

Preface

This book is oriented to optoelectronic device physicists and engineers who want to enter into the realm of quantum calculations for modeling and development of their devices.

As regards quantum mechanics, device physicists generally know their fundamentals and the extent to which they shape the matters of their study; however, given the complexity of the subject matter, time constraints mean that they only become involved in the simplest quantum calculations.

The common background of solid state device physicists and engineers is related to generation and recombination of electron hole pairs and their transport, but in most cases these mechanisms are used in a phenomenological way and no attempt to model the underlying physical mechanism is undertaken. The same can be said about the energy spectrum of the semiconductors used. Contrastingly, balance analyses are frequent in this background.

Among these phenomena, the energy spectrum and mechanism of absorption are considered as properties of the material and their engineering is not considered. With the advent of nanotechnology, this has ceased to be true; the spectrum and the absorption properties can be engineered. Thus they should no longer be treated as a phenomenological input of the device modeling.

Quantum dots (QDs) and quantum wells (QWs) in semiconductors have a typical size range of 2–20 nm compared to atomic unit cells which are 0.5–0.6 nm. In solid state physics, attempts at applying standard quantum mechanical techniques usually require calculation cells with 10,000 atoms or more, which is about the limit of what is feasible even with high-performance computers.

It is the difference between the two characteristic length scales—the mesoscopic nanostructure and the microscopic crystal unit cell—that makes the problem so large. Luckily, within a good approximation, we can decouple the problem into its mesoscopic and microscopic parts. This reduces the complexity of the problem significantly, making it easier to handle both in terms of computation and analysis. Applying the so-called $k \cdot p$ techniques to nanostructures serves this purpose; this book is devoted to such techniques.

The mathematical tool more commonly applied by device physicists, due to its simplicity and powerful intuitive content, is the effective mass Schrödinger equation associated to a quantum dot or well. The fundamentals and domain of application are explained in the book. Indeed, the book begins by applying this method to a single effective mass equation with a simple square-potential quantum dot with parallelepiped geometry. Despite its simplicity, the example yields a rich set of consequences, which are studied in detail. Furthermore, this simple example will be a crucial component of the more complex situations to be studied later where several mass equations are used.

The studies in this book are centered on zincblende materials. The highest efficiency solar cells available today are made of these materials as well as most LED diodes. These crystallize in the T_d symmetry group, giving a number of general properties to their respective Hamiltonians, which are thoroughly utilized.

In this book we propose and develop a new $k \cdot p$ Hamiltonian, which we name the Empiric $k \cdot p$ Hamiltonian (EKPH). The EKPH uses four bands: the conduction band (*cb*) and three valence sub-bands: the heavy holes (*hh*), light holes (*lh*) and split-off (*so*) sub-bands. Using the EKPH the full energy spectrum introduced by the quantum nanostructure can be obtained in a few seconds using a laptop. The calculation of the photon absorption coefficients, involving over one thousand transitions, may be obtained in 1.5 hours.

In this book the EKPH is primarily applied to quantum dot and quantum well solar cells. The main validation of the EKPH is the reasonable agreement between the results it produces and those measured in real devices. As further validation, reasonable agreement has also been achieved for the GaAs band-to-band photon absorption. These validations are presented in the book. The accuracy of this fast and simple model is sufficient for many applications in device engineering.

As a comparison, the commonly used eight-band Luttinger-Kohn Hamiltonian, modified by Pikus and Bir for the incorporation of strains induced by the nanostructures, is also presented. This so-called LKPB Hamiltonian is applied using a very simple strain field in order to give the constant band offsets used along this book. Using this method, the time taken for calculation of the quantum efficiency of a quantum dot device is about 170 hours and the results are less accurate with respect to the experimental data than those obtained with the EKPH. Of course, the LKPB Hamiltonian is much more accurate than our EKPH as the proper strain field is adopted. Also, times may be shorter if faster calculation techniques are used. Nonetheless, in all we think that our EKPH Hamiltonian serves as a more useful feedback for the development of better optoelectronic devices than the LKPB Hamiltonian.

Photon Absorption Models in Nanostructured
Semiconductor Solar Cells and Devices

Luque, A.; Mellor, A.V.

2015, XIII, 202 p. 59 illus., Softcover

ISBN: 978-3-319-14537-2