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NANOTECHNOLOGY

BASIC CALCULATIONS FOR ENGINEERS AND SCIENTISTS

LOUIS THEODORE

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Basic Calculations for Engineers and Scientists

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Nature is neutral. Man has wrestled from nature the power to make the world a desert or to make the deserts bloom. There is no evil in the atom; only in men's souls.

—Adlai Stevenson, 1952

Ill can he rule the great, that cannot reach the small.

—Edmund Spenser, 1596

The small and tiny shall become all-powerful

—L. Theodore, 2006

Preface

It is not a secret that the teaching of a nanotechnology course will soon be required in most engineering and science curricula. It is also generally accepted as one of the key state-of-the-art courses in applied science. The need to develop an understanding of this general subject matter for the practicing engineer and scientist of the future cannot be questioned.

One of the problems with nanotechnology is that its range of subject matter is so broad that nearly every engineering and science discipline falls under the nano umbrella; in effect, it is interdisciplinary. Adding to the confusion is that no clear-cut definition of nanotechnology has emerged since its infancy nearly a half century ago. The reader will soon note that the author has not laid claim to an end-all definition, but rather refers to nanotechnology simply as nanotechnology.

This project was a unique undertaking. Rather than prepare a textbook on nanotechnology, the author considered writing a problem-oriented book because of the dynamic nature of this emerging field. Ultimately, it was decided to prepare an overview of this subject through illustrative examples rather than to provide a comprehensive treatise. One of the key features of this book is that it could serve both academia (students) and industry. Thus, it offers material not only to individuals with limited technical background, but also to those with extensive industrial experience. As such, it can be used as a text in either a general engineering or science course and (perhaps primarily) as a training tool for industry.

As is usually the case in preparing a manuscript, the question of what to include and what to omit has been particularly difficult. However, the problems and solutions in this work attempt to address principles and basic calculations common to nanotechnology.

This basic calculations workbook is an outgrowth of the 2005 John Wiley & Sons book "Nanotechnology: Environmental Implications and Solutions". The desirability of publishing a workbook that focuses almost exclusively on nanotechnology calculations was obvious following the completion of that book.

This book contains nearly 300 problems related to a variety of topics of relevance to the nanotechnology field. These problems are organized into the following four Parts or Categories:

Chemistry Fundamentals and Principles
Particle Technology
Applications
Environmental Concerns

Each Part is divided into a number of problem Sections (or Chapters), with each set containing anywhere from 8 to 12 problems and solutions. The interrelationship between the problems is emphasized in all Parts.

The general approach employed involved the use of solved illustrative examples. However, introductory paragraphs are included in each Part and each Section. The remainder of the text consists of solved examples. In each Part, these have been chosen to emphasize the most important basic concepts, issues, and applications that arise in the topic covered by that Part.

Another feature of this work is that the solutions to the problems are presented in a stand-alone manner. Throughout the book, the problems are laid out in such a way as to develop the reader's technical understanding of the subject in question. Each problem contains a title, problem statement, data, and solution, with the more difficult problems located at or near the end of each problem set (Section). Although some of the topics are somewhat segmented and compartmentalized (relative to each other), every attempt was made to present and arrange each subject in a logical order.

The author cannot claim sole authorship to all the problems and material in this book. The main sources that were employed in preparing the problems included numerous Theodore Tutorials (plus those concerned with the professional engineering exam) and the Reynolds, Jeris and Theodore 2004 Wiley-Interscience text, "Handbook of Chemical and Environmental Engineering Calculations". Finally, the author wishes to acknowledge the National Science Foundation for supporting several faculty workshops that produced a number of problems appearing in this work.

The author also wishes to thank Dr. Albert Swertka, Professor Emeritus of Physicis, U.S. Merchant Marine Academy, for contributing an outstanding write-up in layman terms on "Quantum Mechanics". It can be found in the Appendix. This material was included for those readers interested in obtaining a (better) understanding of how quantum mechanics is related to nanotechnology.

Somehow, the editor usually escapes acknowledgement. I was particularly fortunate to have Bob Esposito ("Espo" to us) of John Wiley & Sons serve as my editor. His advice, support, and encouragement is appreciated.

It is the hope of the editor and author that this basic calculations text provides support in developing an understanding of nanotechnology, and that it will become a useful resource for the training of engineers and scientists in mastering this critical topic area.

Louis Theodore
January 2006

Introduction

Technical individuals have traditionally conducted calculation-related studies using one of a combination of the following approaches (see Figure A):

1. Macroscopic level
2. Microscopic level
3. Molecular level

These studies generally involve the application of a conservation law, e.g., mass, energy, and momentum. For example, if one were interested in determining changes occuring at the inlet and outlet of a system under study, the conservation law is applied on a "macrocopic" level to the entire system. The resultant equation describes the overall changes occuring to the system without regard for internal variations *within* the system. This approach is usually employed in a Unit Operations (for chemical engineers) course. The microscopic approach is employed when detailed information concerning the behavior *within* the system is required, and this is often requested of and by technical personnel. The conservation law is then applied to a differential element within the system, which is large compared to an individual molecule, but small compared to the entire system. The resultant equation is then expanded, via an integration, to describe the behavior of the entire system. This has come to be defined by some as the *transport phenomena approach*. The molecular approach involves the application of the conservation law to individual molecules. This leads to a study of statistical and quantum mechanics – both of which are beyond the scope of this text.

Approaches (1) and (2) are normally in the domain of the engineer, while (2) and (3) are employed by the scientist, particularly the physicist. In a very real sense, this

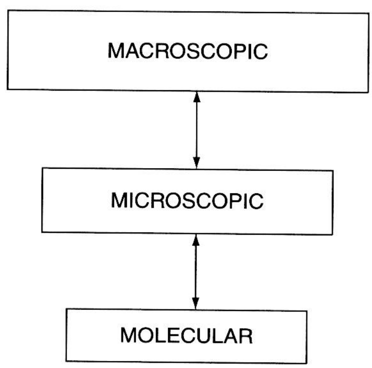

Figure A Engineering and Science Approaches

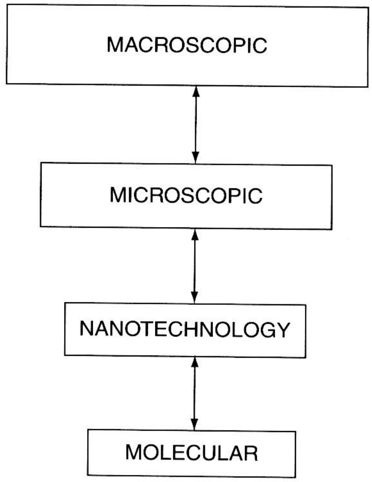

Figure B Nanotechnology Approach

text emphasizes (1), since it has been written for the practicing engineer and scientist, and attempts to provide solutions to real-world nanotechnology applications. Not withstanding this, material in Part 1 delves into some science principles and fundamentals, and an abbreviated introduction to quantum mechanics can be found in the Appendix.

However, nanotechnology has disrupted the above classical approach to the describing behavior of systems. The nanotechnology field today belongs somewhere between (2) and (3), i.e., between the microscopic and molecular approaches (Figure B).

Nanoparticles cannot be correctly described by applying either the microscopic or molecular method of analysis. This new, so-called, in-between field gives rise to some very unusual physics.

This unusual behavior results because the (physical, chemical, and so on) properties are a strong function of the size of the substance. At microscopic or macroscopic sizes, one chunk of iron (an element) has the exact same properties of another chunk of iron. At the molecular level, an atom of iron has the exact same properties of another atom of iron. However, something happened on the way to the forum ... when the size of the iron particle is in the nano range. The chemical, physical, mechanical, electrical, etc., properties of these bulk materials are different in the nanometer range. Further, a 10 nanometer particle has different properties than a particle of different size, e.g., 20 nanometers. (Note: A nanometer is one billionth of a meter; thus, one nanometer equals 10^{-9} meters.) The same phenomena is experienced with iron oxide or any other solid particle. What does all of this mean? It permits a new way to vary and control the properties of materials. In effect, one need only change the size of the particle rather than its composition.

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