HEAT TRANSFER PHYSICS, SECOND EDITION

This graduate textbook describes atomic-level kinetics (mechanisms and rates) of thermal energy storage, transport (conduction, convection, and radiation), and transformation (various energy conversions) by principal energy carriers. The approach combines the fundamentals of molecular orbitals-potentials, statistical thermodynamics, computational molecular dynamics, quantum energy states, transport theories, solid-state and fluid-state physics, and quantum optics. The textbook presents a unified theory, over fine-structure/molecular-dynamics/Boltzmann/macroscopic length and time scales, of heat transfer kinetics in terms of transition rates and relaxation times, and its modern applications, including nano- and microscale size effects. Numerous examples, illustrations, and homework problems with answers to enhance learning are included. This new edition includes applications in energy conversion (including chemical bond, nuclear, and solar), expanded examples of size effects, inclusion of junction quantum transport, and discussion of graphene and its phonon and electronic conductances. New appendix coverage of phonon contributions to the Seebeck coefficient, Monte Carlo methods, and ladder operators is also included.

Massoud Kaviany is a Professor in the Department of Mechanical Engineering and in the Applied Physics Program at the University of Michigan, where he has been since 1986. His area of teaching and research is heat transfer physics, with a particular interest in porous media. His current projects include atomic structural metrics in high-performance thermoelectric materials (both electron and phonon transport) and in laser cooling of solids (including *ab initio* calculations of photon-electron and electron-phonon couplings), and the effect of pore water in polymer electrolyte transport and fuel cell performance. His integration of research into education is currently focused on heat transfer physics, treating the atomic-level kinetics of transport and interaction of phonon, electron, fluid particle, and photon in a unified manner. It combines *ab initio* (fine structure), molecular dynamics, Boltzmann transport, and macroscopic treatments, but on increasing length and times scales. He is author of the monographs *Principles of Heat Transfer in Porous Media* (2nd Ed.) and *Principles of Convective Heat Transfer* (2nd Ed.), and the undergraduate textbooks *Principles of Heat Transfer* and *Essentials of Heat Transfer*. He received the College of Engineering's Education Excellence Award in 2003. He is an editor of the *Journal of Nanoscale and Microscale Thermophysical Engineering* and is on the editorial board of the *International Journal of Heat and Mass Transfer* and several other international journals. He is an ASME Fellow (since 1992) and an APS Fellow (since 2011), was Chair of the ASME Committee on Theory and Fundamental Research in Heat Transfer (1995–98), and is the recipient of the 2002 ASME Heat Transfer Memorial Award (Science) and the 2010 Harry Potter Gold Medal (Thermodynamics Science).

Heat Transfer Physics

Second Edition

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To curiosity, reason, doubt,

dialogue, understanding, tolerance,

and humility.

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Preface

Heat is atomic motion of matter, and temperature indicates the equilibrium distribution of this motion. Nonequilibrium atomic motions, created for example by a temperature gradient, result in heat transfer. Heat transfer physics describes the thermodynamics and kinetics (mechanisms and rates) of energy storage, transport, and transformation by means of principal energy carriers. Heat is energy that is stored in the temperature-dependent motion and within the various particles that make up all matter in all of its phases, including electrons, atomic nuclei, individual atoms, and molecules. Heat can be transferred to and from matter by one or more of the principal energy carriers: electrons† (either as classical or quantum entities), fluid particles (classical particles or quantum particles), phonons (lattice-vibration quantum waves, i.e., quasi-particles), and photons‡ (quantum particles). The state of the energy stored within matter or transported by the carriers can be described by a combination of classical and quantum statistical mechanics. The energy is also transformed (converted) between the various carriers. All processes that act on this energy are ultimately governed by the rates at which various physical phenomena occur, such as the rate of particle collisions in classical mechanics. It is the combination of these various processes (and their governing rates) within a particular system that determines the overall system behavior, such as the net rate of energy storage or transport. Controlling every process, from the atomic level (studied here) to the macroscale (covered in an introductory heat transfer course), are the laws of thermodynamics, including conservation of energy.

The focus of this text is on the heat transfer behavior (the storage, transport, and transformation of thermal energy) of the aforementioned principal energy carriers at the atomic scale. The specific mechanisms are described in detail, including elastic/inelastic collisions/scattering among particles, quasi-particles, and waves. Particular attention is given to the time scales over which energy transport or

† For semiconductors, the holes are included as energy carriers. For electrolytes, ion transport is treated similarly.

‡ Here, *photon* refers to both the classical (Maxwell) and the quantum (quasi-particle, Schrödinger) descriptions of the electromagnetic waves.

transformation processes occur, so that the reader gains some sense of how they compare with one another, as well as how they combine to produce overall system energy storage–transport–transformation rates. The approach taken here begins with a survey of fundamental concepts of atomic-level physics. This survey includes a look at the energy within the electronic states of atoms, as well as interatomic forces and potentials. Various theories of molecular dynamics and transport are also described. After this overview, in-depth, quantitative analyses are performed for each of the principal energy carriers, including analysis of how they interact with each other. This combination should allow for the teaching of a thorough introduction of heat transfer physics within one semester, without prolonged preparation or significant prerequisites. In general, several areas of physics are relevant to the study of heat transfer: (a) atomic–molecular dynamics, (b) solid state (condensed matter), (c) electromagnetism, and (d) quantum optics. No prior knowledge of these areas is necessary to appreciate the material of this text (a knowledge of introductory heat transfer is assumed).

Crystalline solids and their vibrational and electronic energies are treated first. This discussion is followed by an examination of energies of fluid particles and their interactions with solid surfaces. Then the interactions of photons with matter are posed with photons as EM waves, as particles, or as quasi-particles.

The text is divided into seven chapters, starting with the introduction and preliminaries of Chapter 1, in which the microscale carriers are introduced and the scope of the heat transfer physics is defined. Chapter 2 is on molecular electronic orbitals, interatomic and intermolecular potentials, molecular dynamics, and an introduction to quantum energy states. Chapter 3 is on microscale energy transport and transition kinetics theories, including the Boltzmann transport equation, the Maxwell equations, the Langevin stochastic transport equation, the Onsager coupled transport relation, and the Green–Kubo fluctuation–dissipation transport coefficients and relations. Chapters 4, 5, 6, and 7 cover the transport and interactions of phonons, electrons, fluid particles, and photons, respectively.

The size effects (where the system size affects the atomic-level behavior) on transport and energy conversion, for each principal carrier, are considered at the ends of Chapters 4 to 7. This allows for reference to applications in nanostructured and microstructured systems.

Some of the essential derivations are given as appendices. Appendix B gives the Green–Kubo relation, Appendix C gives the minimum phonon conductivity relations, Appendix D gives the phonon boundary resistance, Appendix E gives the Fermi Golden Rule, and Appendix F gives the particle energy distribution (occupancy) functions for bosons (phonons and photons), fermions (electrons), and Maxwell–Boltzmann (fluid) particles. Appendix G is on contributions to the Seebeck coefficient from various charge-carrier interactions, including with phonons. Appendix H is on the Monte Carlo method used for the simulation of energy carrier transport. Appendix I is on the ladder operators used for the carrier state transition by creation (raising) and annihilation (lowering).

Some end-of-chapter problems are provided to enhance understanding and familiarity and to allow for specific calculations. When needed, computer programs are also used. A full, digital solutions manual is available.

In general, vectors (lowercase) and tensors (uppercase) are in bold type. A nomenclature, an abbreviations list, and a glossary of relevant terms are given at the end of the text. Numbers in parenthesis indicate equation numbers. The periodic table of elements, with the macroscopic (bulk) and atomic properties, is given in Appendix A (in Tables A.1 and A.2), along with the tables of the universal and derived constants and unit prefixes.

It is hoped that this treatment provides an idea of the scope and some of the fundamentals of heat transfer physics, along with some of the most recent findings in the field.

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