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Light absorption properties of a nanowire/quantum-dot hybrid nanostructure array



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ABSTRACT

The light absorption properties of a nanowire/quantum-dot hybrid nanostructure array are investigated. By growing multilayer InAs quantum dots on the sidewalls of GaAs nanowires, not only the absorption spectrum of GaAs nanowires is extended by quantum dots, but also the light absorption of quantum dots is dramatically enhanced due to the light-trapping effect of the nanowire array. By optimizing the nanowire and quantum dot parameters, a maximum photocurrent increment of 2.8 mA/cm² is obtained by incorporating 5 layer InAs quantum dots into a 3 μ m high GaAs nanowire array, 4.6 times of its thin-film counterpart. Mode analysis demonstrates that the fundamental mode in the nanowire has a dominate influence on the QD absorption in the wavelength range beyond GaAs bandgap.

1. Introduction

The incorporation of nanostructure with lower bandgap, such as quantum dots (QDs) or quantum well (QW) into a single junction solar cell has been proposed as a promising way to enhance the light absorption by extending the absorption spectrum [1-4]. It has been widely reported that, by inserting multilayer of InAs QDs into GaAs solar cells, isolated intermediate band can be formed within the GaAs bandgap [5-8]. Therefore, photons with energy lower than GaAs bandgap can be absorbed and contribute to the photo current. However, in most of the reported works, the QDs layers are grown on planar substrates, which means additional anti-reflection layers must be employed for light-trapping. In recent years, multilayer of QDs have been successfully fabricated on sidewalls of nanowires (NWs), which offers an innovative approach to combine the advantage of the two kinds of nanostructures [9-13]. The absorption spectra of NWs can be extended by QDs, while the vertical-aligned NW array can dramatically enhance the absorption of QDs due to the excellent light trapping ability [14-17]. Moreover, the NW/QD hybrid structure can be fabricated on low cost Silicon substrates, which makes it promising for low cost, high efficiency solar cells [18].

In this paper, the optical properties of a GaAs/InAs NW/QD hybrid nanostructure array are analyzed by three-dimensional finite-difference time-domain (3D-FDTD) simulations. The considered structure consists of a vertical-aligned NW array with each NW containing 5 layers of QDs arranged perpendicular to the NW growth axis. The absorption spectra of the hybrid structure with different NW radii and periods are calculated, and the underlying physics is discussed by modal analysis.

2. Model and simulation methodology

According to our previous studies [9], the fabrication of the NW/QD hybrid structures can be realized by using a Thomas Swan Closed Coupled Showerhead (CCS) metal organic chemical vapor deposition (MOCVD) system. In those works, Trimethylgallium (TMGa), trimethylindium (TMIn), and arsine (AsH₃) were used as precursors. The carrier was hydrogen. An Au-coated GaAs substrate was loaded into the MOCVD reactor and annealed under AsH₃ ambient to form Au-Ga alloyed particles as catalyst. The GaAs NWs were grown in the first place, and then the first shell of InAs QDs was deposited by switching off TMGa and raising the temperature. After the growth of the InAs QD layer, the GaAs spacer shell was radially grown on the InAs QDs. The multilayers of QDs structures were realized by repeating the combination of InAs QDs and GaAs spacer shell for certain times.

Fig. 1(a) shows a single unit of the GaAs/InAs NW/QD hybrid nanostructure array. The structure consists of a hexagon GaAs NW with 5 layers of QDs arranged perpendicular to the NW growth axis. The thickness of each QD layer is 2 nm. Each QD layer contains a 1.11 nm wetting layer (WL) and hundreds of QDs, and the mean radius and height of the QDs are 5.2 nm and 0.6 nm, the density of the QDs is 125 QD/ μ m².

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Fig. 1. The schematic drawings of a single unit of the NW/QD hybrid nanostructure array and its thin-film counterpart.

The QD layers are modeled by treating InAs QDs, WL and GaAs material surrounding QDs as an effective medium. The wavelength dependent complex refractive index of the effective medium is calculated by a volume weighted superposition of the QDs, WL and GaAs material as described in [19], which is expressed by Eq. (1).

$$\alpha_{eff} = F_{OD}\alpha_{OD} + F_{WL}\alpha_{WL} + F_{GaAs}\alpha_{GaAs} \tag{1}$$

where $F_{\rm QD}$, $F_{\rm WL}$ and $F_{\rm GaAs}$ are the volume fractions of QD, WL and GaAs materials in the effective medium, respectively. The absorption coefficient of InAs QDs and WLs are obtained from [19], with same QD size and density. Other material parameters are obtained from [20]. Absorption spectra of the hybrid structure are calculated by FDTD Solutions software package (Lumerical Solutions, Inc.). Periodic boundary conditions are used in *x*, *y* directions to model an infinite array in a single unit cell, and PML boundary condition is applied in *z* direction. The period of the NW/QD hybrid nanostructure array is defined by the size of the simulation region. The thin-film structure containing QD layers is also simulated for comparison. The thickness of the thin-film structure is set to be equal with the NW length, and the volume of QD layers in thin-film structure is set to be the same with that in NW/QD hybrid structure.

3. Results and discussion

The absorption spectra of GaAs NW array with and without QD layers are shown in Fig. 2(a). The radius and height of the NW are 100 nm and 3 μ m, and the array period is 540 nm. By introducing QD layers, the absorption of GaAs NWs is dramatically enhanced and the absorption spectrum is extended to 950 nm. To analyze the absorption enhancement effect induced by QDs, the reflection and transmission spectra are plotted in Fig. 2(b) and (c). At wavelength region from 500 to 870 nm, the NWs with QD layers have lower transmission compared with those without QDs, while the reflection of the two structures are almost identical. That means the QD layers have stronger light



Fig. 2. The absorption (a), reflection (b) and transmission (c) spectra of the NW/QD hybrid nanostructure array with and without QD layers. The absorption spectra of the thin-film structures with and without QD layers (d).

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