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Short communication

Comparison of optical properties of Si and ZnO/CdTe core/shell nanowire arrays

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ABSTRACT

The systematic computations of the short-circuit current density have been performed for Si and ZnO/CdTe core shell nanowire arrays of 1 μm height in order to optimize the structural morphology in terms of nanowire diameter and period. It is found that the best structural configuration for Si leading to the ideal short-circuit current density of 19.6 mA/cm^2 is achieved for a nanowire diameter and period of 315 nm and 350 nm, respectively. In case of ZnO/CdTe, the ideal short circuit current density is of 24.0 mA/cm^2, the nanowire diameter and period is of 210 nm and 350 nm, respectively. It is shown that the optimal configuration is more compact in the case of Si nanowire arrays than in the case of ZnO/CdTe nanowire arrays. Since Si has a smaller absorption coefficient than CdTe, a larger amount of material is needed and thus more compact nanowire arrays are required. It is also revealed that core–shell nanowire arrays made of ZnO/CdTe more efficiently absorb light than that of Si, making this device a good candidate for the next generation of nanostructured solar cells.

1. Introduction

Semiconductor nanowire (NW) arrays are promising building blocks for solar cells since they can efficiently trap light [1–4] as compared to planar layers with the same amount of materials. In thin film solar cells, such arrays can be used to efficiently couple incident light in the film underneath by benefiting from anti-reflecting properties of the array. Hence, the NW can be fabricated on top of the thin film solar cells [5]. Another promising configuration consists in directly absorbing the light within the NW arrays. This structure benefits from the long optical path within the NW length and by exploiting a radial junction of core shell type, a shorter path for carrier collection corresponding to the NW radius is achieved, leading to a smaller carrier recombination rate. An increasing interest has been devoted to the growth of NWs on top of low cost substrates such as metals [6], glass substrates [7] or transparent conductive oxides [8,9] by using low cost techniques. An experimental photoconversion efficiency as high as 7.9% has already been reported for Si core shell NW arrays [10].

It has early been shown [11–13] that the NW arrays can more efficiently absorb the light than conventional thin film solar cells for a given amount of materials. Moreover, it has been revealed that an optimization of the array structural morphology such as the NW diameter (D), period (P) and height is of great importance in order to improve the efficiency of the light trapping. Theoretical studies have found that the optimum geometrical configuration in terms of NW period and diameter is in the range of a few hundreds of nanometers [14]. Huan et al. [15] have systematically investigated hexagonal NW arrays embedded in air in order to find the best configuration; the optimal geometry for direct band-gap semiconductor materials has been determined. For indirect bandgap materials like Si, an increase in the NW height leads to a further increase in the optical absorption even in the case of NWs longer than 100 μm [15]. The same conclusion can be drawn from the work of Foldyna et al. [16] who studied Si NW arrays on silver substrate. Since no absorption optimum can be found for Si by increasing the NW height, the present work focuses on the optimization of an array of 1 μm height.

Increasing efforts have also been dedicated to the development of nanostructures based on ZnO owing to its ability to grow within the NW morphology by a wide variety of growth methods such as chemical vapour deposition [17], chemical bath deposition [8] or electro-deposition [18]. Such NWs can be covered with

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CdSe [19], ZnS [20], ZnSe [21], or CdTe [8,22] in order to create a type II band alignment. This alignment is expected to separate electrons from holes without any doping. Also, CdTe is a very efficient absorbing material with a high absorption coefficient and a bandgap energy of 1.5 eV at room temperature. It has been shown that CdTe nanograins can uniformly cover ZnO NWs by vapour phase epitaxy [23], electrodeposition [22], close space sublimation [8] or successive ionic layer adsorption and reaction [24]. However, the photovoltaic properties of the resulting solar cells made from ZnO/CdTe core shell NW arrays are still fairly poor, showing the crucial importance to design the structure by systematic computations.

In this paper, we compare the absorption properties of Si(p)/Si(n) and ZnO/CdTe core shell NW arrays in order to find the best absorbing structure. This study has been carried out by simulating the structure using a three-dimensional (3D) rigorous coupled wave analysis (RCWA) tool developed at universities of Moscow and Bologna [25] and a commercial finite difference time domain (FDTD) tool (Lumerical FDTD Solutions).

Section 2 is devoted to a brief explanation of the different computational methods. Sections 3 and 4 describe the structures simulated and the simulation methodology while, in Section 5, the results are discussed.

2. Principles of the computational methods

In this paper, all of the computational methods solve Maxwell's equations assuming that there is neither charge nor current.

FDTD method consists in introducing a space and time mesh that must satisfy the stability criterion in order to converge [26]. Maxwell's equations are solved by replacing the system with finite difference equation on a space-mesh. This has early been done by Yee [26]. He introduced a cell where the fields are spatially offseted from one to another in order to intrinsically model a perfect conductor at the border of the calculation windows.

The Yee cell presents an obvious disadvantage while trying to model unbounded mediums because light is reflected back to the structure at the border of the simulation window. Berenger et al. [27] have shown that perfectly match layer (PML) can be used to model semi-infinite structure since it absorbs radiations going out of the calculation window. Unfortunately, the reflection of light is not null for all incident angle on the PML and can be decreased by considering several layers of PML. Thus the three main parameters describing the PML are its normal incident reflection, its polynomial order and the number of PML layers considered.

Other kind of boundary conditions can be applied; among them, the periodic boundary condition consists in matching the field from one side of the calculation window to the other one [28].

Furthermore, the convergence is achieved for certain time since the method solves the Maxwell's equation in space and time.

Thus, the parameters that ensure the convergence of the FDTD technique are the space step, the computation time, the normal reflectance and the order of the PML and the number of PML layer.

In our setup, PMLs have been implemented at each boundary of the calculation volume in z (propagative) axis while in the x and y axis, periodic boundary conditions have been set. In this paper, all the results that are simulated with the FDTD methods have considered a uniform grid of 4 nm, a third order PML with a normal reflection of 10^{-30} and 84 PML layers. The simulation has been stopped when the time achieved 2000 fs.

In RCWA [29,30], the Maxwell's equations are solved by considering a monochromatic wave. The simulated structure is divided into several layers with a constant profile in the xy plane. For each layer, the Fourier's series decompositions are performed along the x and y axis, which automatically periodize the structure. The different layers are then assembled, such that the fields at the interface are continuous. Since this method relies on Fourier's series decomposition, the single parameter responsible for convergence is the number of harmonics. In this paper, the simulation has been performed with 24 harmonics for each x and y axis.

Based on the above statement, RCWA technique is more suitable for the simulation of periodic structure and the convergence is easier to achieve since it depends only on the number of harmonics considered whereas, in the case of the FDTD, mainly five parameters influence the convergence of the field. Based on our experience, RCWA tool converges faster than FDTD tool. However, since FDTD is a widely used and mature technique, it is used to make sure that the results given by RCWA are consistent.

In order to compute the reflection and transmission of planar structures, the transfer matrix method (TMM) [31] is used. Like in the case of RCWA method, the structure is divided into several layers having different optical properties. A matrix is calculated for each layer by using analytical formulas. It permits to link the electric and magnetic field at one side to those at the other side of the layer. Thus, the product of all these matrices models the propagation of the field in the structure. From this total matrix, it is then possible to deduce the reflection and transmission of the structure.

3. Geometry of the investigated structures

In this paper, two core shell NW array structures have been taken into account, as depicted in Fig. 1. The first structure in Fig. 1(a) consists of a cylindrical NW of Si on Al-doped ZnO on glass substrate. This structure corresponds to the device fabricated in [9]. Fig. 1(b) describes a simplified version of the structure grown in Ref. [8], which consists of ZnO/CdTe core shell NW arrays deposited on undoped ZnO on glass. The thicknesses of the CdTe layer and of the thin ZnO layer underneath have been fixed as 40 and 300 nm, respectively. The NW height has been kept constant and equal to 1 μm whereas both the NW diameter and period have been optimized. For all of the calculations considered, the incident light has been considered perpendicular to the substrate surface and polarized along x.

4. Simulation methodology

Since the aim of this paper is to determine the core shell NW array structures that better absorb light, the spectral absorptance has systematically been calculated for Si and ZnO/CdTe NWs. The NW period has been varied in the range of 200–700 nm while the ratio of the NW diameter over its period in the range of 0.5–1. The spectral absorptance has been integrated using Eq. (1) in order to calculate the ideal short-circuit current density assuming that every generated electron–hole pairs are collected.

$$J_{sc} = \frac{q}{h \cdot c} \int A(\lambda) \cdot I(\lambda) \cdot \lambda \cdot d\lambda \quad (1)$$

In Eq. (1), $A(\lambda)$ is the wavelength-dependent optical absorptance, $I(\lambda)$ denotes the ASTM AM1.5g solar irradiance taken from Ref. [32], λ is the wavelength. q, h and c are fundamental physics constants: electron charge, Plank constant and light celerity, respectively. The integration has been performed from 300 nm to 1200 nm every 5 nm in the case of Si: indeed, the sun power is negligible below 300 nm and Si does not absorb light anymore above 1200 nm. In the case of ZnO/CdTe, the integration has been performed from 300 nm to 830 nm for similar reasons.

The results of the RCWA tool have been compared with literature data given in Refs. [11,12]. The structure simulated to confirm the tool validity consists of Si NW arrays with 50 nm diameter, 100 nm periodicity and 1160 or 4660 nm height embedded in air.