Introduction

It is the intellect's ambition to seem
no longer to belong to an individual.
Human, All Too Human, *F. Nietzsche*

If one tells the truth, one is sure, sooner or later, to be found out.
(Phrases and Philosophies for the Use of the Young, *O. Wilde*)

This book has grown out of my own research interests in semiconductor multilayers, which date from 1980. It therefore runs the risk of being far too limited in scope, of prime interest only to the author, his colleagues and his research students. I hope that this is not the case, and of course I believe that it will be found useful by a large number of people in the field; otherwise I would not have written it. Nevertheless, knowledgeable readers will remark on the lack of such fashionable topics as the quantum-Hall effect, Coulomb blockade, quantized resistance, quantum tunnelling and any physical process that can be studied only in the millikelvin regime of temperature. This has more to do with my own ignorance than any lack of feeling that these phenomena are important. My research interests have not lain there. My priorities have always been to try to understand what goes on in practical devices, and as these work more or less at room temperature, the tendency has been for my interest to cool as the temperature drops. The essential entities in semiconductor multilayers are electrons and phonons, and it has seemed to me fundamental to the study and exploitation of these systems that the effect of confinement on these particles and their interactions be fully understood. This book is an attempt to discuss what understanding has been achieved and to discover where it is weak or missing. Inevitably it emphasizes concepts over qualitative description, and experimentalists may find the paucity of experimental detail regrettable. I hope not, though I would appreciate their point, but the book is long enough as it is, and there are excellent review articles in the literature.

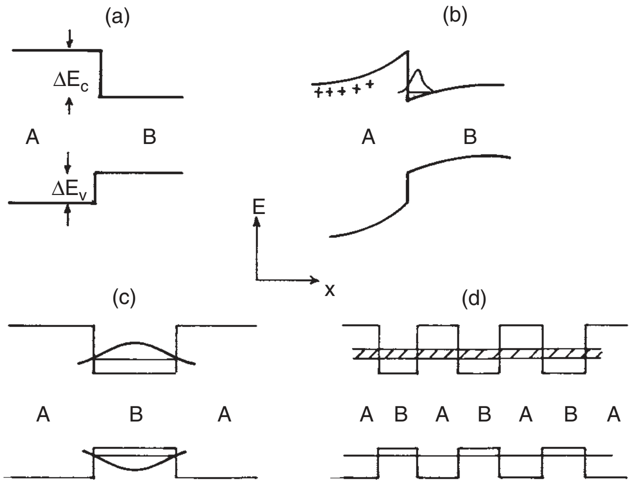

Fig. 1 Types of multilayered structures: (a) Single heterojunction, (b) Modulation-doped heterojunction, (c) Quantum well, (d) Superlattice.

At the risk of being boring, let me remind the reader what a semiconductor multilayer is about. There are several kinds of layered structure, of which those shown in Fig. 1 are the most common. They are interesting only insofar as they have a dimension that is smaller than the coherence length of an electron, in which case the electron becomes quantum confined between two potential steps. The free motion of the electron is then confined to a plane and many of its properties stem from this two-dimensional (2D) space. Electrons are not 2D objects and never could be, but for brevity they are usually referred to as 2D electrons when they are in the sort of layered structure shown in Fig. 1. The most striking effects are the quantization of energy into subbands, as depicted in Fig. 2 and Fig. 3, and the consequent transformation of the density-of-states function as shown in Fig. 4 for 3D, 2D, 1D and 0D electrons. Scattering events must now be classified into intrasubband, intersubband and capture processes, as indicated in Fig. 3. All of this is qualitatively well understood. The real problem here concerns the description of the confined-electron wavefunction (Fig. 5), which involves solving the Schrödinger equation in an inhomogeneous system. This problem is as basic as one can get in a multilayer system and calls for a comprehensive pseudopotential band structure computation. But for me, and anyone interested in further describing scattering events, this approach is too computer-intensive and inflexible, though in some cases there may be little alternative. An attractive (because simple) approximation is to take as known and unchanged the Bloch functions in each bulk medium and connect them at the interface, satisfying the

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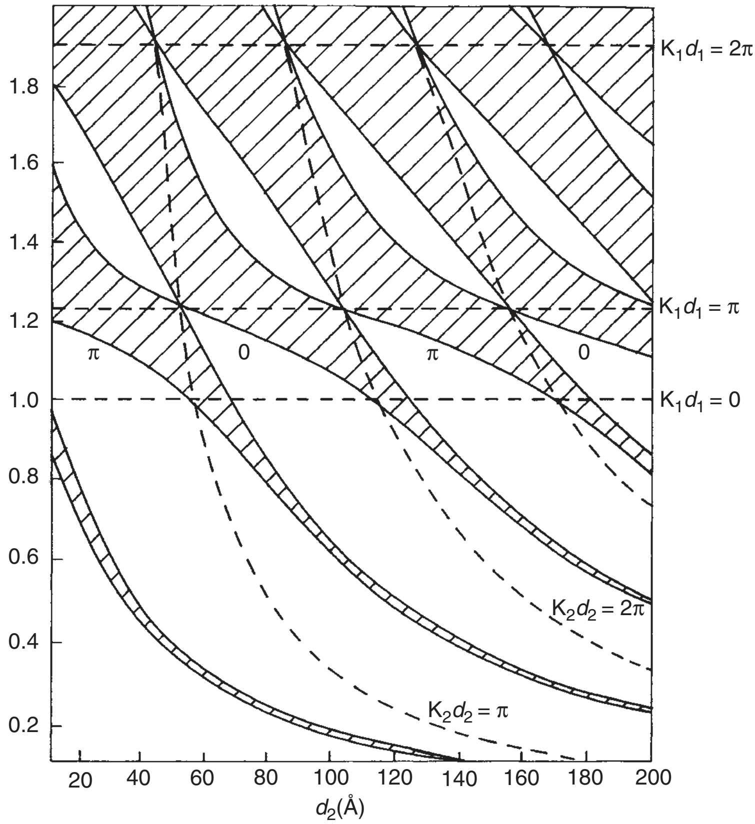

Fig. 2 Subband structures in a GaAs/$Al_{0.3}Ga_{0.7}As$ superlattice with 100 Å ($=d_1$) barriers. The energy is in units of $V_0 = 0.2$eV and d_2 is the well-width.

usual condition of current continuity. An even more attractive approximation is to forget about the cell-periodic part of each Bloch function and have a rule for joining the envelope functions. This is the effective-mass approximation. It is widely used and the energy levels it predicts are close to what is observed in a number of practical cases. Why it works so well is by no means obvious. A discussion of this basic issue will be found in Chapter 2.

Identical problems are found in connection with the confinement of optical phonons (Fig. 6). Adjacent media with different elastic and dielectric properties obviously affect the propagation of elastic waves, but whereas the appropriate boundary conditions for long-wavelength acoustic modes are well known, those for optical modes are not. The interaction between electrons and optical phonons is arguably the most important in semiconductor physics so it is truly important to know how optical modes are confined in a layer. Once again one can resort to

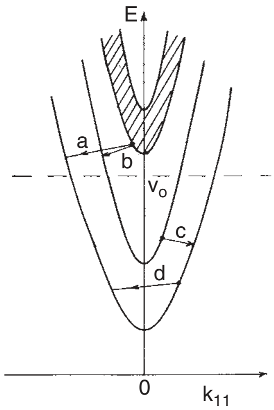

Fig. 3 Subband E–k_{11}, diagram (k_{11} is the wavevector plane). The transitions denote: a, b, capture into the well; c, intersubband scattering; d, intrasubband scattering.

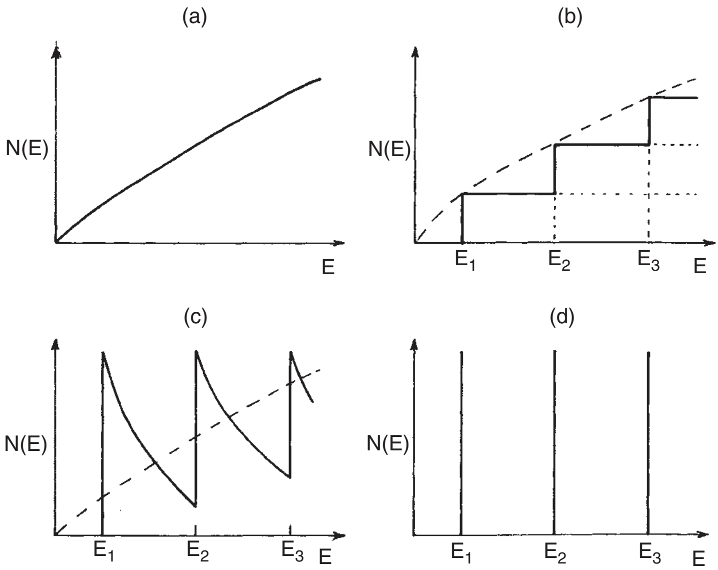

Fig. 4 Density states function of energy: (a) 3D; (b) 2D; (c) 10; (d) 0D.

extensive numerical computation of the relevant lattice electrodynamics, but, for the same reason as in the case of electrons, what is needed is a reliable envelope-function theory. This has proved to be difficult to come by, as the discussion in Chapter 3 amply illustrates.

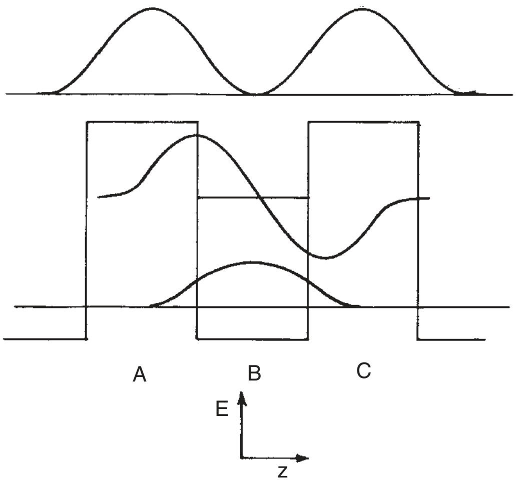

Fig. 5 Ground and excited state wavefunctions for an electron in a superlattice.

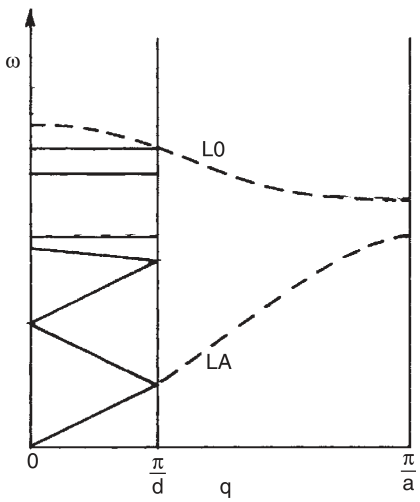

Fig. 6 Phonon dispersion influenced by mechanical/electrical mismatch at a heterojunction. Acoustic modes exhibit folding, optical modes exhibit confinement.

The whole question of envelope-function theory versus numerical computation – effectively continuum theory versus discrete theory – is extremely interesting. Though there is no earthly reason why it should do so, it tends to invoke a partisan response in the practitioners of the two approaches and may occasionally reveal a distinct difference in philosophy: the back-of-the-envelopers want general principles, generally applicable; the number-crunchers want to get at least one system right. The two approaches are complementary and, in principle, mutually supportive. General principles can be gleaned from computation; computation can test the validity of general principles. Being only dimly computer literate I am afraid that, inevitably, envelope-function theory and its usage permeate this book, and readers expecting discourses on the calculations of band structure or lattice dynamics or on Monte Carlo or molecular dynamics simulations will be disappointed.

Modelling the confinement of optical modes has proved to be unusually controversial. The controversy has focussed on the boundary conditions, and although much is now clear, there is still uncertainty regarding the elasticity of optical displacement. Happily, in systems where the vibratory mismatch is large the results of macroscopic and microscopic theory agree. (Oddly enough, the situation in perhaps the first system studied – the free-standing slab of NaCl – is still somewhat unclear.) In these systems the different polarizations of optical modes hybridize and it is possible to give a reliable account of confinement. Beginning with an account of bulk modes in Chapter 4, the description of vibratory modes proceeds to confinement in a quantum well, superlattice and other structures in Chapters 5, 6 and 7.

A central issue is the interaction between an electron and an optical mode in a quantum well, and this is treated in Chapter 8. This particular topic has a history. Before the hybridization of optical modes was understood there were several simple models advanced describing this interaction. Many important aspects of these models arose from electron confinement and remain relevant. Moreover, the scattering rate derived from bulklike phonons and that derived from the so-called dielectric-continuum model prove to be quite close to that derived from hybrid theory and microscopic theory, at least in the system AlAs/GaAs. It seemed worthwhile to an author devoted to simple models to start the book with an account of these models in Chapter 1.

There are other scattering mechanisms apart from the electron–phonon interaction. Charged-impurity and interface-roughness scattering often determine the mobility of electrons, and, of course, there is always alloy scattering in alloys. These processes are described in Chapter 9. Electron–electron scattering is also described there. It shares many grave problems with charged-impurity scattering that are difficult to solve, and it cannot be said with confidence that the rapid thermalization observed in optical experiments is fully explained by electron–electron scattering. A somewhat different topic, also in the same chapter, is the phenomenon of phonon scattering. Optical phonons are produced in abundance by hot electrons and may themselves become hot and take on any drifted motion of the electrons. How far they do so depends upon their lifetime and how rapidly they scatter. Hot-phonon effects are frequently observed when the density of electrons is large.

A substantial population of electrons has a direct effect on all scattering mechanisms through its screening action. Screening is a complex phenomenon, particularly so when more than one subband is involved. The whole topic occupies Chapter 10, and it could easily occupy a complete book.

I have a similar sentiment regarding Chapter 11, which gets down to the statistics of scattering in a population of electrons. Two-body scattering events are all very well to study on their own, but experiments generally look at populations, not individuals – average quantities, not instances – so it is necessary to look at the distribution function when the system is prodded optically or electrically, and to look at how energy and momentum are relaxed and how that depends on dimensionality. In this, for simplicity, I have sometimes committed the heresy of ignoring any phonon confinement. This is not serious for acoustic phonons.

In writing this book I have been keenly aware that references to all the work that has been done in this field are far from being comprehensive. I have told myself that this is not a review article, after all, but I feel that a suitable acknowledgement may not have been made in every case. I hope I am wrong.

Where I am most certainly not wrong is the feeling that much of this book owes its existence to my friends and colleagues at Essex, Cornell and elsewhere. Mohamed Babiker and Nick Constantinou have contributed enormously, and my account of the confinement of optical phonons and their interaction with electrons has been informed significantly by our collaboration over the years. There have been similarly important inputs from Collin Bennett and erstwhile collaborators Martyn Chamberlain, Rita Gupta and Frances Riddoch. The Platonic forms of theory are often grossly distorted in reality and I am grateful to my experimentalist colleagues Pam Bishop, Mike Daniels, Naci Balkan and Anthony Vickers for their attempts, not always successful, to anchor my feet to the ground. In a similar vein I am invigorated by the thought that semiconductors are actually useful, which my annual wintering in Lester Eastman's department at Cornell has reinforced in a delightfully stimulating way, especially by my interaction with graduate engineers like Luke Lester, Sean O'Keefe, Glen Martin, Matt Seaford and Trung LeTran. And, of course, I am grateful to Brad Foreman, whose graduate work at Cornell on quasi-continuum theory illuminated the whole field of optical-phonon confinement, and Mike Burt at British Telecom, whose analysis of the effective-mass approximation stimulated us all. My admiration of analytic theory generated in the former Soviet republics is almost as fervent as my admiration of its literature. It was, therefore, lucky for me to benefit from a

Royal Society Fellowship held by Nicolai Zakhleniuk from Kiev, taken up at Essex, and the insights gained regarding the electron distribution function were exceptionally germane.

Books are not written in a vacuum. This one was written at home in between, as is no doubt usual, myriad other things from professional duties and obligations to gardening. During its production my wife suffered all kinds of chores with remarkable good nature (which only occasionally degenerated into frightening hysteria) and I am indebted to her for her extraordinary efforts on my behalf. Nor did my offspring escape. In an extended encounter with what is known as an equation editor Aaron Ridley developed a remarkable talent, and in certain calculations of power-loss rates Melissa Ridley discovered numerical skills hitherto dormant. Both took to unfamiliar tasks with great good nature, and their contributions were much appreciated.

1

Simple Models of the Electron–Phonon Interaction

Teach us delight in simple things.
The Children's Song, *R. Kipling*

1.1 General Remarks

Evidently, the advent of mesoscopic layered semiconductor structures generated a need for a simple analytic description of the confinement of electrons and phonons within a layer and of how that confinement affected their mutual interaction. The difficulties encountered in the creation of a reliable description of excitations of one sort or another in layered material are familiar in many branches of physics. They are to do with boundary conditions. The usual treatment of electrons, phonons, plasmons, excitons, etc., in homogeneous bulk crystals simply breaks down when there is an interface separating materials with different properties. Attempts to fit bulk solutions across such an interface using simple, physically plausible connection rules are not always valid. How useful these rules are can be assessed only by an approach that obtains solutions of the relevant equations of motion in the presence of an interface, and there are two types of such an approach. One is to compute the microscopic band structure and lattice dynamics numerically; the other is to use a macroscopic model of long-wavelength excitations spanning the interface. The latter is particularly appropriate for generating physical concepts of general applicability. Examples are the quasi-continuum approach of Kunin (1982) for elastic waves, the envelope-function method of Burt (1988) for electrons and the wavevector-space model of Chen and Nelson (1993) for electromagnetic waves and excitons. Some of this will be discussed in later chapters in connection with the boundary conditions that are useful for electrons and phonons.

Effective-mass theory has proved to be remarkably good for describing the situation for electrons and holes (although a rigorous justification for its use has not been available until recently), but obtaining a theory of equivalent simplicity for optical phonons has been more problematic. Historically, boundary problems connected with phonons were ignored in calculations of the electron–phonon interaction, and only confinement effects associated with electrons were taken into account. A review of these calculations is given later. It turns out that in some cases the estimate of the scattering rate obtained by using a bulk phonon spectrum is a reasonable approximation. An account of this work is in any case a good introduction to the electron–phonon interaction, where differences from the bulk interaction are solely due to electron confinement.

Nevertheless, the folding of the acoustic-mode spectrum and the confinement of optical modes are readily observable in spectroscopy. In many cases the effect of folding can be ignored, as far as the interaction with electrons is concerned, but the same cannot be said about optical-mode confinement. Early models of optical-mode confinement are described later, after which we return to the polar interaction between electrons and optical phonons to describe the effect of phonon confinement using these early models. In doing so we will assume that the confinement of electrons is adequately described by particle-in-a-box, effective-mass theory, with boundary conditions entailing the continuity of wave amplitude and of $m^{*-1} d\psi/dz$ (Friedman, 1956; BenDaniel and Duke, 1966).

1.2 Early Models of Optical-Phonon Confinement

The effects of confinement (Fig. 1.1) are clearly seen in a number of studies of Raman scattering from zone-centre modes in the GaAs/$Ga_x Al_{1-x}$ system, and this work has been reviewed by Klein (1986), Cardona (1989, 1990) and Menendez (1989). The typical range of wavevectors, **k**, observed by Raman scattering is of order 10^4 to $10^5\,cm^{-1}$ and it is found that k is quantized in correspondence with the observed quantization of phonon frequency. In the GaAs/AlAs system, $k = n\pi/a_0(m + \gamma)$, where n is an integer greater than zero, a_0 is the thickness of a monolayer of GaAs in the direction perpendicular to the planes (usually [100], in which case $a_0 \approx 2.8$ Å), m is the number of monolayers in the GaAs layer, and γ is a correction to the expected relationship $k = n\pi/a_0 m$, which would apply if the interfaces between GaAs and AlAs were infinitely rigid. It is found that $\gamma \approx 1$ as if the effective interfaces coincided with the Al ions immediately adjacent to the GaAs. Observed frequencies falling in between modes of this scheme are usually interpreted as interface modes of the type first described for an ionic slab by Fuchs and Kliewer (1965). Raman experiments thus confirm the existence of optical-mode confinement and the presence of other frequencies, plausibly identified as interface modes (Fig. 1.2).