LECTURE NOTES IN PHYSICS

K. Busch
A. Powell
C. Röthig
G. Schön
J. Weissmüller
(Eds.)

CFN Lectures on Functional Nanostructures

Volume 1

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G. Schön J. Weissmüller (Eds.)

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Editors

Kurt Busch
University of Central Florida
Dept. of Physics and College
of Optics and Photonics: CREOL & FPCE
Orlando, FL 32816, USA

Gerd Schön
Universität Karlsruhe (TH)
Institut für Theoretische
Festkörperphysik
76128 Karlsruhe, Germany

Annie Powell
Universität Karlsruhe (TH)
Institut für Anorganische Chemie
Engesserstr. 15
76131 Karlsruhe, Germany

Jörg Weissmüller
Forschungszentrum Karlsruhe
Institut für Nanotechnologie
Postfach 3640
76021 Karlsruhe, Germany

Christian Röthig
Universität Karlsruhe (TH)
DFG-Centrum für Funktionelle
Nanostrukturen
Wolfgang-Gaede-Str. 1
76131 Karlsruhe, Germany

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Preface

This book contains a selection of lectures from the first CFN Summer School on Functional Nanostructures which took place from September 24^{th} to September 27^{th}, 2003 in Bad Herrenalb in the Black Forest of Germany. The DFG-funded CFN, or Center for Functional Nanostructures, was founded in July 2001 at the Universität Karlsruhe (TH) and the Forschungszentrum Karlsruhe. Additional funding comes from the State of Baden-Württemberg and from the home institutions, Universität and Forschungszentrum. The mission of the CFN is to investigate nanoscale functional materials within the following broad research areas:

A Nanophotonics
B Nanoelectronics
C Molecular Nanostructures
D Nanostructured Materials

The CFN is made up of a wide range of research groups from 15 different Institutes in Karlsruhe bringing a variety of scientific backgrounds together. The Center thus provides a melting pot where various talents can be combined to address the problems associated with creating functional nanoscale materials. At the same time, the members of the Center are acutely aware of the need to develop a common language to facilitate communication amongst the various disciplines, and thus the idea of holding Summer Schools to bring groups across the four research areas together evolved. The remit of the Summer Schools is to allow members of the CFN and external participants to exchange ideas and explain research methods and strategies through a series of lectures designed both to introduce unfamiliar concepts and discuss the benefits and problems associated with various research methods including many which are highly specialised.

Chapters 1–4 of these Lecture Notes are devoted to research area A (Nanophotonics), Chaps. 5–9 to B (Nanoelectronics) while the last two chapters give a flavor of research areas C (Molecular Nanostructures) and D (Nanostructured Materials).

The lecture notes we have brought together here represent a selection of the presentations made at the Summer School in 2003 and are designed to provide a useful starting point for those interested in learning more about this rapidly developing area of science. It is hoped that they will not only provide a useful working text, but also arouse interest in our activities in Karlsruhe within the CFN.

We would like to take this opportunity to thank all the authors who have contributed to this volume for their valuable input as well as all the participants at the Summer School for helping to make this interdisciplinary venture such a success.

Karlsruhe,
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Kurt Busch
Annie Powell
Christian Röthig
Gerd Schön
Jörg Weissmüller

List of Contributors

Wolfgang Belzig
Department of Physics
and Astronomy,
University of Basel,
Klingelbergstraße 82,
4056 Basel, Switzerland

Gunnar Böttger
Technische Universität
Hamburg-Harburg,
Eißendorfer Straße 38,
21073 Hamburg, Germany

Kurt Busch
Department of Physics
and School of Optics:
CREOL & FPCE,
University of Central Florida,
Orlando, FL 32816, USA
and
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe (TH),
76128 Karlsruhe, Germany

Manfred Eich
Technische Universität
Hamburg-Harburg,
Eißendorfer Straße 38,
21073 Hamburg, Germany

Igor V. Gornyi
Forschungszentrum Karlsruhe,
Institut für Nanotechnologie (INT),
Postfach 3640,
76021 Karlsruhe, Germany

Eugeniyus L. Ivchenko
Eugeniyus L. Ivchenko
A.F. Ioffe Physico-Technical Institute,
Russian Academy of Sciences,
194021 St. Petersburg, Russia

Heinz Kalt
Institut für Angewandte Physik
and DFG-Center for Functional
Nanostructures,
Universität Karlsruhe (TH),
76128 Karlsruhe, Germany

Jürgen König
Institut für Theoretische Physik III,
Ruhr-Universität Bochum,
44780 Bochum, Germany

Jan Martinek
Institut für Theoretische
Festkörperphysik,
Universität Karlsruhe (TH),
76128 Karlsruhe, Germany
and
Institute for Materials Research,
Tohoku University,
Sendai 980-8577, Japan
and
Institute of Molecular Physics,
Polish Academy of Sciences,
60-179 Poznań, Poland

Sergei Mingaleev
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe (TH),
76128 Karlsruhe, Germany
and
Bogolyubov Institute
for Theoretical Physics,
03143 Kiev, Ukraine

John H. Perepezko
University of Wisconsin-Madison,
Department of Materials Science
and Engineering,
1509 University Avenue,
WI 53706, USA

Dmitri G. Polyakov
Forschungszentrum Karlsruhe,
Institut für Nanotechnologie (INT),
Postfach 3640,
76021 Karlsruhe, Germany

Markus Schmidt
Technische Universität
Hamburg-Harburg,
Eißendorfer Straße 38,
21073 Hamburg, Germany

Lasha Tkeshelashvili
Institut für Theorie
der Kondensierten Materie,
Universität Karlsruhe (TH),
76128 Karlsruhe, Germany

Florian Weigend
Forschungszentrum Karlsruhe,
Institut für Nanotechnologie (INT),
Postfach 3640,
76021 Karlsruhe, Germany

Jürgen Weis
Max-Planck-Institut
für Festkörperforschung,
Heisenbergstraße 1,
70569 Stuttgart, Germany

Heiko B. Weber
Forschungszentrum Karlsruhe,
Institut für Nanotechnologie (INT),
Postfach 3640,
76021 Karlsruhe, Germany

Contents

Solid State Theory Meets Photonics: The Curious Optical Properties of Photonic Crystals

Kurt Busch[1,2], Sergei F. Mingaleev[1,3], Matthias Schillinger[1], Daniel Hermann[1], and Lasha Tkeshelashvili[1]

[1] Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany
[2] Department of Physics and School of Optics: CREOL & FPCE, University of Central Florida, Orlando, FL 32816, USA
[3] Bogolyubov Institute for Theoretical Physics, 03143 Kiev, Ukraine

1 Introduction

The past decades have seen dramatic advances in microstructuring technology. Today, a wide variety of structures with feature sizes ranging from a couple of micrometers all the way down to a few tens of nanometers are routinely fabricated with precision better than ten nanometers. In addition to these improvements in fabrication quality, the variety of materials that can be processed is growing continuously. These advances in materials science are paralleled by the development of novel and improvement of existing laser sources that allows one to generate electromagnetic fields with previously unattainable energy densities as well as temporal and spatial coherences. Bringing together advanced microfabrication technologies with sophisticated laser systems lies at the heart of Nano-Photonics: The control over the flow of light on length scales of the wavelength of light itself through microstructured optical materials ("photonic metamaterials") with carefully designed properties.

A particularly prominent class of metamaterials are the so-called Photonic Crystals (PCs) which consist of a microfabricated array of dielectric materials in two or three spatial dimensions. The resulting combination of microscopic scattering resonances from individual elements of the periodic array and Bragg scattering from the corresponding lattice is very similar to the propagation of electron waves in electronic crystals and, as a result, leads to the formation of an energy bandstructure for electromagnetic waves. The most dramatic modification of the photonic dispersion relation in these systems occurs when the photonic bandstructure of suitably engineered PCs exhibits frequency ranges over which the light propagation is forbidden irrespective of the direction of propagation [1,2]. The corresponding subclass of PCs that exhibit such a Photonic Band Gap (PBG) are commonly referred to as Photonic Band Gap materials and may be regarded as a "Semiconductor for Light" [3]. In fact, this analogy of PBG materials to electronic semiconducting materials may be reaching very far and the current state of PBG research suggests that this field is at a stage comparable to the early years of semiconductor technology shortly before the in-

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vention of the solid state electronic transistor. If this analogy continues to hold, one may find PBG materials at the heart of a 21st century revolution in optical technologies similar to the revolution in electronics we have witnessed over the latter half of the 20th century.

In this chapter, we want to outline how the vast knowledge about electron propagation in crystalline solids may be employed to determine the optical properties of PCs in general and of PBG materials in particular. In Sect. 2, we introduce photonic bandstructure computations as the central tool for obtaining the photonic dispersion relation, the corresponding eigenmodes (Bloch functions), and related physical quantities such as group velocities, group velocity dispersion as well as total and local density of states. In Sect. 3, we discuss how the existence of a PBG may be utilized for the design of (linear) waveguiding structures through the deliberate incorporation of defects. In addition, we outline the qualitatively new physics that may arise in the case of nonlinear and quantum optical phenomena in PBG materials. Finally, in Sect. 4, we discuss a novel approach to obtain a fully quantitative lattice model for PCs using the solid-state theoretical concept of Wannier functions that allow us to efficiently carry out accurate simulations of PC-based devices. We employ this approach to develop novel concepts and design for functional elements based on the infiltration of individual pores in two-dimensional PBG materials.

2 Photonic Bandstructure Computation

Photonic bandstructure computations determine the dispersion relation of infinitely extended defect-free PCs. In addition, they allow us to design PCs that exhibit PBGs and to accurately interpret measurements on PC samples. As a consequence, photonic bandstructure calculations represent an important predictive as well as interpretative basis for PC research and, therefore, lie at the heart of theoretical investigations of PCs. For instance, the first convincing evidence for the very existence of PBGs has come from the seminal theoretical work of the Iowa State group [4], where it has been reported that certain structures with diamond symmetry exhibit complete three-dimensional (3D) PBGs.

2.1 Photonic Bandstructure and Bloch Functions

More specifically, the goal of photonic bandstructure computations is to find the eigenfrequencies and associated eigenmodes of the wave equation for the perfect PC, i.e., for an infinitely extended periodic array of dielectric material. For the simplicity of presentation, we restrict ourselves in the remainder of this chapter to the case of TM-polarized radiation propagating in the plane of periodicity (x, y)-plane of two-dimensional (2D) PCs. In this case, the wave equation in the frequency domain (harmonic time dependence) for the z-component of the electric field reads

$$\frac{1}{\epsilon_{\mathrm{p}}(\boldsymbol{r})}\left(\partial_x^2+\partial_y^2\right)E(\boldsymbol{r})+\frac{\omega^2}{c^2}E(\boldsymbol{r})=0\,. \tag{1}$$

Here c denotes the vacuum speed of light and $\boldsymbol{r} = (x, y)$ denotes a two-dimensional position vector. The dielectric constant $\epsilon_{\mathrm{p}}(\boldsymbol{r}) \equiv \epsilon_{\mathrm{p}}(\boldsymbol{r} + \boldsymbol{R})$ is periodic with respect to the set $\mathcal{R} = \{n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2; (n_1, n_2) \in \mathcal{Z}^2\}$ of lattice vectors $\boldsymbol{R}$ generated by the primitive translations $\boldsymbol{a}_i$, $i = 1, 2$ that describe the structure of the PC. Equation (1) represents a differential equation with periodic coefficients and, therefore, its solutions obey the Bloch-Floquet theorem

$$E_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{a}_i) = e^{i\boldsymbol{k}\boldsymbol{a}_i}\, E_{\boldsymbol{k}}(\boldsymbol{r})\,, \tag{2}$$

where $i = 1, 2$. The wave vector $\boldsymbol{k} \in$ 1st BZ that labels the solution is a vector of the first Brillouin zone (BZ) known as the crystal momentum. As a result of this so-called reduced zone scheme, the photonic bandstructure acquires a multibranch nature that is associated with the backfolding of the dispersion relation into the 1st BZ. This introduces a discrete index n, the so-called band index, that enumerates the distinct eigenfrequencies and eigenfunctions at the same wave vector $\boldsymbol{k}$ [5]. Furthermore, (2) suggests that the Bloch function $E_{n\boldsymbol{k}}(\boldsymbol{r})$ for band n and wave vector $\boldsymbol{k}$ can be written in a form

$$E_{n\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\boldsymbol{r}}\, u_{n\boldsymbol{k}}(\boldsymbol{r})\,, \tag{3}$$

representing a plane wave that is modulated by a lattice periodic function $n\boldsymbol{k}(\boldsymbol{r})$ [5].

A straightforward way of solving (1) is to expand all the periodic functions into a Fourier series over the reciprocal lattice $\mathcal{G}$, thereby transforming the differential equation into an infinite matrix eigenvalue problem, which may be suitably truncated and solved numerically.

For instance, for a PC consisting of pores (radius r, dielectric constant ϵ_b) in a background material (dielectric constant ϵ_b), the periodic dielectric constant $\epsilon_{\mathrm{p}}(\boldsymbol{r})$ may be written as

$$\frac{1}{\epsilon_{\mathrm{p}}(\boldsymbol{r})} = \frac{1}{\epsilon_a} + \left(\frac{1}{\epsilon_b} - \frac{1}{\epsilon_a}\right) \sum_{\boldsymbol{R}} S(\boldsymbol{r} - \boldsymbol{R}) \tag{4}$$

$$= \sum_{\boldsymbol{G}} \eta_{\boldsymbol{G}}\, e^{i\boldsymbol{G}\cdot\boldsymbol{r}}\,, \tag{5}$$

where $S(\boldsymbol{r} - \boldsymbol{R})$ takes on the value one if $|\boldsymbol{r}| \leq r$, and is zero elsewhere. The Fourier coefficients $\eta_{\boldsymbol{G}}$ are given by

$$\eta_{\boldsymbol{G}} = \frac{1}{V_{\mathrm{WSC}}} \int_{\mathrm{WSC}} d^2r\, \frac{1}{\epsilon_{\mathrm{p}}(\boldsymbol{r})}\, e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}\,. \tag{6}$$

Here, we designate the volume of the Wigner-Seitz cell (WSC) by V. Similarly, following the Bloch-Floquet theorem we expand $E(\boldsymbol{r})$ for a given wave vector $\boldsymbol{k}$ as

$$E_{\boldsymbol{k}}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} A_{\boldsymbol{G}}^{\boldsymbol{k}}\, e^{i(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}}\,. \tag{7}$$