Phonons in Nanostructures

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Phonons in nanostructures

This book focuses on the theory of phonon interactions in nanoscale structures with particular emphasis on modern electronic and optoelectronic devices.

The continuing progress in the fabrication of semiconductor nanostructures with lower dimensional features has led to devices with enhanced functionality and even to novel devices with new operating principles. The critical role of phonon effects in such semiconductor devices is well known. There is therefore a pressing need for a greater awareness and understanding of confined phonon effects. A key goal of this book is to describe tractable models of confined phonons and how these are applied to calculations of basic properties and phenomena of semiconductor heterostructures.

The level of presentation is appropriate for undergraduate and graduate students in physics and engineering with some background in quantum mechanics and solid state physics or devices. A basic understanding of electromagnetism and classical acoustics is assumed.

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Mitra Dutta dedicates this book to her parents
Dhiren N. and Aruna Dutta

and

Michael Stroscio dedicates this book to
his friend and mentor Morris Moskow and
his friend and colleague Ki Wook Kim

Preface

This book describes a major aspect of the effort to understand nanostructures, namely the study of phonons and phonon-mediated effects in structures with nanoscale dimensional confinement in one or more spatial dimensions. The necessity for and the timing of this book stem from the enormous advances made in the field of nanoscience during the last few decades.

Indeed, nanoscience continues to advance at a dramatic pace and is making revolutionary contributions in diverse fields, including electronics, optoelectronics, quantum electronics, materials science, chemistry, and biology. The technologies needed to fabricate nanoscale structures and devices are advancing rapidly. These technologies have made possible the design and study of a vast array of novel devices, structures and systems confined dimensionally on the scale of 10 nanometers or less in one or more dimensions. Moreover, nanotechnology is continuing to mature rapidly and will, no doubt, lead to further revolutionary breakthroughs like those exemplified by quantum-dot semiconductor lasers operating at room temperature, intersubband multiple quantum-well semiconductor lasers, quantum-wire semiconductor lasers, double-barrier quantum-well diodes operating in the terahertz frequency range, single-electron transistors, single-electron metal-oxide–semiconductor memories operating at room temperature, transistors based on carbon nanotubes, and semiconductor nanocrystals used for fluorescent biological labels, just to name a few!

The seminal works of Esaki and Tsu (1970) and others on the semiconductor superlattice stimulated a vast international research effort to understand the fabrication and electronic properties of superlattices, quantum wells, quantum wires, and quantum dots. This early work led to truly revolutionary advances in nanofabrication technology and made it possible to realize band-engineering and atomic-level structural tailoring not envisioned previously except through the molecular and atomic systems found in nature. Furthermore, the continuing reduction of dimensional features in electronic and optoelectronic devices coupled with revolutionary advances in semiconductor growth and processing technologies have opened many avenues for increasing the performance levels and functionalities of electronic and optoelectronic devices. Likewise, the discovery of the buckyball by Kroto *et al.* (1985) and the carbon nanotube by Iijima (1991) led to an intense worldwide program to understand the properties of these nanostructures.

During the last decade there has been a steady effort to understand the optical and acoustic phonons in nanostructures such as the semiconductor superlattice, quantum wires, and carbon nanotubes. The central theme of this book is the description of the optical and acoustic phonons in these nanostructures. It deals with the properties of phonons in isotropic, cubic, and hexagonal crystal structures and places particular emphasis on the two dominant structures underlying modern semiconductor electronics and optoelectronics – zincblende and würtzite. In view of the successes of continuum models in describing optical phonons (Fasol *et al.*, 1988) and acoustic phonons (Seyler and Wybourne, 1992) in dimensionally confined structures, the principal theoretical descriptions presented in this book are based on the so-called dielectric continuum model of optical phonons and the elastic continuum model of acoustic phonons. Many of the derivations are given for the case of optical phonons in würtzite crystals, since the less complicated case for zincblende crystals may then be recovered by taking the dielectric constants along the c-axis and perpendicular to the c-axis to be equal.

As a preliminary to describing the dispersion relations and mode structures for optical and acoustic phonons in nanostructures, phonon amplitudes are quantized in terms of the harmonic oscillator approximation, and anharmonic effects leading to phonon decay are described in terms of the dominant phonon decay channels. These dielectric and elastic continuum models are applied to describe the deformation-potential, Fröhlich, and piezoelectric interactions in a variety of nanostructures including quantum wells, quantum wires and quantum dots. Finally, this book describes how the dimensional confinement of phonons in nanostructures leads to modifications in the electronic, optical, acoustic, and superconducting properties of selected devices and structures including intersubband quantum-well semiconductor lasers, double-barrier quantum-well diodes, thin-film superconductors, and the thin-walled cylindrical structures found in biological structures known as microtubulin.

The authors wish to acknowledge professional colleagues, friends and family members without whose contributions and sacrifices this work would not have been undertaken or completed. The authors are indebted to Dr C.I. (Jim) Chang, who is both the Director of the US Army Research Office (ARO) and the Deputy Director of the US Army Research Laboratory for Basic Science, and to Dr Robert W. Whalin and Dr John Lyons, the current director and most recent past director of the US Army

Research Laboratory; these leaders have placed a high priority on maintaining an environment at the US Army Research Office such that it is possible for scientists at ARO to continue to participate personally in forefront research as a way of maintaining a broad and current knowledge of selected fields of modern science.

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Michael Stroscio and Mitra Dutta

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Chapter 1

Phonons in nanostructures

There are no such things as applied sciences, only applications of sciences.
Louis Pasteur, 1872

1.1 Phonon effects: fundamental limits on carrier mobilities and dynamical processes

The importance of phonons and their interactions in bulk materials is well known to those working in the fields of solid-state physics, solid-state electronics, optoelectronics, heat transport, quantum electronics, and superconductivity.

As an example, carrier mobilities and dynamical processes in polar semiconductors, such as gallium arsenide, are in many cases determined by the interaction of longitudinal optical (LO) phonons with charge carriers. Consider carrier transport in gallium arsenide. For gallium arsenide crystals with low densities of impurities and defects, steady state electron velocities in the presence of an external electric field are determined predominantly by the rate at which the electrons emit LO phonons. More specifically, an electron in such a polar semiconductor will accelerate in response to the external electric field until the electron's energy is large enough for the electron to emit an LO phonon. When the electron's energy reaches the threshold for LO phonon emission – 36 meV in the case of gallium arsenide – there is a significant probability that it will emit an LO phonon as a result of its interaction with LO phonons. Of course, the electron will continue to gain energy from the electric field.

In the steady state, the processes of electron energy loss by LO phonon emission and electron energy gain from the electric field will come into balance and the electron will propagate through the semiconductor with a velocity known as the saturation velocity. As is well known, experimental values for this saturated drift velocity generally fall in the range 10^7 cm s^{-1} to 10^8 cm s^{-1}. For gallium arsenide this velocity is about 2×10^7 cm s^{-1} and for indium antimonide 6×10^7 cm s^{-1}.

For both these polar semiconductors, the process of LO phonon emission plays a major role in determining the value of the saturation velocity. In non-polar materials such as Si, which has a saturation velocity of about 10^7 cm s^{-1}, the deformation-potential interaction results in electron energy loss through the emission of phonons. (In Chapter 5 both the interaction between polar-optical-phonons and electrons – known as the Fröhlich interaction – and the deformation-potential interaction will be defined mathematically.)

Clearly, in all these cases, the electron mobility will be influenced strongly by the interaction of the electrons with phonons. The saturation velocity of the carriers in a semiconductor provides a measure of how fast a microelectronic device fabricated from this semiconductor will operate. Indeed, the minimum time for the carriers to travel through the active region of the device is given approximately by the length of the device – that is, the length of the so-called gate – divided by the saturation velocity. Evidently, the practical switching time of such a microelectronic device will be limited by the saturation velocity and it is clear, therefore, that phonons play a major role in the fundamental and practical limits of such microelectronic devices. For modern integrated circuits, a factor of two reduction in the gate length can be achieved in many cases only through building a new fabrication facility. In some cases, such a building project might cost a billion dollars or more. The importance of phonons in microelectronics is clear!

A second example of the importance of carrier–phonon interactions in modern semiconductor devices is given by the dynamics of carrier capture in the active quantum-well region of a polar semiconductor quantum-well laser. Consider the case where a current of electrons is injected over a barrier into the quantum-well region of such a laser. For the laser to operate, an electron must lose enough energy to be 'captured' by the quasi-bound state which it must occupy to participate in the lasing process. For many quantum-well semiconductor lasers this means that the electron must lose an energy of the order of a 100 meV or more. The energy loss rate of a carrier – also known as the thermalization rate of the carrier – in a polar-semiconductor quantum well is determined by both the rate at which the carrier's energy is lost by optical-phonon emission and the rate at which the carrier gains energy from optical-phonon absorption. This latter rate can be significant in quantum wells since the phonons emitted by energetic carriers can accumulate in these structures. Since the phonon densities in many dimensionally confined semiconductor devices are typically well above those of the equilibrium phonon population, there is an appreciable probability that these non-equilibrium – or 'hot' – phonons will be reabsorbed. Clearly, the net loss of energy by an electron in such a situation depends on the rates for both phonon absorption and phonon emission. Moreover, the lifetimes of the optical phonons are also important in determining the total energy loss rate for such carriers. Indeed, as will be discussed in Chapter 6, the longitudinal optical (LO) phonons in GaAs and many other polar materials decay into acoustic phonons through the Klemens' channel. Furthermore, over a wide range of temperatures and phonon wavevectors, the lifetimes of longitudinal optical phonons in GaAs vary from a few picoseconds to about 10 ps (Bhatt *et al.*, 1994). (Typical lifetimes for other polar semiconductors are also of this magnitude.) As a result of the Klemens' channel, the 'hot' phonons decay into acoustic phonons in times of the order of 10 ps. The LO phonons undergoing decay into acoustic phonons are not available for absorption by the electrons and as a result of the Klemens' channel the electron thermalization is more rapid than it would be otherwise; this phenomenon is referred to as the 'hot-phonon-bottleneck effect'.

The electron thermalization time is an important parameter for semiconductor quantum-well lasers because it determines the minimum time needed to switch the laser from an 'on' state to an 'off' state; this occurs as a result of modulating the electron current that leads to lasing. Since the hot-phonon population frequently decays on a time scale roughly given by the LO phonon decay rate (Das Sarma *et al.*, 1992), a rough estimate of the electron thermalization time – and therefore the minimum time needed to switch the laser from an 'on' state to an 'off' state – is of the order of about 10 ps. In fact, typical modulation frequencies for gallium arsenide quantum-well lasers are about 30 GHz. The modulation of the laser at significantly higher frequencies will be limited by the carrier thermalization time and ultimately by the lifetime of the LO phonon. The importance of the phonon in modern optoelectronics is clear.

The importance of phonons in superconductors is well known. Indeed, the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity is based on the formation of bosons from pairs of electrons – known as Cooper pairs – bound through the mediating interaction produced by phonons. Many of the theories describing the so-called high-critical-temperature superconductors are not based on phonon-mediated Cooper pairs, but the importance of phonons in many superconductors is of little doubt. Likewise, it is generally recognized that acoustic phonon interactions determine the thermal properties of materials.

These examples illustrate the pervasive role of phonons in bulk materials. Nanotechnology is providing an ever increasing number of devices and structures having one, or more than one, dimension less than or equal to about 100 ångstroms. The question naturally arises as to the effect of dimensional confinement on the properties on the phonons in such nanostructures as well as the properties of the phonon interactions in nanostructures. The central theme of this book is the description of the optical and acoustic phonons, and their interactions, in nanostructures.

1.2 Tailoring phonon interactions in devices with nanostructure components

Phonon interactions are altered unavoidably by the effects of dimensional confinement on the phonon modes in nanostructures. These effects exhibit some similarities