Preface

As the advances in nanosciences and nanotechnology open ways to new engineering concepts, understanding and modeling thermal transport at nanoscales are becoming crucial for the success of future applications and discoveries. Traditional transport theories are typically applicable to bulk objects. Among all, the Fourier law of heat transfer and the Ohm law of electricity are valid for relatively large systems, as opposed to the molecular regime where both continuum and local thermodynamic equilibrium approximations become questionable. With the increasing focus on smaller length and shorter time scales, the intricate effects of energy carriers, including electromagnetic waves, electrons, and phonons, need to be considered in the analyses of transport phenomena. The development of new theories requires a knowledge of the true physics concerning these energy carriers and corresponding scattering mechanisms. In addition to theory, future engineers need to be exposed to approximations, models, and solution methodologies to tackle the complexities of these new and challenging applications.

The focus of this monograph is on thermal transport modeling from nano- to micro-scale levels, starting from 1 nm. Since one of the primary objectives of nanoscale engineering is material removal within a range of 1–100 nm, we use the term *micro/nanomachining* and *nanomanufacturing* throughout the manuscript. The equations and solution methodologies presented here are valid for a number of practical problems, and some for larger bulk systems. We present them coherently and specifically for electron-beam-based applications. The emphasis here is on the particle theories, specifically for electrons and phonons. All the theoretical details are provided, starting from first principles; nevertheless, all the physical concepts introduced need to be further evaluated experimentally, which is left to future studies.

The first chapter of the monograph presents a short review of micro/nanomachining and nanomanufacturing within a historical context. Transport theories for different energy carriers are briefly outlined to follow the discussions given in later chapters. A general description of an example problem is presented, which is considered as a test case for the numerical simulations conducted in the rest of the monograph.

Transport mechanisms at the micro/nanoscale levels are described in Chap. 2, and a summary of the fundamental concepts is given. Properties and behavior of electrons, phonons, and to some extent, photons, are discussed. The Boltzmann transport equation (BTE) is introduced, and its physical meaning is explained. After that, different equations which stem from the BTE are outlined, including the conservation of momentum and energy equations, the moments of the BTE, the electron-beam transport equation (EBTE), the radiative transfer equation (RTE), the phonon radiative transport equation (PRTE), and the electron transport equation (ETE). The RTE, which is quite well-known in the heat transfer community, provides a starting point for understanding the transport equations for electrons and phonons. It should be understood, however, that the RTE is not applicable to radiative transfer at nanoscales; for that the Maxwell equations need to be introduced, which is beyond the scope of this work. The chapter, discusses the governing equations for the modeling of electron-phonon transport, including the Fourier Law, the two-temperature model (TTM) and the dual-phase lag (DPL) model. Finally the details of the electron-phonon hydrodynamic equations (EPHDEs) are presented, which allow the calculation of energy transfer due to the motion of energy carriers within the medium. Two flow charts are provided at the end of the chapter to put all these models in perspective and to help the reader to choose the right set of models for a given scenario.

Chapter 3 is devoted to the discussion of Monte Carlo (MC) methods, which are known to be quite versatile and extensively used for the solution of the BTE in different geometries. First, a general introduction is given for MC methods and the probability density functions. After that, two different solution techniques, called continuous slowing-down approach (CSDA) and the discrete inelastic scattering (DIS), are outlined for the solution of the EBTE. Finally, MC methods for the ETE and the PRTE are discussed.

In Chap. 4, we focus on the solution of the EBTE with a MC method. Different electron scattering mechanisms inside a participating medium are discussed, and the derivations of the electron properties needed in the MC simulation are given. In Chap. 5, the EBTE is coupled with the Fourier heat transfer formulation to predict micro/nanomachining with a single carbon nanotube (CNT) probe. In addition, extending the concept to an array of probes for sequential machining is discussed.

The Fourier law is not necessarily applicable to modeling thermal transport at nanometer scales. In Chap. 6, we determine the range of its validity by comparing the Fourier conduction model with the TTM, where electron and lattice energies are treated separately before coupling of the corresponding energy equations. Comparisons between these two sets of solutions allow the reader to decide under what micro/nanomachining conditions the Fourier law can readily be used.

We present two advanced electron-phonon modelings in Chap. 7. In the first one, we consider the EPHDEs to describe the electrical and thermal behaviors of the metal semiconductor field effect transistors (MESFETs). In the second, the construction of a MC simulation is described for the electronic thermal conduction to predict the so-called pseudo-temperature profiles of electrons at nanoscale, considering the ballistic nature of electrons. Chapter 8 is devoted to an overview of parallel-computation methodologies used to solve the transport equations. Different parallelization strategies and architectures are discussed. The same problem considered in Chap. 6 is solved using the TTM and the increase in computational speed is discussed for different clusters.

With the feature of decreasing size, micro/nanomachining is likely to converge with molecular processes. At such a small scale, the continuum models need to be re-evaluated. Once implemented properly, we can obtain the required insight to thermal transport during a micro/nanomachining process using molecular dynamics (MD) simulations. In effect, MD simulations mimic physical experiments, albeit over a relatively small computation domain, due to the requirements for extensive computational resources. In Chap. 9, a review and discussion of MD simulations are outlined. We present a simple example where the MD simulations are coupled with an MC method used to model electron-beam propagation. Finally, general conclusions are drawn and future works required improving the modeling of micro/nanomachining applications are summarized in Chap. 10.

This monograph is intended to serve as a reference rather than a comprehensive textbook. It is written as a handy resource for students and researchers working on the numerical and theoretical aspects of thermal transport phenomena at micro- and nanoscales. Naturally, the subject areas covered here are biased toward our own research efforts, and by no means is it claimed that all the models for all potential applications are discussed. Specific emphasis is on particle theories, and on electrons and phonons as energy carriers. Even though laser-beam based machining can be modeled with the use of similar approaches, no specific attempt is made to discuss the details of laser-matter interactions. In addition, even though "near field radiation transfer" must be considered for nanoscale machining, and even though we have an active research program on the subject, we decided not to include it in this monograph as it requires discussion of "wave" approaches. Readers are encouraged to refer to other textbooks, supplementary materials, and the ever growing body of literature for additional and the most recent information related to these problems. Among all relevant references, we would like mention two relatively new textbooks on the subject, by Chen [30] and Zhang [222], for additional discussion on nanoscale transport phenomena.

This book grew out of Basil Wong's Ph.D. dissertation [208] at the University of Kentucky. However, both the breadth and depth of the discussion provided in the dissertation have significantly been enhanced since then. Additional theoretical approaches, models, comparisons and further practical information are included in Chaps. 8 and 9, based on the work of three other students. Ravi Kumar and Illay "Victor" Kunadian contributed to the discussion of the parallelization algorithms and hardware presented in Chap. 8; they worked on nanoscale thermal transport during their respective MS theses. Details of MD simulations in Chap. 9 are provided by Jaime A. Sánchez, who has recently completed his Ph.D. under M.P. Mengüç.

During the preparation of this monograph we had extensive discussions with several researchers and students. Professors R. Ryan Vallance (George Washington University), Apparao Rao (Clemson University), Sungho Jin (University of California, San Diego), who are our collaborators in a related NSF NIRT grant, have contributed significantly to our understanding of micro/nanomachining applications. Several graduate students, including Jaime A. Sánchez, King-Fu Hii, Ravi Kumar, Ellie Hawes, Mathieu Francoeur, Illay "Victor" Kunadian and Matt Robinson, helped us to sharpen our views on thermal transport and proofread many parts of the text. Professors A. Rao of Clemson University, Z. Zhang of Georgia Tech, and T. Okutucu of METU, Ankara, provided valuable insight into different aspects of our discussions. We gratefully acknowledge their help and contributions. In the end, however, all omissions and mistakes are solely our responsibility.

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