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Type III solar cells based on quantum dots

BACHELOR'S THESIS

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Abstract

In this thesis the extensive study of possible and surly optimal materials for Quantum Dot Solar Cells (QDSCs) will be provided to the reader. One will have the opportunity to develop a rather current image of the necessary parts in their architecture which will be supported with an abundant description of the important aspects in engineering a photovoltaic device. With an introduction of its kind we will try to convey a basic but sufficient knowledge of standard terms, light with matter interaction, light spectrum analysis, quantum dots description with their behaviour and a photovoltaic device operation theory with certainly needed quantities that one has to find in order to properly describe a solar cell. In many parts we will try to outline possible enlargement of that information. With the objective of creating a possibly competitive QDSC the description of methods that we used will be included with a related to them characteristics. One will also be able to use this paper as a review of today's development phase and current technological state of the other scientific groups all around the world. After a successful development of a solar cell, the analysis and comparison will definitely be provided.

Dedication

I would like to dedicate ...

Declaration

I hereby declare that the present bachelor's thesis was composed by myself and that the work contained herein is my own. I also confirm that I have only used the specified resources. All formulations and concepts taken verbatim or in substance from printed or unprinted material or from the Internet have been cited according to the rules of good scientific practice and indicated by footnotes or other exact references to the original source.

The present thesis has not been submitted to another university for the award of an academic degree in this form. This thesis has been submitted in printed and electronic form. I hereby confirm that the content of the digital version is the same as in the printed version. I understand that the provision of incorrect information may have legal consequences.

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Acknowledgements

Thanks

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Chapter 1

Introduction

We, as a society nowadays, are in constant demand for energy. Although, even with the development of calculating, conducting and studying it, we don't really know what the energy is, we are depending on that abstract quantity. One might probably say that to study physics is to endure to study energy in its every possible form. There's a brilliant quote from Bill Bryson that: "Energy is liberated matter, matter is energy waiting to happen." What might be incredible is that from this strictly mathematical quantity we can deduct anything. And what's also important it is as arbitrary as it gets, depending only on one's reference. From energy we can create few more important quantities such as *power* P , which is simply the energy provided per unit time, so:

$$E = \int P(t) dt$$

The energy will be represented in J (Joules) or eV (electron volt), which directly describes energy of elementary charge body ($e \approx 1.602 * 10^{-19}C$) in 1V (Volt) potential.

$$1eV = 1.602 * 10^{-19}J$$

Power will be then represented in W (Watts) ($W = \frac{J}{s}$).

The rise of energy consumption has proven that in the future we will almost certainly require even more. From Global Energy Perspective paper [3] we can learn that:

- Global energy demand will reach plateau at around 2035 despite strong population expansion and economic growth thanks to emphasis on renewable sources, more efficient service industries or more efficient industrial regions
- The energy demand and economic growth became "decoupled" for the first time in history
- Renewables will provide more than half the electricity after 2035

The reader is strongly recommended to take a look at the document.

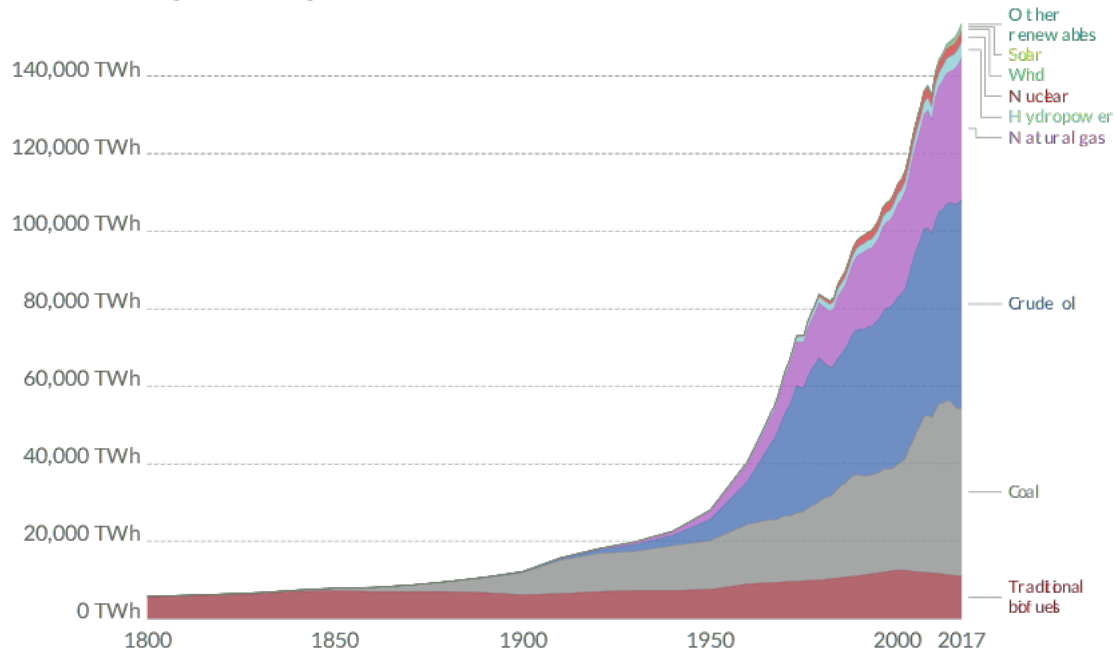
With saying that we can produce energy there's a slick trick given with the phrase. Energy cannot be simply created, it is just converted from another source so nothing is ever lost or miraculously made. The problems we need to struggle

with are then being able to obtain as much energy from the energy source as it is possible and of course, as humankind society is governed by money, keep the cost lowest. There is plenty of different energy sources that we learned to receive energy from. In Figure 1.1 we can see the most vivid ones nowadays. But with the human demand fulfilment come great damages and soon depleting resources of many energy sources such as fossil fuels.

Global primary energy consumption

Global primary energy consumption, measured in terawatt-hours (TWh) per year. Here 'other renewables' are renewable technologies not including solar, wind, hydropower and traditional biofuels.

Our World
in Data



Source: Vaclav Smil (2017) and BP Statistical Review of World Energy

Figure 1.1: Energy sources contribution in world scale [2]

The necessity of searching new possible ways to harness it through renewable sources has become a global issue. Our concern of the environment had never been that serious before. Not only the change of methods for energy production must be enhanced because of this demand but we need to be strictly aware of the World's urging trepidation of Global Warming of which evidence is provided for example here [6].

Among all of the ideas created in a past few decades, solar energy is believed by many to be the most reliable and promising. It can be directly converted into electricity, heat or chemical energy and our only star seems to be an infinite power resource for us. In the last ten years the world solar PV electricity production has grown impressively, being almost three times bigger in 2016, than in 2010 [7]. In theory, the Sun has the potential to fulfil earth's energy demand if it is not for the technology. Annually, nearly 10^{18} EJ of energy reaches our planet and of that 10^4 EJ is claimed to be harvestable. The possibility of converting the solar energy into electric energy has been studied since discovery of the basic photovoltaic effect and the development of semiconductor technologies.

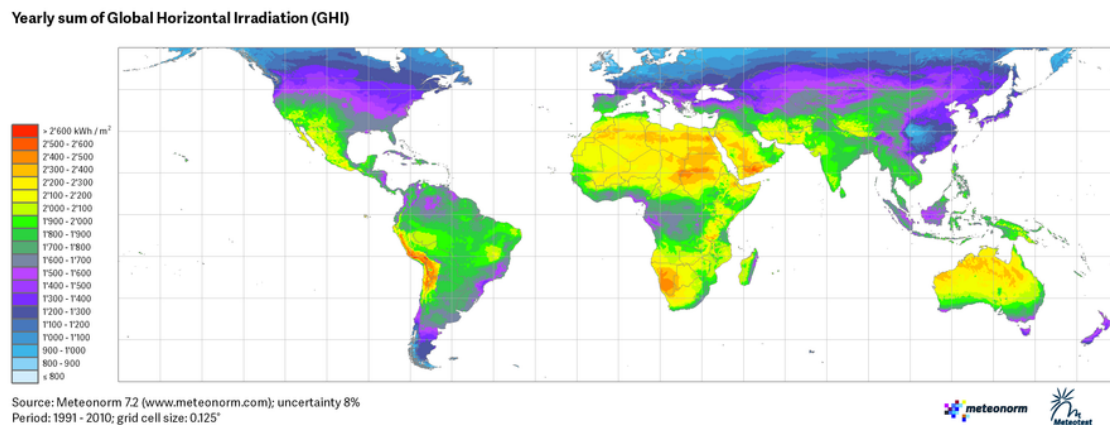


Figure 1.2: Annual yearly sum of Global Horizontal Irradiation [5]

Chapter 2

Theory

With this chapter the introduction of some theoretical concepts will be provided. Certainly some of chapters below could be omitted without missing the final result and its meaning. Nevertheless, even if the paper is laced with rather practical analysis and effects, a physicist should be sure to understand the aspects of an experiment well, not just to have a better insight into the outcome but also to be sure that during the process no foolish mistakes are made and to be able to find new methods to improve the research. Therefore, few parts will just be a reminder and introduction to notation used or to ensure the understanding and some will be treated as an inquiry of what might be searched to describe it further.

2.1 Classical and semi classical theory of light and light with matter interaction

As in the photovoltaic physics we are constantly struggling with light itself we should be know what the light actually is and how it interacts with matter in many, rather curious and different ways. Why is that so that matter looks the way it does and what of its properties can we control. In this chapter we will embrace the phenomena just to create an image of what we are dealing with.

2.1.1 Basic properties of electromagnetic field

Before we actually begin we need to state some classic information about the physics of electric charges. The electromagnetic field is represented by two generally complex vectors, even though the physical result that we are expecting is ought to be real. Those vectors are \mathbf{E} – *electric field* and \mathbf{B} – *magnetic induction*. The properties of those fields are of course described by the *Maxwell's equations*. For them we shall also introduce two more important quantities ρ – *the electric charge density* and \mathbf{j} – *electric current density* vector. We can define them in this way:

$$e = \int \rho dV \quad (2.1.1.1)$$

$$I = \int_S \mathbf{j} \cdot d\mathbf{S} \quad (2.1.1.2)$$

Where I is electric current.

The four Maxwell equations in differential form are:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \rightarrow \text{Faraday's induction law} \quad (2.1.1.3)$$

$$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{j} + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right) \rightarrow \text{Ampere's circuital law} \quad (2.1.1.4)$$

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0} \rightarrow \text{Gauss's law} \quad (2.1.1.5)$$

$$\nabla \cdot \mathbf{B} = 0 \rightarrow \text{Gauss's law for magnetism} \quad (2.1.1.6)$$

To freely describe the properties of the fields interacting macroscopically with material objects we here we can also introduce standard auxiliary fields with polarization and magnetisation of a macroscopic medium. Those vectors are \mathbf{D} – *the electric displacement* and \mathbf{H} – *the magnetic vector*. From Gauss's law for magnetism there is a straight implication that no magnetics monopoles exist and Gauss's law may be also treated as electric charge density definition.

$$\mathbf{D}(\mathbf{r}, t) = \epsilon_0 \mathbf{E}(\mathbf{r}, t) + \mathbf{P}(\mathbf{r}, t) \quad (2.1.1.7)$$

$$\mathbf{H}(\mathbf{r}, t) = \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) - \mathbf{M}(\mathbf{r}, t) \quad (2.1.1.8)$$

Where \mathbf{P} is a *polarization vector* and \mathbf{M} is *magnetization vector*. And with them our former equations change to:

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \rightarrow \text{Faraday's induction law} \quad (2.1.1.9)$$

$$\nabla \times \mathbf{H} = \left(\mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} \right) \rightarrow \text{Ampere's circuital law} \quad (2.1.1.10)$$

$$\nabla \cdot \mathbf{D} = \rho \rightarrow \text{Gauss's law} \quad (2.1.1.11)$$

$$\nabla \cdot \mathbf{B} = 0 \rightarrow \text{Gauss's law for magnetism} \quad (2.1.1.12)$$

If we put divergence on the Ampere's law, we can then place Gauss's theorem in the equation because of the exchangeability of partial derivatives and from that we can simply derive so called equation for *charge conservation*:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (2.1.1.13)$$

The field is said to be static if all quantities are independent of time and, of course, no currents are present. This is the special case but we cannot be so lucky every time. Optical fields are usually sources of very rapid time variety but one may deal with it thanks to the possibility to average the field over macroscopic time interval which is mostly the case in for photovoltaic needs, where for example the light source is a distant star.

Relations for substances under influence of those fields can be very complicated. There is a special case that can make life easier as well. If the material is *isotropic* (all its properties are identical in every direction) they take a simple form of:

$$\mathbf{j} = \sigma \mathbf{E} \rightarrow \text{Ohm's law} \quad (2.1.1.14)$$

$$\mathbf{D} = \epsilon \mathbf{E} \quad (2.1.1.15)$$

$$\mathbf{B} = \mu \mathbf{H} \quad (2.1.1.16)$$

Here σ is called *conductivity*, ϵ is a *dielectric constant* and μ is *magnetic permeability*. Normally, all of those are tensors. In the case of scalar conductivity we can separate macroscopic media in three different categories: conductors, semiconductors and isolators. The same goes for magnetic permeability. With $\mu < 1$ the substance is said to be diamagnetic, $\mu > 1$ paramagnetic and so with $\mu \gg 1$ ferromagnetic. Obviously this description is rather intuitive and treated as a general theory. For example for exceptionally strong fields the area of non-linear optics is needed to be got into which provides higher power terms of fields in the above equations. Also, the case where we need to include relativistic effects by extracting previous values of \mathbf{E} acting on charges is not included as well. The information will be expanded later when needed, but if the reader wants to really expand following discussion understanding, it can be done via [1] [4].

2.1.2 Boundary conditions at discontinuity

2.1.3 Energy of electromagnetic field, the Poynting vector

2.1.4 Wave equation

2.1.5 Scalar waves and wave packets

2.1.6 Vector waves

2.1.7 Refraction and reflection of classical electromagnetic wave

2.2 Physics and properties of solids and semiconductors

2.2.1 Physics and properties of solids

The most common distinction between solids is taking their resistivity as a criterion. We can distinguish three main categories for them - metals, semiconductors and isolators. Within that we can also provide temperature differences beneath them as for the metals, the resistivity goes down with the temperature increase and for the rest of them it is quite the opposite.

Also, as it will be later extended, when we light a semiconductor or an isolator we can clearly observe so called *absorption threshold*.

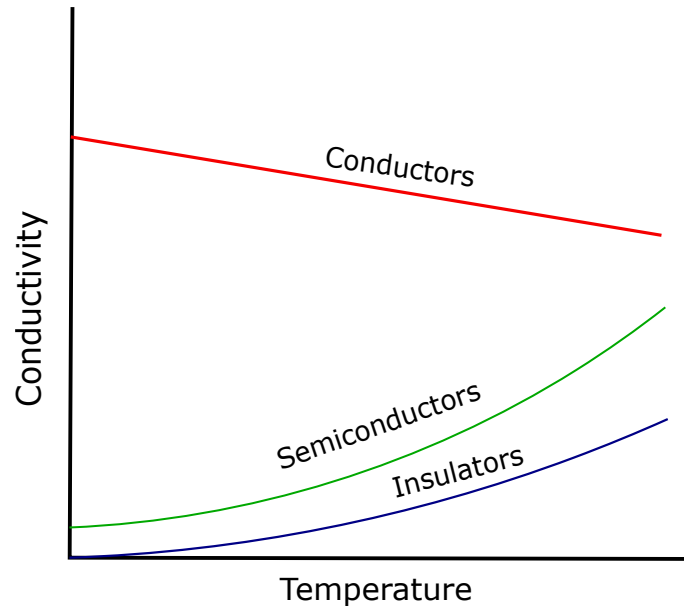


Figure 2.1: Demonstrations of conductivity behaviour of different types of solids

2.2.2 Drude model of free carriers

The discovery of electron in 1897 had the great impact on the first attempt to describe properties of solids. Fairly early, just three years later, Drude constructed his first theory which based on the usage of quite successful kinetic theory, which described the behaviour of gases. Starting with metals he imagined a gas of electrons which are identical solid spheres moving randomly in straight lines. They change directions by collisions and of course no other forces than that of the very quick collisions are taken into account. As metals are neutral, Drude deduced that much heavier and steady particles are compensating negative electron charge. Strictly, that kind of model provides us with the crystal structure but back then, Drude assumed (and for great deal of metals it's fairly true), that only valence electrons are important and they move freely through the whole metal. The basic assumptions for the model are:

1. Between collisions, interactions electron-electron and electron-ion are able to be neglected. The first one is called *independent electron approximation* and the second is called *free electron approximation*.
2. Only the collisions are important. They are approximately instantaneous

events that alter the velocity of the electron. The electron-electron scattering is one of the least important scattering mechanisms in metals. Nevertheless with others, very often, in describing conducting electrons it is not important to describe all mechanisms deeply.

3. We can assume that the period in which an electron isn't making any collision is τ (*relaxation time*) and thus the probability that electron is undergoing a collision in any infinitesimal time period dt is $\frac{dt}{\tau}$. This of course means that τ is average time and it is independent of both velocity and position \rightarrow therefore also time.
4. Thermal equilibrium is achieved only through collisions.

Electrical Conductivity

Drude model can describe, with certain accuracy, the Ohm's law $V = IR$. Resistance R is a quantity which is dependent of the dimensions of the material, therefore resistivity, which has been mentioned before can be used.

$$\mathbf{E} = \rho \mathbf{j} \quad (2.2.2.1)$$

The current density j is the same as in former section, when we were describing Maxwells equations. If n electrons move with velocity \mathbf{v} in time period dt and through area A we get that charge connected with that quantities is $-nevAdt$ so current density is:

$$\mathbf{j} = -nev\mathbf{v} \quad (2.2.2.2)$$

and is just a net current because of random electron movement. Also, let's assume that electron has a velocity \mathbf{v}_0 at time t_0 just after a collision and additional velocity $\frac{-\mathbf{E}e\tau}{m}$ from the external field, we can take average through long time period. The random velocity \mathbf{v}_0 disappears and therefore, connecting with 2.2.2.2 we get that:

$$\mathbf{j} = \sigma \mathbf{E} \quad (2.2.2.3)$$

$$\sigma = \frac{ne^2\tau}{m} \quad (2.2.2.4)$$

2.2.3 Crystal structure and Bloch theorem

2.2.4 Energy structure

2.2.5 Bigger world of carriers

2.2.6 Non-equilibrium processes

2.2.7 Carrier injection

2.2.8 Recombination

2.2.9 Semiconductor junctions

2.3 Quantum dots and nano-structures

2.4 Introduction to quantum description of light

2.5 Theory of photovoltaic devices

2.6 Solar cell parameters

2.7 Third generation solar cells, QDSCs and review

Chapter 3

Cell architecture

Chapter 4

Depositions and parameters

Chapter 5

Results

Chapter 6

Future possibilities

Chapter 7

Conclusion and outlook

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