attention as solids.

2. The first part of the book is devoted to fundamentals. Thus, at a later stage of discussing *what* happens to materials, explaining *why* becomes much easier. Except for the most elementary differential and integral calculus, no reference to other texts is necessary, and the book is self-contained.

3. Supposedly different classes of systems are compared and their *common* features stressed, with the objective of building up a coherent picture of materials.

4. The book has been written with the various possible backgrounds of the learner in mind. A reader who already happens to be familiar with a particular topic (or who is not interested in a particular class of materials, properties, or fundamental explanations . . . ) can safely skip a section or even an entire chapter. The flexible structure of the text as well as frequent cross-references assure that he or she will not get lost afterward.

5. Explaining properties on the molecular level involves using statistical mechanics once in a while. Now, statistical mechanics is considered to be a difficult subject, often taught only at the graduate level and based on something nebulous and impossible to prove called the ergodic hypothesis. In this book, essential ideas concerning ignorance and information are explained first, and then statistical mechanics is derived from these notions. Thus (1) one learns some information theory, a discipline that also has many uses outside of materials science, for instance in decision making and business management as well as in everyday life; (2) learning the rudiments of statistical mechanics becomes incomparably easier than by the traditional route; (3) statistical mechanics automatically acquires a firm foundation (and, incidentally, so does thermodynamics). There is one more discipline introduced for the first time into a textbook on materials science, namely the theory of graphs.

6. While as complete a range as possible is covered, a strict upper limit has been imposed in advance on the volume of this book. As already mentioned, the material can be learned in one semester. Incidentally, this limitation resulted in the hardest part of my work: to ask, of each single item, is it of primary importance, and to be discussed in detail? Is it of secondary importance, and only to be mentioned? Or is it of tertiary importance, and in a book of this size to be omitted completely? Such decisions were easy in certain instances but quite difficult in others.

The book as constructed may be useful for several categories of readers:

1. Students of science, such as physics or chemistry. They should find that pieces of knowledge, which they have already acquired, are brought

together, along with things they have not encountered. Moreover, as compared to an engineer, a chemist who finds himself working in industry is distinctly handicapped, for instance by his limited knowledge of mechanical properties of materials. This book should supply a remedy for that.

2. Students of engineering. What I have already called bridges between molecular physics and macroscopic treatment are essential in their case.

3. Students and researchers who are just beginning materials science, but who intend to remain in this field. They may treat this book as an introduction before embarking on study of more voluminous works and specializing in a particular branch of the discipline.

4. Engineers and scientists working in industry. The *what* and *how* are well known to them; it is the *why* they are looking for. Frontiers of science, and university programs in consequence, now change so rapidly that people are already talking about periodical recycling of graduates through university mills. An alternative is self-study of books such as this one. The fact that we include topics that haven't yet found their way into standard curricula ought to be helpful.

This book owes much to many people. First of all, students helped by their questions, by demands for more detailed explanations, and sometimes by comments. Second, I consulted quite a few experts on various specific points, and they reviewed sections of the book related to their specific fields. Last but not least, teachers helped both by their knowledge and by their experience in explaining things. On purpose, my list of consultants includes physicists, chemists and chemical engineers, metallurgists, mechanical engineers, computer scientists, electrical engineers, and mathematicians. By accident, this list covers several continents.

I cannot possibly give here the names of all those people who helped, even if I am really indebted to them all. At least the names of those who helped to structure the whole book and of those who reviewed entire chapters should be recorded: I. E. Chambouleyron (University of Buenos Aires and Center for Advanced Studies, Mexico City); Roger Connan (University of Strasbourg I); Dinkar Deshpande (Indian Institute of Technology, Bombay); Michael Falk (National Research Council of Canada, Halifax); C. D. Graham, Jr. (University of Pennsylvania); Arthur E. Grosser (McGill University); Thelma M. Hardman (University of Reading); Jorge Helman (Center for Advanced Studies, Mexico City); Aleksander Kreglewski (Texas A & M University); Bernard Morrill (Swarthmore College); Jacques Prud'homme (University of Montreal); Stuart A. Rice (The University of Chicago); Rustum Roy (Pennsylvania State University); G. M. Schneider (Ruhr University, Bochum); Neil S.

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WITOLD BROSTOW

*Mexico City,  
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# Important Symbols

$A$	Helmoholtz function
$A_\mu$	Landau potential
$B$	second virial coefficient; magnetic induction
$C$	heat capacity; third virial coefficient
$D$	electric displacement
$E$	Young modulus; electric field strength
$F$	Force; function (appears in general equations, usually followed by a specification what $F$ can stand for)
$G$	Gibbs function
$H$	enthalpy; magnetic field strength
$I$	electric current
$J$	Massieu function
$K$	degree Kelvin (used to denote both the Kelvin scale and the temperature unit in Kelvin and in centigrade scales)
$M$	mass per mole
$M_m$	magnetization
$N$	number of particles or units
$N_A$	Avogadro constant
$P$	pressure
$Q$	canonical partition function
$R$	distance
$R_g$	radius of gyration
$S$	entropy
$T$	thermodynamic temperature
$U$	energy
$V$	volume
$Y$	Planck function
$Z$	charge number of ion

xx IMPORTANT SYMBOLS

$a$	relative activity; matrix entry
$c$	capacitance
$e$	electronic charge
$f$	activity coefficient; geometric coordination number
$g$	radial distribution function
$h$	Planck constant
$j$	electric current density
$k$	Boltzmann constant
$l$	length
$m$	mass
$p$	probability
$q$	electric charge; partition function
$t$	centigrade temperature
$u$	pair interaction energy
$v$	velocity
$x$	mole fraction
$z$	structural coordination number
$\Xi$	grand partition function
$\Omega$	number of permutations
$\alpha$	isobaric expansivity
$\beta$	polarizability
$\varepsilon$	engineering strain; permittivity
$\varepsilon_r$	dielectric constant
$\eta$	viscosity
$\theta$	angle
$\kappa$	electrical conductivity
$\kappa_s$	adiabatic compressibility
$\kappa_T$	isothermal compressibility
$\lambda$	absolute activity; wavelength
$\mu$	chemical potential; dipole moment
$\mu_m$	permeability
$\nu$	frequency; Poisson ratio
$\rho$	density
$\sigma$	engineering stress
$\tau$	shear stress; time
$\phi$	volume fraction
$\chi_e$	electric susceptibility
$\chi_m$	magnetic susceptibility

**PART I**

# **FOUNDATIONS**

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