Introduction to Theoretical and Computational Fluid Dynamics

By Constantine Pozrikidis, Oxford University Press, 1997, New York, 675 pp., $75.00

This excellent textbook by Professor Pozrikidis wonderfully fulfills its author's stated mission of providing a balanced treatment of theoretical *and* computational approaches to the engaging field of fluid dynamics. As researchers, practitioners, educators and students of this field, we are all aware of the large selection of advanced textbooks available for the study of fluid dynamics. However, it is generally true that books which are suitable for learning the fundamental concepts contain very little, if any, coverage of computational methods. Similarly, specialized texts for computational fluid dynamics are usually not appropriate for a first graduate course in fluid mechanics, aimed at introducing the concepts. The principal strength of this textbook is that it successfully bridges the gap between fundamental concepts and numerical techniques, both of which are needed for proper analysis of fluid motion.

The book focuses on incompressible laminar flows of Newtonian fluids. Chapter 1 provides a thorough introduction to the kinematics of fluid flow, making full use of vector and tensor calculus and differential geometry (which are separately reviewed in an appendix). The chapter includes unique and insightful descriptions of material lines, surfaces and volumes; curvature; streamline coordinates; vortex lines and vortex sheets, in addition to the more standard topics. Chapter 2 further discusses kinematics in terms of vorticity and expansion rate, also introducing the scalar and vector potentials and the stream function. Green's functions and multipoles are also introduced, as are integral representations and vorticity-induced flows. Chapter 3 introduces the stress tensor and provides a complete derivation of the conservation laws describing fluid motion in their various forms. A very detailed and illuminating description is provided (more so than in any other textbook) of the boundary conditions at solid surfaces and fluid interfaces, including such issues as vorticity at a free surface. Chapter 4 introduces hydrostatics, with an emphasis on determining the shapes of free surfaces governed by the Young-Laplace equation. Chapter 5 analyzes a number of fundamental flow fields which can be found analytically or by simple numerical computation: steady and transient unidirectional flows, stagnation point flows, rotating disk flows, point force and point source flows, and so on. Chapter 6 provides a surprisingly thorough introduction to the subject of low-Reynolds-number hydrodynamics, including the fundamental singular solutions, boundary integral representations, reciprocal theorem, generalized Faxen relations, unsteady Stokes flows, and lubrication equations among others. Chapter 7 on irrotational flows, together with Chapter 10 on the boundary-integral method for potential flow, provides one of the most complete treatments of two- and three-dimensional potential flows using analytical and numerical methods in the literature. Chapter 8 describes boundary layers, including axisymmetric and three-dimensional ones with unsteady effects. Chapter 9 provides a nice introduction to (linear) hydrodynamic stability analysis for internal, external, interfacial and free-surface flows. Chapter 11 focuses on vortex motion and so-called vortex methods. Finally, the last two chapters, 12 and 13, focus primarily on finite-difference methods. The former introduces the methods in the context of the unsteady convective-diffusion equation, providing a fairly comprehensive review of the relevant explicit and implicit numerical methods in one, two and three space dimensions. Chapter 13 applies the finite-difference method to incompressible fluid flow, using the vorticity-stream function formulation, the marker-and-cell method in the primitive variables, the pressure Poisson equation, operator splitting, and so on.

Most sections have two sets of homework problems, the first being of a theoretical nature (to be solved by paper and pencil) and the second being computational in scope and requiring the preparation of a computer program by the student. Each chapter also includes a separate comprehensive list of references, providing a good resource for pursuing a topic in more depth. Theoretical topics not covered in the book include turbulence, compressible flows, waves, and non-Newtonian fluids; numerical methods which are not discussed include finite-element, finite-volume, and spectral methods. However, the topics which are covered (outlined above) are introduced at a fundamental level and with deep insight and understanding for both analytical and numerical treatments.

In the short time that I have had a copy of the book, I have found it to be a valuable resource to me and to my graduate students. As an active researcher and educator in fluid dynamics for the past 15 years, I still find that each time I read a section of this book, I learn something new or gain additional insight. Professor Pozrikidis should be congratulated for this truly valuable contribution to our profession. This textbook will be of immense value to students, researchers and practitioners of fluid dynamics.

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The Surface Science of Metal Oxides

by V. E. Henrich and P. A. Cox, Cambridge University Press, Cambridge, U.K., 1994, 464 pp. hardcover $99.95; paperback $39.95

Over the past several decades, the use of ultra-high-vacuum surface spectroscopic techniques to study the structure, reactivity, and electronic properties of well-defined surfaces of macroscopic single crystals has led to an increasingly detailed understanding of the physical properties of the surfaces of metals and to a lesser extent semiconductors. Only recently, however, have these studies been extended to include another technologically important class of materials, metal oxides. In *The Surface Science of Metal Oxides* Henrich and Cox provide an excellent introduction to this emerging area of study.

The book begins by providing a brief overview of the technological importance of metal oxides and a historical perspective on the study of their surfaces. Chapter 2 focuses on the structure of metal oxides. Since the surface structure of a material is related to its

bulk structure, this chapter starts with a discussion of the most common bulk lattice structures. The discussion focuses on how these lattice structures result from the ionic nature of oxides and the relationships between bulk and surface structure. As pointed out by the authors, there have been relatively few detailed studies of the structures of oxide surfaces. Thus, this section focuses for the most part on surfaces resulting from ideal termination of the bulk. For those systems that have been studied in detail, however, descriptions of real surfaces and surface reconstructions are included. For each class of oxides, a table of references to experimental studies (primarily LEED results) is provided. The end of this chapter includes a brief discussion of steps and defects on oxide surfaces. Although it would have been good if a discussion of the use of calculational approaches to predict oxide surface structure were included, overall this chapter provides a good introduction.

The following three chapters focus on the physical properties of metal oxide surfaces. Chapter 3 is devoted to vibrational properties, specifically lattice phonon modes. Although this chapter is written with the novice in mind, a general knowledge of solid state physics is useful in understanding the origin of the equations that describe lattice vibrations. The bulk of this material deals with the characterization of surface phonon modes using high-resolution electron energy loss spectroscopy (HREELS) and to a lesser extent IR and Raman spectroscopies. A brief section on the use of HREELS to study adsorbate vibrations on oxide surfaces is also included. This latter section would have been better placed in Chapter 6, which focuses on adsorption on oxide surfaces.

The electronic properties of nontransition and transition metal oxide surfaces are discussed in Chapters 4 and 5, respectively. Chapter 4 is effectively divided into three parts: the electronic structure of metal oxide surfaces, experimental methods of surface electronic structure determination, and case studies of the electronic properties of nontransition metal oxide surfaces. The first section provides an introduction to the various models which describe the bulk electronic structure of oxides. This is followed with a discussion of how bulk defects and doping can alter electronic and optical properties. As was the case with Chapter 3, this discussion is on a rather basic level and is intended to provide the reader with an introduction to the subject, rather than a detailed theoretical framework for describing electronic properties. A section on electronic excitations in oxides describes band gap excitations in insulating oxides and conduction band plasmons in semiconducting oxides. This is followed with a discussion of the electronic properties of metal oxide surfaces and how these properties may differ from those of the bulk. The role of surface defects such as oxygen vacancies and surface band-bending in semiconducting oxides on surface electronic properties are also mentioned.

The second part of Chapter 4 provides a very brief introduction to the experimental techniques most commonly used to characterize the electronic properties of metal oxides. The bulk of this discussion focuses on photoemission spectroscopies such as XPS and UPS. The remainder of this chapter provides an excellent review of previous studies of the electronic properties of nontransition metal oxide surfaces. The bulk of this material deals with MgO, Al_2O_3, ZnO, and SnO_2. The first two serve as examples of insulators, while the latter two serve as semiconductors. Topics of discussion include variations in surface electronic properties with crystallographic orientation and the electronic properties of surface defects. The influence of surface treatments such as sputtering and annealing on surface electronic properties is also illustrated.

Chapter 5 begins with a survey of the electronic structure of transition metal oxides. The approach used here is to highlight the differences between transition and nontransition metal oxides. The authors do a nice job of illustrating how inclusion of the *d*-orbitals in the valence states for transition metal oxides result in complex behavior. As with the discussion of electronic properties in Chapter 4, this section does not provide detailed theoretical descriptions, but rather introduces the most important parameters and provides simple examples which illustrate their effect. Specific subjects covered here include variable oxidation states and nonstoichiometry, the failure of simple band models, and crystal field splitting. The remainder of the chapter uses a variety of examples from the literature to illustrate these effects on transitional metal oxide surfaces. This section provides a fairly comprehensive review of previously published surface science studies of transition metal oxides.

Chapter 6 deals with chemisorption on metal oxides. Although this chapter does not provide a comprehensive review of the literature in this area, it provides a good introduction to the study of adsorbates on oxides and is an excellent starting point for anyone interested in this area of study. The initial portion of this chapter is broken into sections on specific adsorbates such as H_2, H_2O, CO, CO_2 and SO_2. There are also sections on the interaction of organic molecules with oxide surfaces. These sections are rather brief, however, and it would have been nice if the authors had spent a little more time on this material, since this is of critical importance in many applications such as catalysis and chemical sensors. The latter portion of the chapter focuses on the adsorptive properties of different classes of metal oxides. The chapter is well referenced and contains numerous tables that point to a wide range of chemisorption studies. Researchers new to the field will no doubt find this a valuable resource.

Overall, this book provides an excellent introduction to the field of surface science of metal oxides. It has relatively few shortcomings and is likely to become the classic text in this area. It already occupies a prominent spot on my bookshelf and should be required reading for anyone new to the field.

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Polymer Devolatilization

R. Albalak, ed., Marcel Dekker, New York, 1996, 772 pp. $225.00

This monograph is a successful update concerning the state of the art in the highly specialized area of devolatilization of polymer solutions, emphasizing the work of the past decade. The book attempts to cover the physico-chemical and transport foundations (Chapters 2–7), the technology and design principles of the most commonly used devolatilizers (Chapters (9–13), and several case studies on selected polymer/solvent combinations (Chapter 14–17), followed by chapters on the perceived future developments (Chapter 18) and the laboratory techniques currently used for analysis of the vapor phase (Chapter 19). The appendices provide data on the vapor-liquid equilibria, albeit only a subset of the property functions required for a rational interpretation of devolatilization. The book is supplemented by a compi-