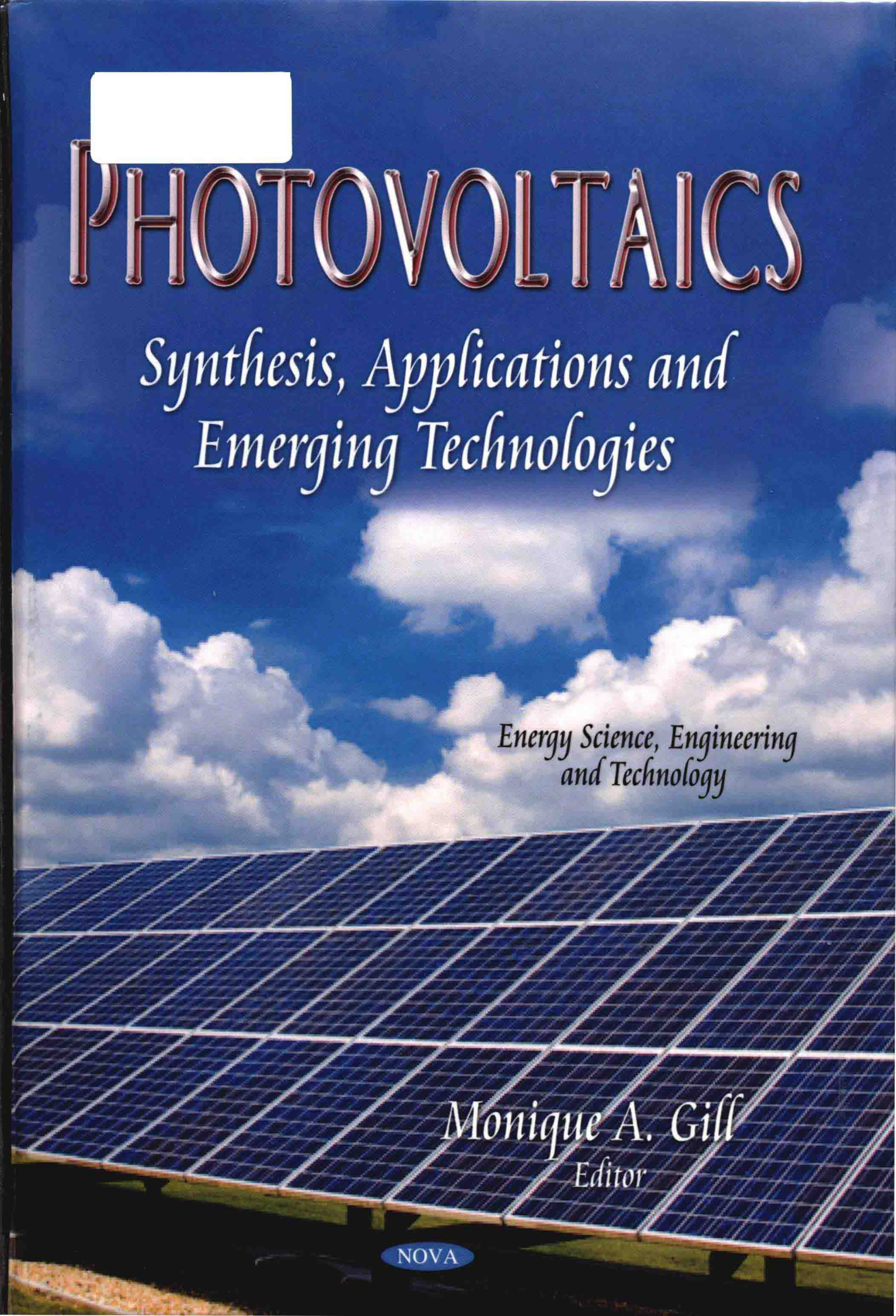
PHOTOVOLTAICS

Synthesis, Applications and Emerging Technologies

Energy Science, Engineering and Technology



Monique A. Gill
Editor

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ENERGY SCIENCE, ENGINEERING AND TECHNOLOGY

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SYNTHESIS, APPLICATIONS AND EMERGING TECHNOLOGIES

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EDITOR

nova publishers
New York

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Photovoltaics : synthesis, applications and emerging technologies / editor, Monique A. Gill.
pages cm. -- (Energy science, engineering and technology)
Includes index.
ISBN 978-1-63117-843-6 (hardcover)
1. Photovoltaic power generation. 2. Photovoltaic cells. I. Gill, Monique A., editor of compilation.
TK1087.P469 2014
621.3815'42--dc23
2014013788

Published by Nova Science Publishers, Inc. † New York

ENERGY SCIENCE, ENGINEERING AND TECHNOLOGY

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PREFACE

Increasing demands on energy has necessitated the development of large-scale, low-cost, renewable energy. Solar energy is highly attractive and extremely promising as the energy reaching the earth from the sun is orders of magnitude larger than today's global energy consumption and is quiet, requires low maintenance, has no restrictions on size, can be located close to the point on consumption, and is a clean, direct and efficient mode of energy conversion. The challenge lies in making solar power economically competitive while working with the materials readily available in abundance along with all their inherent constraints, also using those materials as economically as possible. Novel materials and structures are constantly being investigated for possible application in the area of photovoltaics (PVs). This book begins by discussing nanostructure-based PVs. It then continues to provide information on several topics that include the environmental impacts from end-of-life disposal of PVs; photocured polymer electrolyte membranes for dye-sensitized solar cells; economic analysis of support policies in PV systems; indoor PVs; effect of urban density on PV performance; and PV effects in nanoscale ferroelectrics.

Increasing demands on energy has necessitated the development of large-scale, low-cost, renewable energy. Solar energy is highly attractive and extremely promising as the energy reaching the earth from the sun is orders of magnitude larger than today's global energy consumption and is quiet, requires low maintenance, has no restrictions on size, can be located close to the point on consumption, and is a clean, direct and efficient mode of energy conversion. The challenge lies in making solar power economically competitive while working with the materials readily available in abundance along with all their inherent constraints, also using those materials as economically as possible. Novel materials and structures are constantly being investigated for possible application in the area of photovoltaics (PVs). Lately, various nanoparticle-polymer-based solar cells have demonstrated reasonable power conversion efficiencies (PCE), about 9%. Theoretical predictions suggest that higher efficiencies are achievable through nanocrystal-based approaches due to the outstanding optoelectronic properties and multi-exciton generation capabilities of semiconductor nanocrystals (NCs). Hence, these hybrid solar cells have the potential to provide cost-effective, high-efficiency solutions for PV, although significant challenges need to be overcome.

Chapter 1 discusses several approaches in pursuit of efficient light absorption in materials. Group-IV materials such as silicon (Si) and germanium (Ge) are desirable for optoelectronic applications due to their high abundance, cost-effectiveness, and high compatibility with the existing technology but as they are indirect band gap materials, they inherently have poor optoelectronic properties at room temperature. Approaches such as point defects, optically excited Raman lasers, quantum confinement in Si NCs, utilizing rare earth dopants, bonding of III-V semiconductor structures onto Si chips, integration of active conjugated-polymers with Si, synthesis of tensile-strained semiconductor heterostructures and NCs to modify their band structure and obtain favorable optical properties which result in improved carrier mobilities have been tried to address the challenge.

Band engineered nanoparticles (NPs) and NCs provide improvements in the primary photoconversion process by increasing the energy absorbed from the electromagnetic spectrum that may otherwise be lost as heat in bulk semiconductors and thin films. Such NS may be embedded in a suitable matrix for application in PV and could be a potential solution to surpass the ~33% Shockley-Queisser (SQ) limit for PCE, leading us towards viable "third generation" PV devices. This approach also offers great flexibility, allowing us to combine various materials to maximize the range of wavelengths absorbed by the materials which could lead to higher efficiencies for PVs. Also, various nanostructured materials are being experimented for the contact layers. The following sections discuss the synthesis and characterization of the structural and optoelectronic properties of such nanostructures (NSs) and their advantages for high efficiency PV.

In Chapter 2 is presented the global solar photovoltaic (PV) deployment that enjoyed exponential growth in the past decade. As the industry grows, large future end-of-life PV waste volumes will need to be managed. It is likely that recycling will be a dominant strategy as in the case of the European Union, where end-of-life collection and recycling will be mandatory beginning 2014 under the recast Waste from Electrical and Electronic Equipment Directive. However, PV deployment is globalizing beyond the European Union into emerging markets. Given the presence of various metals in PV modules, some stakeholders have raised concerns regarding potential environmental impacts if PV modules are disposed of in unlined landfills instead of sanitary landfills or instead of being recycled. Potential adverse health or environmental impacts associated with disposal of utility-scale (25 MWac) volumes of PV modules in an unlined landfill were evaluated by fate and transport modeling using U.S. EPA Delisting Risk Assessment Software (DRAS). Estimated surface and groundwater media concentrations of Cd and Pb, and associated cancer risks and non-cancer hazards were below human health and ecological screening limits. The hazard index under basic landfill conditions was an order of magnitude lower than under acidic conditions, which is notable as landfills have predominantly neutral to slightly basic conditions over their lifetime. Estimated environmental concentrations of Pb from crystalline silicon PV were comparable to concentrations of Cd from cadmium telluride PV, indicating that responsible disposal is important for all PV technologies. Potential impacts may be further limited by use of sanitary landfills or with high value recycling, with the latter providing the important benefit of resource recovery. The DRAS default assumption is Toxicity Characteristic Leachate Procedure (TCLP) data for waste with a fragment size of 1 cm. Experimental crushing of cadmium telluride PV modules in landfill conditions was conducted to evaluate the representativeness of the leachate data used in the DRAS modeling. On average approximately three-quarters of the crushed module fragments were larger than 1 cm, and 99% of module fragments were larger than 0.1 mm. The glass-laminate-glass bond of individual broken module fragments was maintained, and when analyzed without further size reduction, the landfill fragments are non-hazardous based on TCLP and Soluble Threshold Limit Concentration (STLC) testing.

The photovoltaic market is currently dominated by silicon technology, but emerging devices such as Dye-Sensitized Solar Cells (DSSCs) are drawing increasing attention, due to their easy fabrication, low cost and high conversion efficiency. However, one of the major problems limiting the long-term stability of these devices and their subsequent large-scale industrial production is the volatilization of the liquid electrolytes traditionally employed. Furthermore, a liquid also presents technological drawbacks with respect to its effective encapsulation in an electronic device.

In order to solve this problem and improve the technological perspectives of DSSCs, many studies have been focused on the preparation of quasi-solid electrolytes, in which a polymer network is exploited to effectively retain the redox mediator. In Chapter 3, the photoinduced polymerization has attracted large attention, demonstrating to be the most effective preparation method for these polymer electrolytes. In fact, among other advantages, it is a rapid, economic, functional and environmentally friendly process, besides being easily transferable to an industrial scale.

In this chapter, the fabrication and characterization of free-standing UV-cured polymer electrolyte membranes and their integration in quasi-solid DSSCs is reported. In particular, the first part of the chapter describes the dye-sensitized solar cell working principles and the photopolymerization process. In the second part, devoted to the new electrolytes, the discussion concerns the selection of peculiar monomers useful to obtain a specific 3D network, the development of smart fillers used to selectively improve the photovoltaic parameters, and the physico-chemical correlation between charge transport properties and polymer backbone architectures.

The development of the photovoltaic (PV) sector in the last decade was spurred by the implementation of various support strategies aimed at reducing the gap between PV energy cost and the energy price for conventional generation. The deployment of support policies has pushed the reduction of PV energy costs, but despite this PV is still not very competitive and its development still requires adequate support mechanisms, simple grid connection procedures, and so on.

Chapter 4 provides a technical-economic analysis of investments in PV systems, evaluating the positioning of the main European markets (Germany and Italy), with the purpose of highlighting the main differences in the implementation of support policies in the two top countries. Several case studies are examined, differentiated in relation to the rated power (from 3 kW to 1 MW) and the type of plant (ground-mounted and rooftop PV systems). The profitability indexes in terms of the payback period (PBP), net present value (NPV) and the internal rate of return (IRR) are evaluated throughout the reference period. The chapter is expected to be very useful for policy makers, energy producing industries and national Governments to estimate the profitability of PV investments in the two selected countries, predicting how the PV sector will evolve in each of the two EU states.

The uncertainty introduced by non-dispatchable generation, e.g. photovoltaic, affects the daily operation and planning of electric networks. To study this uncertainty, it is common to model the performance of photovoltaic units from a prediction of solar radiation. In Chapter 5 a method to predict this photovoltaic generation is proposed.

The purpose of this prediction is to obtain the output electrical power from the photovoltaic generator as a random variable. This random variable can be used in studies where it is considered appropriate to take into account the uncertainties, e.g. probabilistic load flow.

The clearness index and the fraction of diffuse radiation, which are considered random variables, are the basis of the model proposed. An expression that gives the global radiation on a sloped surface is obtained, depending on the input variables that are the clearness index and the fraction of diffuse radiation. After that, another expression that gives the output electrical power from the photovoltaic generator, also as a function of the input random variables, is reached.

Cumulants method is used to solve equation for output electrical power from a photovoltaic generator. To characterize the output random variable obtained, Gram-Charlier expansion is used.

The model proposed in this work takes into account the random nature of solar radiation, dependent on the geographical location where the solar panels are installed, and the hour and day of the year in which the simulation is performing. This approach allows determining the output electrical power from a photovoltaic generator at any place and hour as random variable.

Support schemes for solar PV have widely been adopted in the world. There is a voluminous literature on the theoretical and empirical analysis of different instruments to support renewable energy sources in genera and solar PV in particular. Chapter 6 has mostly focused on the effectiveness and efficiency criteria, although other criteria have also been included in some analyses. However, what is missing is a comprehensive framework which includes all relevant assessment criteria.

In addition, the assessment criteria have been treated in an isolated manner, although these criteria interact between each other.

Therefore, the aim of this paper is to close those gaps in the literature by providing a comprehensive framework which integrates all the relevant assessment criteria, explicitly considering their interactions. The results are deemed useful in order to undertake future multicriteria analyses of support schemes for solar PV.

The use of photovoltaic devices within buildings is also known as Indoor Photovoltaics (IPV). IPV has gained rising interest in the last years, when both the development of energy efficient electronics with an average power demand of a few micro watt and the introduction of narrow banded artificial light sources took place. This has opened new application fields for IPV, such as to power wireless sensor systems in intelligent buildings, with limiting efficiencies close to 50% for fluorescent lighting and even higher for LED spectra.

Chapter 7 provides the basic theory, recent progress, and future aspects of IPV devices. Aspects of IPV characterization are explained and referenced to methods from Standard Test Conditions following IEC 60904-3 Ed. 2 (2008). Typical indoor irradiance conditions and the resulting theoretical photovoltaic efficiency limits for ideal and real cells under these conditions are discussed. The calculated limits are compared to recent progress in research and industrial devices. The chapter closes with a discussion of current and future optimization strategies.

The development of sustainable materials in thin film form is a prerequisite for their potential deployment in future photovoltaic technologies. While cost, performance, and recently carbon footprint have been essential factors in materials selection, other equally important factors such as materials abundance (supply chain), chemical risk (toxicity), and recycling/reuse at end of life (cradle-to-cradle approach) have emerged as the new paradigm shift in the deployment of sustainable alternative energy technologies. Many concerted research efforts have been directed at the development of thin films that are able to guarantee optimal characteristics in terms of abundance, environmental compatibility, and photoactivity. Iron disulfide (pyrite) stands out as an excellent candidate for competitive photovoltaic technologies, as it meets all sustainability criteria in addition to its attractive technical capabilities. For over three decades, several investigations have been carried out to develop pyrite in thin film form and highlighted the potential of pyrite in future large-scale production of solar cells. Chapter 8 focuses on the review and discussion of different fabrication methods of pyrite thin films.

Buildings consume more than 40% of global energy use and are responsible for 33% of global greenhouse gas emissions. Hong Kong, being one of the most densely populated cities in the world, has buildings consuming over 90% of total electricity annually. Out of the various renewable energy sources, solar power using photovoltaic cells is considered the most suitable for wide-scale implementation in a densely populated city with a large number of high rises. To quantify the potential, a methodology was devised to determine the amount of Building Integrated Photovoltaic (BIPV) and Non-BIPV panels that may be installed on the rooftop and façades of selected existing buildings as well as in open space. With a database of building stock being established, a detailed site survey can then be conducted for the sampled buildings in order to determine and verify the feasible areas for PV installation. This methodology can be applied to other similar cities with a large number of high-rise buildings. In addition, the challenges and details of actual projects with different types of BIPV are described in Chapter 9. Operating measurements from the projects can then be used for design verification and further practical design considerations. Coupled with practical operating experience, this methodology can be used to evaluate the effect of urban density on photovoltaic (PV) performance.

Light matter interactions in nanoscale ferroelectric materials have received growing interest over the last years due to new developments in scientific instrumentation and novel materials that allow for the study of so far scarcely investigated and /or hidden nanoscale phenomena. Domain walls in complex oxides have especially been in focus opening new pathways for a number of possible applications. Recently an anomalous photovoltaic effect in ferroelectric $BiFeO_3$ thin films was reported that arises from a unique, new mechanism - namely, structurally driven steps of the electrostatic potential at nanometer-scale domain walls. In conventional solid-state photovoltaics, electron–hole pairs are created by light absorption in a semiconductor and separated by the electric field spanning a micrometer-thick depletion region. The maximum voltage these devices can produce is equal to the semiconductor electronic bandgap. Interestingly, domain walls can give rise to a fundamentally different mechanism for photovoltaic charge separation, which operates over a distance of 1–2 nm and produces voltages that are significantly higher than the bandgap. The authors present in Chapter 10, the charge separation that happens at previously unobserved nanoscale steps of the electrostatic potential that naturally occur at such ferroelectric domain walls. Their nanoscopic size and flexible arrangement using thin film growth engineering solutions and applied external electric fields offer unique possibilities for novel concepts in oxide based photovoltaics.

CONTENTS

In: Photovoltaics
Editor: Monique A. Gill, pp. 1-35

ISBN: 978-1-63117-843-6

Chapter 1

NANOSTRUCTURE-BASED PHOTOVOLTAICS

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Abstract

Increasing demands on energy has necessitated the development of large-scale, low-cost, renewable energy. Solar energy is highly attractive and extremely promising as the energy reaching the earth from the sun is orders of magnitude larger than today's global energy consumption and is quiet, requires low maintenance, has no restrictions on size, can be located close to the point on consumption, and is a clean, direct and efficient mode of energy conversion. The challenge lies in making solar power economically competitive while working with the materials readily available in abundance along with all their inherent constraints, also using those materials as economically as possible. Novel materials and structures are constantly being investigated for possible application in the area of photovoltaics (PVs). Lately, various nanoparticle-polymer-based solar cells have demonstrated reasonable power conversion efficiencies (PCE), about 9% [1]. Theoretical predictions suggest that higher efficiencies are achievable through nanocrystal-based approaches due to the outstanding optoelectronic properties and multi-exciton generation capabilities of semiconductor nanocrystals (NCs) [2]. Hence, these hybrid solar cells have the potential to provide cost-effective, high-efficiency solutions for PV, although significant challenges need to be overcome.

This chapter discusses several approaches in pursuit of efficient light absorption in materials. Group-IV materials such as silicon (Si) and germanium (Ge) are desirable for optoelectronic applications due to their high abundance, cost-effectiveness, and high compatibility with the existing technology but as they are indirect band gap materials, they inherently have poor optoelectronic properties at room temperature. Approaches such as point defects [3, 4, 5], optically excited Raman lasers [6], quantum confinement in Si NCs [7, 8], utilizing rare earth dopants [9], bonding of III-V semiconductor structures onto Si chips [10], integration of active conjugated-polymers with Si [11], synthesis of tensile-strained semiconductor heterostructures [12] and NCs [13] to modify their band structure and obtain favorable optical properties which result in improved carrier mobilities have been tried to address the challenge.

Band engineered nanoparticles (NPs) and NCs provide improvements in the primary photoconversion process by increasing the energy absorbed from the electromagnetic

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spectrum that may otherwise be lost as heat in bulk semiconductors and thin films. Such NS may be embedded in a suitable matrix for application in PV and could be a potential solution to surpass the ~33% Shockley-Queisser (SQ) limit for PCE, leading us towards viable "third generation" PV devices. This approach also offers great flexibility, allowing us to combine various materials to maximize the range of wavelengths absorbed by the materials which could lead to higher efficiencies for PVs. Also, various nanostructured materials are being experimented for the contact layers. The following sections discuss the synthesis and characterization of the structural and optoelectronic properties of such nanostructures (NSs) and their advantages for high efficiency PV.

Introduction

Nanotechnology offers great promise to revolutionize a vast majority of areas of science and technology as it allows for the manipulation of material properties at the atomic level. Low-dimensional semiconductor structures could provide significant improvement in several applications in the fields of electronics, telecommunications, and energy. NS based PV devices could lead us towards high-efficiency, economical solutions for energy production.

PV devices produce direct current using the light incident upon them. The low dimensions of NSs play a key role in increasing the amount of energy absorbed from the incident light primarily based on two parameters, the material and the size of the NSs. In addition, the band structure of the material may be further influenced by the introduction of strains [13] and doping [14, 15] in these NSs to provide enhanced optoelectronic properties. The key goals of this chapter is to introduce the reader to the basics of semiconductor NSs, approaches for the synthesis of NSs, various techniques used to study their structural and optoelectronic properties, and the fabrication processes for third generation NS-based PV devices.

Semiconductor Material Properties

Crystalline materials have electrons arranged in various energy levels consistent with Pauli's exclusion principle. These energy levels form bands separated by regions of energy where no electrons and wavelike electron orbitals can exist. These forbidden regions of energy caused by interactions between the conduction electrons and the ion cores of the crystal [16] are called "energy gaps" or "band gaps" and strongly influence the electrical and optical properties of materials. Band gaps may be of different widths depending on the properties of the atomic orbitals from which they arise; the band gap is typically inversely proportional to the atomic weight of the material. Sometimes, allowed bands overlap to form a single large band. Electron transfer from one band to the other is possible by means of the processes of carrier generation and recombination.

The upper range of energies of the energy band is called the conduction band. Here, the electrons are allowed to move freely within the crystal lattice. Electrons at these energy levels are mobile charge carriers, responsible for conduction of electric currents in good electrical conductors. The lower range of energy levels where electrons are bound to individual atoms forms the valence band. The bound electrons cannot move freely to be available for conduction.

Electrical and Optical Properties of Semiconductors

Electrical Properties

If allowed energy bands are completely filled or completely empty, no electrons can move in response to an applied electric field and the crystal behaves as an insulator. Partially filled bands give rise to the behavior of conductors (metal). Slightly filled or slightly empty band(s) results in semiconductors which have electrical conductivity values in between that of a conductor and an insulator.

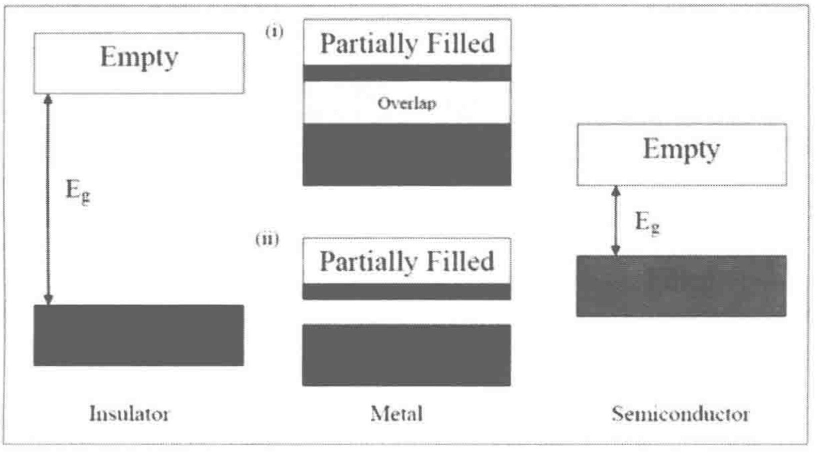

Figure 1. Typical band structure at 0 K for metal, insulator, and semiconductor.

A schematic representation of the band structures of the three types of materials is depicted in Figure 1. The fundamental difference between the band gaps of semiconductors and insulators is that the band gap between the valence band (VB) and conduction band (CB) is much larger in insulators. This prevents electrons being able to get over the larger barrier, therefore resulting in lower, almost negligible electrical conductivity. With thermal energy being a prominent mechanism by which electrons get excited to the conduction band, conductivity of semiconductors is strongly dependent on the temperature of the material.

Optical Properties

The process of optical emission in semiconductors is a result of the transition of an electron from a higher energy level in the CB, across the band gap, into a lower energy level in the VB, and the energy difference being released as a photon, an elementary quantum of light. Therefore, the amount of energy of the emitted photon is dependent on the width of the band gap.

It is possible to stimulate light emission from a semiconductor by means of optical excitation of the material. In doing so, electrons are excited from the VB (E_1) into the CB (E_2) and light emission is stimulated as the excited electrons transition back into the VB to recombine with the hole. The exciting photon energy ($h\upsilon_1$) needs to be at least as much as the band gap energy ($E_2 - E_1$) of the material to be able to excite an electron into the CB. When the electron-hole pairs undergo recombination, the generated photons have energies ($h\upsilon_2$) corresponding to the magnitude of the band gap, as indicated by the schematic in figure 2.

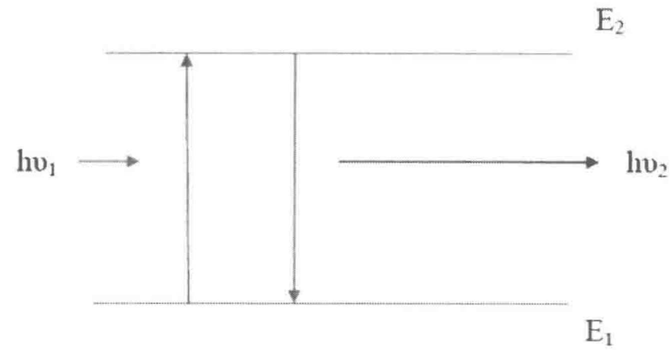

Figure 2. Simplified two energy level model for light emission.

In reality, the energy of the emitted light is slightly lower than the band gap energy. This is attributed to the coulombic attraction between the excited electron and the localized hole it left behind in the VB. The electron-hole pair, referred to as an "exciton" has a lower energy compared to the free unbound electron and hole. Consequently, the energy of the photon released by their recombination is slightly lower than the band gap energy.

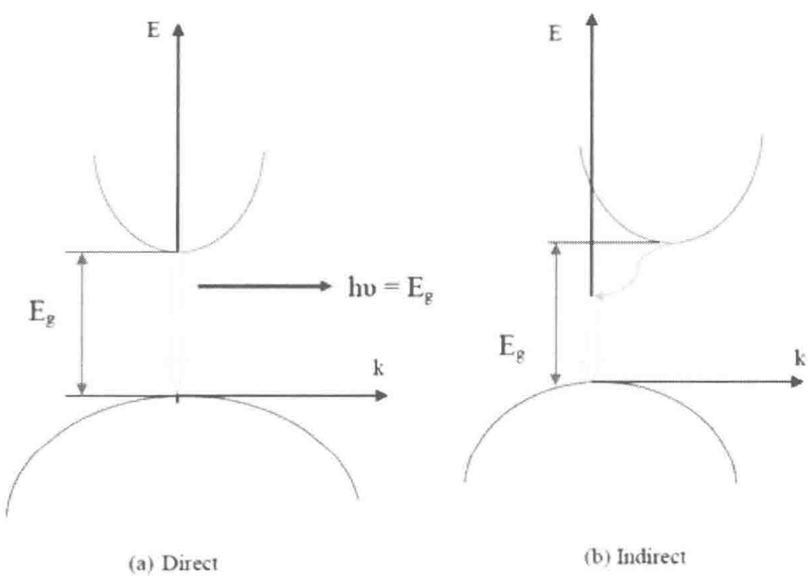

Figure 3. Direct and indirect electron transitions in semiconductors.

Band gaps of semiconductors are classified into direct and indirect types based on the positions of the lowest point in of the CB edge (in green) and the highest point of the VB edge (in red), as shown in figure 3. The bands of energy are distributed along the k-space (reciprocal lattice space) of the crystal in wave-like patterns. If the lowest point of the conduction band occurs at the same k-vector in the Brillouin zone (coordinates in k-space) as