HEAT TRANSFER PHYSICS

*Heat Transfer Physics* is a graduate-level textbook describing the atomic-level kinetics (mechanisms and rates) of thermal energy storage, transport (conduction, convection, and radiation), and transformation (various energy conversions) by principal energy carriers. These carriers are called phonons (lattice vibration waves, also treated as quasi-particles), electrons (classical or quantum entities), fluid particles (classical particles with quantum features), and photons (classical electromagnetic waves, also treated as quasi-particles), as shown in the cover figure. This approach combines fundamentals (through survey and summaries) of the following fields: molecular orbitals/potentials, statistical thermodynamics, computational molecular dynamics (including lattice dynamics), quantum energy states, transport theories (e.g., Boltzmann and stochastic transport and Maxwell equations), solid-state (including semiconductors) and fluid-state (including surface interactions) physics, and quantum optics (e.g., spontaneous and stimulated emission, photon-electron-phonon couplings). These are rationally connected to atomic-level heat transfer (e.g., heat capacity, thermal conductivity, photon absorption coefficient) and thermal energy conversion (e.g., ultrasonic heating, thermoelectric and laser cooling). This book 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 relates it to modern applications (including nanoscale and microscale size effects).

Heat Transfer Physics

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To curiosity, reason, doubt,
dialogue, understanding, tolerance,
and humility.
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Preface

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 combinations of one or more of the principal energy carriers: electrons\(^1\) (either as classical or quantum entities), fluid particles (classical particles with quantum features), phonons (lattice-vibration waves), and photons\(^2\) (quasi-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 will be described in detail, including elastic–inelastic collisions–scattering among particles, quasi-particles, and waves. Particular attention will be given to the various time scales over which energy transport or transformation processes occur, so that the reader will be given 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 ap-

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\(^1\) For semiconductors, the holes are included as energy carriers. For electrolytes, ion transport is treated similarly.

\(^2\) Here, photon refers to both the classical (Maxwell) and the quantum (quasi-particle, Schrödinger) descriptions of the electromagnetic waves.
The approach taken here is to begin with a survey of fundamental concepts of atomic-level physics. This includes looking at the energy within the electronic states of atoms, as well as interatomic forces and potentials. Various theories of molecular dynamics and transport will also be described. Following this overview, in-depth, quantitative analyses will be 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 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 is followed by energies of fluid particles and their interactions with solid surfaces. Then the interactions of photons with matter are posed with photons as EM waves, or 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. Following these, 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.

Some end-of-chapter problems are provided to assist in further understanding and familiarity, and to allow for specific calculations. When needed, computer programs are also used.

In general, vectors (lowercase) and tensors (uppercase) are in bold symbols. A nomenclature and an abbreviation list are given at the end of the text. Numbers in parenthesis indicate equation numbers. A glossary of relevant terminology is also given at the end. 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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