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Length-Scale Dependent Phonon Interactions

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Preface

The concept of a phonon as the elementary thermal excitation in solids dates back to the start of the twentieth century. Phonons are elementary excitations arising from collective simple harmonic oscillations of atoms about their equilibrium sites in crystalline solids. Phonons manifest themselves practically in all properties of materials. For example, scattering of electrons with acoustic and optical phonons limits electrical conductivity. Optical phonons strongly influence optical properties of semiconductors, while acoustic phonons are dominant heat carriers in insulators and technologically important semiconductors. Phonon–phonon interactions dominate thermal properties of solids at elevated temperatures.

The emergence of techniques for control of semiconductor properties and geometry has enabled engineers to design structures whose functionality is derived from controlling electron interactions. Now, as lithographic techniques have greatly expanded the list of available materials and the range of attainable length scales, similar opportunities for designing devices whose functionality is derived from controlling phonon interactions are becoming available.

Currently, progress in this area is hampered by gaps in our knowledge of phonon transport across and along arbitrary interfaces, the scattering of phonons with crystal defects and delocalized electrons/collective electronic excitations, and anharmonic interactions in structures with small physical dimensions. There is also a need to enhance our understanding of phonon-mediated electron–electron interactions. Closing these gaps will enable the design of structures that provide novel solutions and enhance our scientific knowledge of nanoscale electronics and nanomechanics, including electron transport from nanoclusters to surfaces and internal dissipation in mechanical resonators. This becomes particularly important because of the great potential for use of these materials in energy harvesting systems (e.g., photovoltaics and thermoelectrics), next generation devices, and sensing systems.

This book is aimed at developing a somewhat comprehensive description of phonon interactions in systems with different dimensions and length scales. Chapters are written by acknowledged experts and arranged in a sequence that will enable the researcher to develop a coherent understanding of the fundamental concepts related to phonons in solids. Coverage of their propagation and interactions leads eventually into their behavior in nanostructures, followed by phonon interactions-based practical applications, such as thermal transport. There are nine chapters in all: the first five cover theoretical concepts and developments, the next three are devoted to experimental techniques and measurements, and the last chapter deals with fabrication, measurements, and possible technological applications.

The chapter by Tütüncü and Srivastava (Chap. 1) describes theoretical calculations for phonons in solids, surfaces, and nanostructures. Their calculations utilize the density functional perturbation theory (DFPT) and an adiabatic bond charge method (BCM). The authors introduce and explain the concepts of folded, confined, and gap phonon modes in low-dimensional systems (surfaces and nanostructures). The computed results evolve into the size, dimensionality, and symmetry dependence of phonon modes.

The chapter by Wang et al. (Chap. 2) highlights selected concepts in the theory of acoustic and optical phonons in confined systems. They cover the basic concepts of elastic and dielectric continuum models. Examples of phonon confinement in dimensionally confined structures are provided. These include phonons in single-wall carbon nanotubes, phonons in multi wall nanotubes, graphene sheets, graphene nanoribbons, and graphene quantum dots to name just a few. The chapter also touches upon the mechanisms underlying carrier–phonon scattering processes.

In Chap. 3, Srivastava outlines the theories that are generally employed for phonon transport in solids. This chapter describes in detail the steps in deriving the lattice thermal conductivity expression within the single-mode relaxation-time approximation. Explicit expressions for various phonon scattering rates in bulk and low-dimensional solids are provided. Numerical evaluation of scattering rates and the conductivity expression is presented using both Debye's isotropic continuum scheme and a realistic Brillouin zone summation technique based upon the application of the special phonon wave-vectors scheme. Results of the conductivity are presented for selected bulk, superlattice, and nanostructured systems.

The chapter by Garg et al. (Chap. 4) covers "first-principles determination of phonon lifetimes, mean free paths, and thermal conductivities," in selected crystalline materials. The thermal properties of insulating, crystalline materials are essentially determined by their phonon dispersions, the finite-temperature excitations of their phonon populations treated as a Bose–Einstein gas of harmonic oscillators, and the lifetimes of these excitations. The authors present an extensive case study of phonon dispersions, phonon lifetimes, phonon mean free paths, and thermal conductivities for the case of isotopically pure silicon and germanium.

Mingo et al. (Chap. 5) present ab initio approaches to predict materials properties without the use of any adjustable parameters. This chapter presents some of the recently developed techniques for the ab initio evaluation of the lattice thermal conductivity of crystalline bulk materials and alloys as well as nanoscale materials including embedded nanoparticle composites.

The chapter by Hurley et al. (Chap. 6) focuses on the interaction of thermal phonons with interfaces. They show that phonon interactions with interfaces fall into two broad categories, which are defined by interfaces with two different geometries that form the boundary of nanometer size channels (e.g., grain boundaries, superlattice interfaces, nanowires, and thin films). The authors also demonstrate that the Boltzmann transport equation provides a convenient model for considering boundary scattering in nanochannel structures, while for internal interfaces such as the grain boundaries found in polycrystals, it is more natural to consider transmission and reflection across a single boundary. Also addressed are experimental techniques for measuring phonon transport in nanoscale systems, including experimental results using time-resolved thermal wave microscopy on specimens with grain boundaries having known atomic structure.

Yamaguchi (Chap. 7) reviews time-resolved phonon spectroscopy and phonon transport in nanoscale systems. He touches upon time-resolved acoustic phonon measurements using ultrafast laser spectroscopy, with particular emphasis on the methods that are relevant to transport measurements. The chapter discusses tunable acoustic spectroscopy with a combination of picosecond acoustics and laser pulse shaping. The development of the spectrometer demonstrates direct measurement of the group velocity and mean free path of acoustic phonons at variable frequency up to about 400 GHz.

The chapter by Kent and Beardsley (Chap. 8) delves into “semiconductor superlattice sasers at terahertz frequencies”: They discuss the design criteria for the superlattice lasers to be used as the gain medium and acoustic mirrors in saser devices. They elucidate potential applications of sasers in science and technology, viz., nanometer-resolution acoustic probing and imaging of nanoscale structures and devices. They also touch upon more recent developments in the area of THz acousto-electronics, e.g., the conversion of sub-THz acoustic impulses to sub-THz electromagnetic waves using piezoelectric materials.

Lazic et al. (Chap. 9) discuss growth techniques that allow formation of different types of nanostructures, such as quantum wells, wires, and dots on the surface of a single semiconductor crystal for creating surface acoustic wave (SAW) devices. They describe how SAWs propagating on the crystal surface provide an efficient mechanism for the controlled exchange of electrons and holes between these nanostructures. They explore this ability of dynamic SAW fields to demonstrate acoustically driven single-photon sources using coupled quantum wells and dots based on the (Al,Ga)As (311)A material system. Also addressed is the growth of the coupled nanostructures by molecular beam epitaxy, the dynamics of the acoustic carrier transfer between them, and the acoustic control of recombination in quantum dots.

This book has been developed and evolved for more than 2 years and the authors have made every attempt to take into account the latest developments in their fields. We hope that the concepts covered in these chapters will endure and inspire many young scientists to initiate their own research in these exciting and promising fields.

The editors are very thankful to all of the authors for their interest and patience and to the Springer New York staff for their highly professional handling of the production of this volume. They would also like to thank the colleagues who contributed their precious time to reviewing the manuscripts.

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