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Nanostructures for light management in thin-film GaAs quantum dot solar cells

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Abstract: We have investigated structures for thin-film GaAs quantum dot solar cells. Light trapping at quantum dot bands is realized by a triangular grating reflector whose aspect ratio is identified as the main design parameter.

OCIS codes: 040.5350 Photovoltaic; 050.1950 Diffraction gratings; 050.6624 Subwavelength structures

1. Introduction

Thin-film solar cells have an attractive weight-to-power ratio which is especially important in space applications. The performance of traditional III-V single junction solar cells can be enhanced by using multiple junctions or embedding quantum dots (QDs) to broaden the absorption bandwidth. Recently, research efforts have been directed to exploit the concept of intermediate bands provided by the quantum dots. [1] In case of basic GaAs solar cells, high absorption above the bandgap will be complemented by sub-bandgap states of the quantum dots as well as absorption of the wetting layer. Due to inherently low absorption of these states some light management scheme, for example based on light trapping, should be employed to enhance the performance of these devices. [2]

In this presentation, we shall analyze few structures of quantum dot solar cells and explore possibilities to improve absorption especially near and below the band gap of GaAs.

2. Models

Our analysis and design of the top surface grating focuses on the antireflection characteristic, whereas the rear grating is designed and optimized for realizing light trapping at the QD wavelengths. In particular, we have considered diffraction grating configurations, where light-trapping is pursued by coupling light into high diffraction modes propagating outside of the escape cone. These gratings require a period length larger than the incident wavelength.

Device structures

The basic structure of the thin-film solar cell is shown in Fig. 1 (left). The topmost layer is an anti-reflection (AR) layer which can be realized by a conventional thin-film of e.g. silicon nitride (SiNx) or by nanostructured “moth eye” layer [3]. Next layers are highly doped GaAs for contacts, and AlInP window layer to reduce surface recombination at the interface of the active layer. In case of the nanostructured AR the nanocones or pyramids will often be structured in this layer. The absorption layer consist of GaAs embedded with several layers of QDs. On the bottom of the cell we add another AlInP layer and finally a metal mirror made of Ag to reflect light as efficiently as possible. To realize light trapping the bottom of the cell needs to be structured. There are various implementations in the literature to realize light trapping either by periodic gratings, random scattering structures, photonic crystal mirrors or plasmonic nanostructures [4]. Often the structures are optimized for solar cells made of amorphous or crystalline silicon. Due to the inherently different optical characteristics of our thin-film GaAs cells we shall analyze structures to enhance absorption especially near the absorption band of the QDs. The typical External Quantum Efficiency (EQE) of conventional wafer-based GaAs cell and QD/GaAs cell is displayed in Fig. 1 (right). We analyze four different configurations: 1) unpatterned slab without mirrors and photonic structures 2) slab with planar Ag mirror on bottom 3) 2D/3D triangular/pyramidal grating as a scattering element and 4) 2D/3D triangular/pyramidal grating covered with Ag as mirror.

Fig. 1. Cross-section of the solar cell structure with triangular grating (left). EQE of wafer-based regular GaAs cell and QD/GaAs cell, highlighting the extended harvesting provided by the QDs through interband absorption of ground state (GS), excited state (ES) and wetting layer (WL) (right).

Materials optical models

QD layers are made by QDs embedded in a GaAs matrix: the resulting medium is modeled as an equivalent homogeneous medium (GaAs-QD) characterized by absorption coefficient $\Delta\alpha = 4\pi\Delta k/\lambda$ and equivalent refractive index: $n_{\text{GaAs}} + \Delta n$, $k_{\text{GaAs}} + \Delta k$, Δn and Δk being the real and imaginary part of the refractive index of the quantum dot (see Fig. 2). Δk has been estimated from typical literature data [5] and approximated by Lorentz oscillators whose resonance frequency corresponds to the different QD states; Δn is then derived through Kramers-Kronig relations.

Fig. 2. Model of the optical properties of the QD material: absorption coefficient, (left) and real part of the refractive index (right). The absorption was calibrated for a QD thickness of about 4 nm. [5]

Simulation tools

Finite-difference time-domain (FDTD) and Rigorous coupled-wave analysis (RCWA) methods were employed depending on the specific problem. Both methods are available as free software packages. [6,7] The sharp absorption edge imposes a challenge for the FDTD method since the refractive index needs to be modeled with an analytic function to ensure numerical stability. Comparison between different photonic configurations and the optimization of the grating parameters is carried out with reference to the photogenerated current density estimated from the solar cell absorbance, $A(\lambda)$, as

$$J_{ph}(\lambda) = \int_{\lambda_0}^{\lambda_1} q_{el} A(\lambda) SPF(\lambda) d\lambda \quad [\text{A cm}^{-2}] \quad (1)$$

where q_{el} is the elementary charge and the solar photon flux (SPF , cm⁻²s⁻¹ nm⁻¹) is evaluated from a specific air mass solar irradiance, as solar irradiance/photon energy. The estimated photocurrent density provides an upper bound to the achievable short circuit current under the assumption of unitary collection efficiency.

3. Results

The analysis of linear 2D gratings made in AlInP, with triangular cross-section, is summarized in Fig. 3 (left). In these simulations the absorption layer consists of 1580 nm of GaAs and a QD region with 20 stacks of QD layers (about 4 nm thick, with areal density of $6 \times 10^{10} \text{ cm}^{-2}$) separated by a 16 nm GaAs interdot layer. The absorbance spectra shows a marked increase around the GaAs band-edge and in the QD range. We refer with QD photocurrent to the current evaluated from (1) in the QD wavelength range, i.e. integrating between $\lambda_0 = 895 \text{ nm}$ and $\lambda_1 = 1200 \text{ nm}$. This photogenerated current is studied as a function of the grating period (d) and height (h). From the results, the relevant parameter for light-trapping optimization turns to be the aspect ratio defined as the ratio of height to period. For any period in the considered range ($1 \mu\text{m} - 2.8 \mu\text{m}$), the photocurrent is maximum for aspect ratio between 0.32 and 0.36. The optimized grating provides – under 1 sun AM1.5 illumination, – a QD photocurrent of about 1.47 mA/cm^2 , against 0.3 mA/cm^2 and 0.49 mA/cm^2 provided by the unpatterned slab and the slab with planar mirror, respectively. Thus, QD photogeneration is enhanced by about 5 times with respect to a conventional wafer-based configuration. Even higher enhancement is achievable using 3D pyramidal gratings. Experimental evaluation of this structure is on-going.

Fig. 3. Absorbance spectra calculated for various photonic configurations. The triangular grating has height $h = 600 \text{ nm}$ and period $d = 2.5 \mu\text{m}$. (left) QD Photocurrent for 2D triangular grating without silver mirror. (right)

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