European Association for the
Development of Renewable Energies,
Environment and Power Quality (EA4EPQ)

International Conference on Renewable Energies and Power Quality
(ICREPQ'11)
Las Palmas de Gran Canaria (Spain), 13th to 15th April, 2011

Photoabsorption Efficiency Improvement for Photovoltaic Solar Cells by Using the Honeycomb Nanostructures

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Abstract. In this paper we propose a designs of solar cells based on III-V semiconductors which can deliver more efficient, less expensive solar cells. Recently proposed approaches to enhance the efficiency utilize the novel III-V nanomaterials containing quantum dots, and new concepts like intermediate bandgap quantum dot based solar cells promise the efficiency over 50% [1]. Needs for thin flexible space solar cells are supposed to be fulfilled with Inverted Metamorphic Multijunction (IMM) solar [2]. In this paper we consider the alternative design of flexible solar cells, which is based on a honeycomb nanostructure consisting of embedded semiconductor pillars in a flexible film [3]. Such nanostructures are flexible and solar cells therefore are suitable for wider range of applications compared to ones with solid panel design, and are less expensive due to the smaller fraction of the active semiconductor material. However this kind of design may reduce the efficiency of the solar cell due to the volume filling factor..

Key words

Nanostructured, photovoltaic cell, flexible, photoabsorption..

1. Introduction

In this paper we propose a designs of solar cells based on III-V semiconductors which can deliver more efficient, less expensive solar cells. Recently proposed approaches to enhance the efficiency utilize the novel III-V nanomaterials containing quantum dots, and new concepts like intermediate bandgap quantum dot based solar cells promise the efficiency over 50% [1]. Needs for thin flexible space solar cells are supposed to be fulfilled with Inverted Metamorphic Multijunction (IMM) solar [2]. In this paper we consider the alternative design of flexible solar cells which is based on a honeycomb nanostructure consisting of embedded semiconductor pillars in a flexible film [3]. Such nanostructures are flexible and solar cells therefore are suitable for wider range of applications compared to ones with solid panel design, and are less expensive due to the smaller fraction of the active semiconductor material. However this kind of design may reduce the efficiency of the solar cell due to the volume filling factor.

2. Proposed Approach

We intend to show that the proposed nanostructured solar cell have the same efficiency as monolithic cells, while contain the smaller fraction of the active semiconductor material.

We present the models and simulation results that show that the filling factor does not limit the efficiency of such solar cell, in contradiction with the common sense approach, is not valid for such nanostructures. We provide the detailed analysis of such multiscale models (nanostructure feature size is much less than light wavelength), show that the absorption efficiency is more than 90%, and that such nanostructures also work as concentrators, comparable to Goetzberg et al[4].
There are several parameters that describe the efficiency of a solar cell. Usually a recombination rate and a carrier transport have to be calculated in order to obtain a power efficiency of the device or external quantum efficiency. We are primarily interested in the absorption of photons and showing that the efficiency of photoabsorption is not necessarily proportional to the volume filling factor. We will compare a quantum efficiency of the bulk semiconductor to the efficiency of composite structure.

Honeycomb photovoltaic nanostructures, consisting of embedded semiconductor rods in a flexible film, are proposed for flexible solar cell design to make the devices resistant against thermal and mechanical stresses, therefore suitable for wider range of applications compared to ones with solid panel design.. However this may reduce the efficiency of the solar cell due to the

volume filling factor. Here we present the multiscale models for such systems (nanostructure feature size is much less than light wavelength), and simulation results that show that the filling factor does not limit the efficiency. Therefore we show that the common sense approach is not valid for such nanostructures.

An attenuation of a light intensity in the structure is characterized by its penetration depth. Its value is in a range of values of materials used that span over four orders of magnitude. Furthermore, the intensity has terms that decays 100-times faster than the main exponential term. These fast decaying components create a boundary layer with a comparable contribution to energy transmitted into the structure. Hence, the traditional methods have difficulties due to a multiscale nature of the problem. In our approach we solve for the fields on top boundary and then use analytical expressions for the light propagation modes.

3. Problem Formulation and Solution Method

Photoabsorption is a process of capturing a photon that yields a transition of a valence electron to the conductive band. The probability that the captured photon contributes an electron-hole pair (e-h) generation rather than an increase of heat is called a quantum efficiency η and is defined as a ratio of e-h generation rate *G* to photon absorption rate *Nph*

$$\eta = \frac{G}{N_{ph}} \tag{1}$$

A capture of every photon decreases the magnitude of the electromagnetic field inside the structure. The depth where the intensity of the field drops down to 1/*e* is called a penetration depth δ and its inverse an attenuation constant α. Both quantities describe how fast the field in the structure is attenuated.

The quantum efficiency as defined above requires switching from a classical description of an electromagnetic field to a quantum one. By introducing a photoabsorbed power *PG* that contributes the e-h generation and the total absorbed power P_0 we can rewrite (1) into form

$$\eta = \frac{PG}{P_0} \tag{2}$$

If P_0 is an incident power rather than an absorbed power and a portion of the energy of light escapes from the structure, then (1) and (2) are not equivalent but the efficiency η represents the effectiveness of the light capture in the honeycomb structure. Therefore the second definition will be preferred.

A design of a solar cell allows a current and therefore an equilibrium can be developed. However, the generated DC current doesn't interact with the light and is not considered in our analysis. All relevant charges and currents at the considered frequency are implicitly included in the complex permittivity ε of the material. Assuming the time factor $e^{-i\omega t}$, the electromagnetic fields $\vec{E}$, $\vec{H}$ are described by Maxwell equations

$$\nabla \times \vec{\mathbf{E}} = i\omega\mu_0 \vec{\mathbf{H}} \tag{3}$$

$$\nabla \times \vec{\mathbf{H}} = -i\omega\varepsilon \vec{\mathbf{E}} \tag{4}$$

where μ_0 is a permeability of vacuum, ω is an angular frequency of the light and *i* is the imaginary unit. An equivalent way of describing the material properties is to use a reflection coefficient *n* and an extinction coefficient *k*. Then, the absorption coefficient can be calculated from the extinction coefficient *k* and the wavelength in vacuum $\lambda_0 = 2\pi c/\omega$

$$\alpha = \frac{4\pi k}{\lambda_0} \tag{5}$$

The absorption constant α corresponds to the total absorbed power and the density of the absorbed power can be calculated according to

$$p_{ab} = \alpha \cdot \frac{1}{2}\frac{n}{Z_0} |E|^2 \tag{6}$$

where the intrinsic impedance of vacuum $Z_0 = 377\,\Omega$ and *E* is magnitude of the electric field at given point in space.

As a good performance was expected in the homogenization limit, the geometry was simplified to the extent possible by considering only a two dimensional problem. This reduces complexity of the calculation and let us concentrate on the mechanism of absorption in the structure to demonstrate that absorbed energy is not simply proportional to a filling factor of GaAs in alumina.

We consider a periodic structure consisting of vertical slabs of GaAs and Al_2O_3 depicted in Fig. 1. The slabs are oriented in y-z plane and periodically repeat along the x-direction. A volume filling factor of GaAs is

$$FF = b/d \tag{7}$$

This structure fills out the lower semi-space. There is a single-layer antireflection coating to maximize the energy flow into the structure. The incident plane wave of given free space wavelength λ_0 and irradiance I_0 impinges perpendicularly from the top.

A. Maxwell equations governing the problem

The problem is two dimensional because neither the material properties nor the driving field depends on the y-coordinate. The solution can be decomposed into two

polarizations that don't interact with each other: E-mode and H-mode

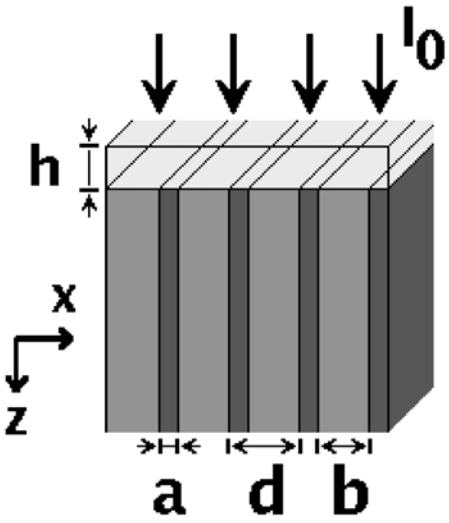

Figure 1: Periodic structure of alumina (thickness a) and GaAs (thickness b) slabs with a period d and an antireflection coating of height h on top of it. An incident light impinges from the top.

$$\vec{\mathbf{E}}_{E-mode} = \hat{y}E_y \tag{8}$$

$$\vec{\mathbf{H}}_{E-mode} = \hat{x}H_x + \hat{z}H_z \tag{9}$$

$$\vec{\mathbf{E}}_{H-mode} = \hat{x}E_x + \hat{z}E_z \tag{10}$$

$$\vec{\mathbf{H}}_{H-mode} = \hat{y}H_y \tag{11}$$

where $\hat{x}$, $\hat{y}$ and $\hat{z}$ are unit vectors of the canonical base. After substituting into Maxwell equations (3,4), the equations for the E_y and H_y components can be derived

$$\nabla^2 E_y(x,z) + \omega^2 \mu_0 \varepsilon(x) E_y(x,z) = 0 \tag{12}$$

$$\nabla \bullet \frac{1}{\varepsilon(x)} \nabla H_y(x,z) + \omega^2 \mu_0 H_y(x,z) = 0 \tag{13}$$

The general solution in terms of variable u (E_y in the E-mode and H_y in the H-mode) has form of a periodic function $u_{per}(x)$ with the period d modified by an exponential factor

$$u(x,z)=u_{per}(x,z)e^{ik_B x} \tag{14}$$

To obtain a solution one usually chooses one period in the x-direction as a computational domain (the z-coordinate bounds depend on the problem). So called Bloch boundary conditions flow directly from (14)

$$u(x_0,z)=u(x_0+d,z)e^{ik_B x} \tag{15}$$

where the Bloch wave number k_B is to be found. Since in our case a normal incidence is considered, there is no preferred direction in x-y plane due to the translational symmetry. Therefore Bloch boundary conditions can be reduced to periodic conditions on the y-z sides of the computational domain

$$u(x_0,z)=u(x_0+d,z) \tag{16}$$

B. Plane Wave Expansion

The plane wave expansion (PWE) method is applied to solve the problem, i.e. the general solution (14) for k_B=0 is expressed as a superposition of plane waves

For our analysis we chose GaAs as a prospective candidate for a photoabsorbing material with a cut-off wavelength of 871 nm. Its internal quantum efficiency was estimated to be 99%. The word *internal* reflects the fact that recombination was not taken into account and needs to be included during an optimization of the structure height. Alumina (Al_2O_3) was chosen for its good mechanical properties and a low heat generation.

However, it is not a photovoltaic material and thus degrades the performance of the structure. The results below give a quantitative estimate of this degradation. Properties of both materials at 827 nm were estimated from various sources and are summarized in Table (not shown).

2. Antireflection layer

Because of the field matching procedure described above and uniqueness of the expansion there will be a plane wave component in the reflected field. For the cell size d sufficiently smaller than the wavelength λ_0 one can expect that the plane wave component will be prevailing. As the ε_r in the air is 1 the plane wave component decays very slowly and carries energy away. Therefore its reflection has to be eliminated by an antireflection layer.

The antireflection layer (Fig. 1) was calculated for the plane wave component and its properties were determined to be $h=\lambda_0/4n$, $n=\sqrt{n_{air}\cdot n_{eff}}$ with $n_{air}=1$ and n_{eff} being the real part of eigenvalue β for the longest propagating mode.

The higher harmonics have different equivalent refraction index β, so they will be reflected even if the plane wave component is totally eliminated. Fortunately, by a good choice of the cell size d it is possible to make the refraction index imaginary, meaning that the higher harmonics will exponentially decay with a distance from the reflecting surface. Then, the energy conservation law implies that these modes cannot carry energy away

because there is no absorption. In order to make β imaginary one needs to request

$$\varepsilon_r - \left(\frac{m}{d/\lambda_0}\right)^2 < 0 \qquad (17)$$

for every value of *m* except *m*=0. Hence for air (ε_r=1), the cell size must be smaller than wavelength

$$d < \lambda_0 \qquad (18)$$

The smaller the cell size *d* is, the more confined to the surface the modes are.

In our simulations the observed total reflected power was less than 2% for cell sizes less than 0.3 λ_0 for both polarizations and all filling factors and it was decreasing with the cell size. These results include the contribution of higher harmonics.

The related eigenproblems were solved by a Matlab*TM* eigenvalue solver. The value β was calculated as a square root of the eigenvalue with a sign chosen so that the imaginary part is positive. A typical Fourier spectrum is depicted in Fig. 2.

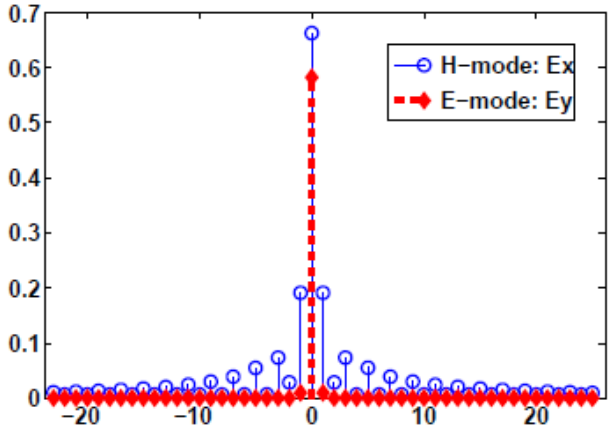

Figure 2: Fourier spatial harmonics of modes in the periodic structure excited by a plane wave incident in the normal direction. Normalized Fourier component amplitude (y-axis) vs. the component number m (x-axis).

3. Discussion of Results

A convergence of the method was checked for d/λ_0=0.12 and filling factors 0.1 and 0.5. It was found that small and large filling factors demand more harmonics to be used. 128 harmonics expansion was found to be satisfactory to achieve about 1% accuracy.

A penetration of the light into the material is given by the most slowly decaying mode. Figure 3 shows a homogenization limit for cell sizes $d<0.1\lambda_0$, i.e. the penetration is independent on the cell size and varies only with the filling factor *FF*. The variation is mild except for *FF*<0.05 where it abruptly increases (Fig.3).

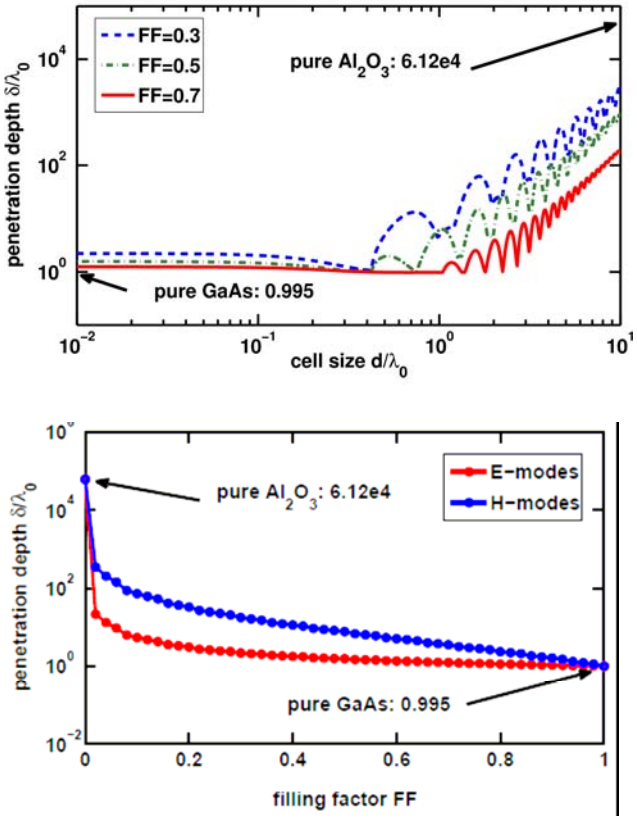

Figure 3: Top: Dependence of the normalized penetration depth δ/λ_0 of 827nm light on a cell size *d* of the periodic structure for three filling factors *FF*. Theoretical penetrations for pure GaAs and pure alumina are shown. E-polarization. Bottom: Penetration vs. filling factor in the homogenization limit for cell size d=50*nm*=0.06λ_0. Comparison between E- and H- modes.

The opposite limit (the cell size *d* is several times larger than λ_0 – not shown) exhibits very large penetration, i.e. a slow absorption. The longer penetration requires a thicker active area to collect the solar power. That in turn means increased recombination, and hence, a lost of efficiency. Fortunately, for cell sizes *d* comparable to the wavelength λ_0 is possible to achieve a penetration depth of several wavelengths. The power efficiency η defined in (2) is almost not affected (Fig. 4), meaning that 99% of the absorbed power contributes e-h generation. However, the current response will be smaller because of increased recombination.

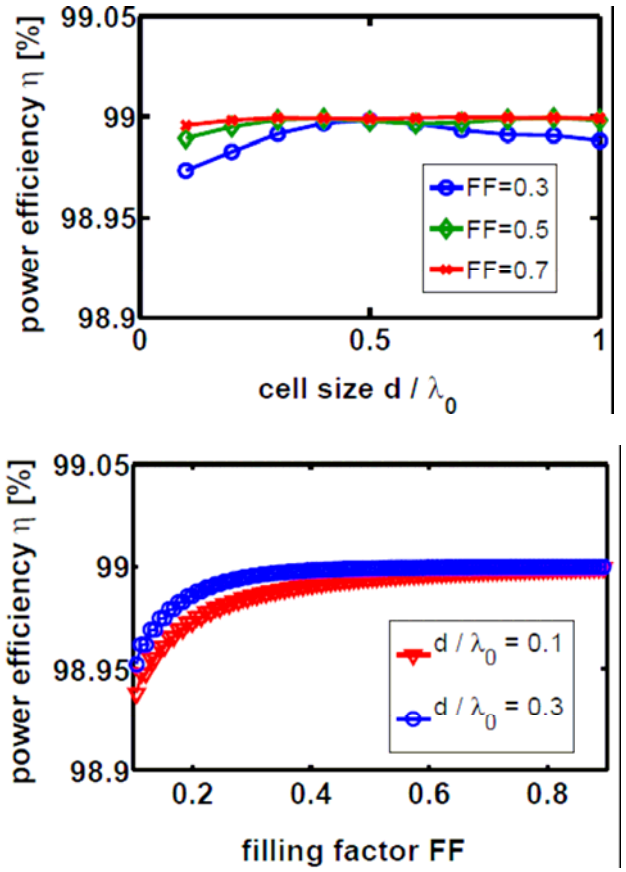

Figure 4: Power efficiency of photoabsorption. An unpolarized incident light is assumed.

When the height of the periodic structure is not big enough, the light won't be absorbed before reaching the boundary and a part of the energy escapes from the structure without being absorbed. To minimize an energy loss and an excessive recombination the height of the active area must be optimized. In the homogenization limit (for $d<0.1\lambda_0$) there is only one dominant mode. The second longest mode has about 100 times shorter penetration depth. This allows to use the dominant exponential decay with an amplitude properly calculated from the boundary condition evewhere but in the vicinity of the boundary.

4. Conclusion

A numerical analysis of a periodical structure consisting of alumina and GaAs slabs driven by an infrared light propagating along the slabs was presented. A significant portion of the work deals with eigenmodes of this structure. It was argued that the analysis of fields can be performed for two independent polarizations thoughout this paper referred to as E- and H-modes. Since the most practical case is when the spatial period *d* of the structure, referred to as a cell size, is smaller than the wavelength an efficiency of photoabsorption was calculated in this region. Equal contributions of both polarizations in the incident light was assumed.

A photoabsorption efficiency was calculated as a ratio of photoabsorbed power to the power entering the periodic structure. It was shown that the resulting efficiency is nearly the one of GaAs. From the energy flux into GaAs was concluded that a diffraction is an important factor increasing the amount of absorbed power at the expense of larger penetration depth.

The absorption constant of the structure is important for calculation of the height of the structure. Although, the light intensity doesn't decay always exponentially (e.g. when two excited modes have similar attenuation constants), it was observed that the mode with the largest attenuation constant is dominant because of its large plane wave component. This allows at least a quantitative estimate of the optimal height of the structure (too high structures has a higher recombination rate so finding a trade-off is necessary).

There are some results that can be extended for GaAs rods or bars buried in alumina. The most important is that when the cross sectional size of alumina is less than or comparable to a wavelength in alumina, the energy from alumina is diffracted into GaAs, and thus, substantially increasing the efficiency of photoabsorption. As a side effect the light attenuation constant is close to the one of GaAs.

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