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Theoretical analysis and modeling of light trapping in high efficicency GaAs nanowire array solar cells

Long Wen,[1] Zhifei Zhao,[1] Xinhua Li,[1,a)] Yanfen Shen,[2] Haoming Guo,[1] and Yuqi Wang[1]
[1]*Key Laboratory of Material Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China*
[2]*MENGYAO Microelectronics Research and Development Center, Shandong University, Jinan 250100, China*

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A rigorous analysis and design of efficient light trapping for Gallium arsenide nanowire array (NWA) solar cells is presented. The influence of the geometric parameters on the optical absorption of NWA has been thoroughly analyzed by using finite-difference time-domain simulations. It is found that the NWA have superior absorption characteristic over thin-film due to the combined effects of intrinsic anti-reflection and efficient excitation of resonant modes. Optimized optical designs are obtained by maximizing the ultimate photocurrent under AM1.5G illumination. The photogeneration profiles under optimized conditions are incorporated into electrical modeling, in which the core-shell NWA solar cells exhibit 22.3% efficiency. © *2011 American Institute of Physics*. [doi:10.1063/1.3647847]

Semiconductor nanowire arrays (NWA) are a topic of intense research recently for photovoltaic applications due to their potential to realize low cost and high energy conversion efficiency solar cells. There are several advantages of such designs over conventional planar thin-film technologies that are noteworthy. By combining intrinsic anti-reflection and efficient absorption enhancement, nanowires (NWs) can achieve near perfect light absorption with reduced material use.[1–4] Meanwhile, NWs with coaxial p-n structure would enable a decoupling of the direction of light absorption from that of carrier collection.[5] While much attention has been focused on silicon based nanowire solar cells, gallium arsenide (GaAs) offers the potential of higher efficiency due to its high absorption coefficient, ideal bandgap, and the potential to implement advanced high efficiency schemes such as multi-junctions.[6–8]

To give clear guidelines for fabricating high-efficiency NWA solar cells, it is necessary to theoretically clarify the optoelectronic properties of such one dimensional systems. Recently, LaPierre has performed a comprehensive electrical simulation of the current-voltage characteristics of GaAs NWA solar cells by considering many practical problems.[9] In their study, conventional optical model based on Beer's law was applied to obtain the illuminated characteristics of NWA solar cells and the optimized devices with only 4.17% photovoltaic efficiency have been demonstrated for a volume filling ratio of 14.8%. However, due to their sub-wavelength dimensions, NWA have unique optical properties as compared with the conventional planar structure. It has been proved by many theoretical and experimental works that NWA with well-defined diameter, length, and filling ratio exhibit much higher absorption than their thin-film counterparts with the same thickness.[1–4,10,11] Hence, suitable simulation techniques with the correct consideration of the optical properties (denoted as light trapping effect) are needed to maximize light absorption efficiency within the structures and evaluate the performance of GaAs NWA solar cells.

In this paper, a coupled optoelectronic simulation is presented to investigate the potential photovoltaic efficiency of GaAs NWA solar cells. First, the influence of geometric parameters on the optical absorption of NWA has been thoroughly analyzed by using finite-difference time-domain (FDTD) simulations.[12] Second, to find an optimized geometry, the ultimate photocurrent was calculated to maximize the light absorption capability of the NWA in the solar spectrum. Finally, the photogeneration profiles under optimized conditions were incorporated into the electrical simulation, in which the core-shell NWA solar cells exhibit 22.3% efficiency. In addition, we compared our coupled model to Beer-Lambert absorption model. We conclude that the optimized geometry could absorbs 500% more photons per unit volume material, implying an effective optical concentration[11] in the NWA.

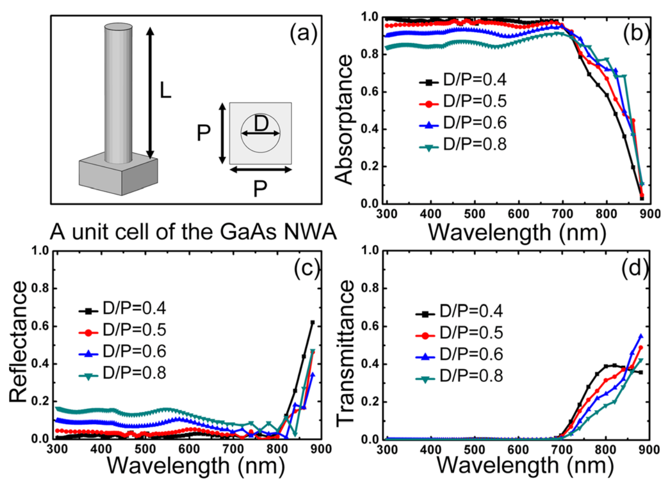

FIG. 1. (Color online) (a) Schematic drawing of the periodic GaAs NWs structure. (b) absorptance, (c) reflectance, and (d) transmittance of GaAs NWA with different fill factors.

a)Author to whom correspondence should be addressed. Electronic mail: xinhuali@issp.ac.cn.

Figure 1(a) shows the schematics of the simulation geometry under study. The system consists of a 200 nm thick GaAs substrate followed by vapor-liquid-solid grown GaAs NWs. The parameters of the structure are the period of the square lattice P, wire diameter D, and wire length L. By placing periodic boundary conditions, the simulations were carried out within this unit cell to model the periodic square-array wire structure. The nanowire length is fixed to 2 μm. Optical simulations were performed using the software package FDTD SOLUTIONS (Lumerical, Inc.).

Figures 1(b)–1(d) show the optical properties of GaAs NWA with different fill factors (D/P) at a fixed diameter of 120 nm. In the visible wavelength region ($\lambda < 700$ nm), from Figs. 1(c) and 1(d), it is obvious that the absorptance is uniquely determined by the reflectance as the transmittance spectra of the four cases are close to zero. This result can be explained by the high extinction coefficient of GaAs in these wavelengths. Meanwhile, as shown in Fig. 1(b), the absorptance decreases with increasing fill factors, which is mainly attributed to the increase in reflection at the top surface of the NWA [Fig. 1(c)]. In long wavelength regime ($\lambda > 700$ nm), due to the insufficient absorption of NWA layer, the incident light will reaches the NWA-substrate interface, resulting in a notable substrate light reflection and transmission [Figs. 1(c) and 1(d)]. The absorptance curve, shown in Fig. 1(b), tends to shift towards larger wavelengths as the fill factor is increased. From these results, we can conclude the optimal filling ratio is determined by the trade-off between the reflection enhancement and transmission suppression with the increase in D/P.

Figure 2(a) shows the optical characteristics of the GaAs NWA with different diameter at a fixed D/*P* of 0.5. The absorptance of a 2.2 μm GaAs thin-film is also plotted for comparison. From Fig. 2(a), the absorptance spectra for all NWAs are maintained above 90% in short wavelengths, which is much higher than the thin-film case due to the lower effective refraction index and thus lower reflection at the top of NWA. When increasing D from 60 to 180 nm, the absorption spectra show a significant increase in long wavelength regime. The results agree well with Gu *et al.*'s report, in which the guided-resonance modes are introduced to explain the dependence of absorption on diameter of periodic GaAs NWA.[13] Similar phenomena are also reported in Silicon NWA.[3,4,14] Due to the large refractive index contrast between the NWs and surrounding air, the electromagnetic field can be coupled efficiently into the NWs at resonances.[15] For small diameter GaAs NWA, with less supporting modes, most of the incident light cannot be guided into the NWs.

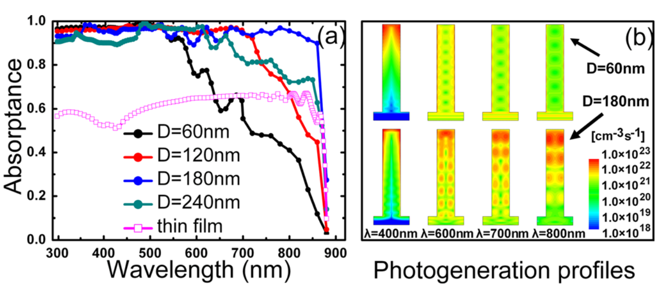

FIG. 2. (Color online) (a) Absorptance of NWA with different diameters. (b) Photogeneration profiles calculated by FDTD simulations.

The incident lights are absorbed in a single path through the NWA, thus the absorptance is much lower than thin-film at long wavelengths due to the low filling ratio. In comparison, NWs with larger diameters induce more supported modes, so that when these modes are well coupled and concentrated within the NWs, the absorption is greatly increased. As can be seen in Fig. 2(a), the absorptance values of the NWA with D = 180 nm remain high across the entire above-bandgap wavelengths. However, a further increase in diameter to 240 nm will lead to a decrease in absorption efficiency due to the increased reflection at the top surface of NWA and the insufficient field concentration at long wavelengths.

To gain a better understanding of the role of guided resonance in the light absorption enhancement, it is necessary to clarify the optical generation distribution around the NWs. Fig. 2(b) plots the vertical cross section of the photogeneration profiles within the NWs (D = 60, 180 nm and D/P = 0.5) under 1 $\mathrm{mW \cdot cm^{-2}}$ illumination at various wavelengths. At $\lambda = 400$ nm, the photogeneration rates are concentrated near the top and sides of the nanowire for both diameters. It is clear from the figure that only a small fraction of the incident wave was transmitted onto the substrate. This can be explained by the short absorption length of GaAs at this wavelength. At long wavelengths (e.g., 600 nm and above), for a NWA with 180 nm diameter, the photogeneration rates are concentrated to several lobes that form along the NWs, indicating strong guided modes confined inside the NWs. In contrast, for the case of D = 60 nm, the optical generation become more homogeneously spread over the NWs with longer wavelength. Clearly, the 180 nm diameter NWA induces much larger optical concentration than the 60 nm diameter one. These results are consistent with the absorptance spectra for both diameters shown in Fig. 2(a).

From the above discussion, it is clear that light absorption of the GaAs NWA is quite sensitive to structural parameters. By proper choice of diameter and fill factor, we find that the absorption of NWA is significantly enhanced. To determine the optimized geometric configuration, we calculate the ultimate photocurrent[11,14] for various diameters and fill factors, assuming that all photogenerated carriers can contributes to photocurrent: $J_{sc} = e/hc \int \lambda A(\lambda) I(\lambda) d\lambda$, where e is the elementary charge, h is Plank's constant, c is the speed of light, I(λ) is AM1.5G spectrum, and A(λ) is the absorptance of NWA. The ultimate photocurrent as a function of the fill factor for different diameters is shown in Fig. 3(a). A general increase of the photocurrent can be observed when increasing D from 60 to 180 nm. This trend arises from the excitation of guided resonance modes, as discussed above. As D is further increased to 220 nm, we observed a rapid drop in photocurrent especially for low D/P value. For a fill factor of 1 (the nanowires are packed side by side), the properties of NWA become comparable to that of the thin-film with an equivalent thickness (the calculated photocurrent of 2.2 μm thin-film is 20.24 $\mathrm{mA/cm^2}$, indicated by the purple star). From the figure, the maximum photocurrent of 29.83 $\mathrm{mA/cm^2}$ was observed for a diameter of 180 nm and D/P of 0.5. Under AM1.5G illumination, the upper limit of achievable photocurrent in GaAs photovoltaic device is 32.5 $\mathrm{mA/cm^2}$, implying that the optimized geometry can absorb more than 90% of the above-bandgap sunlight.

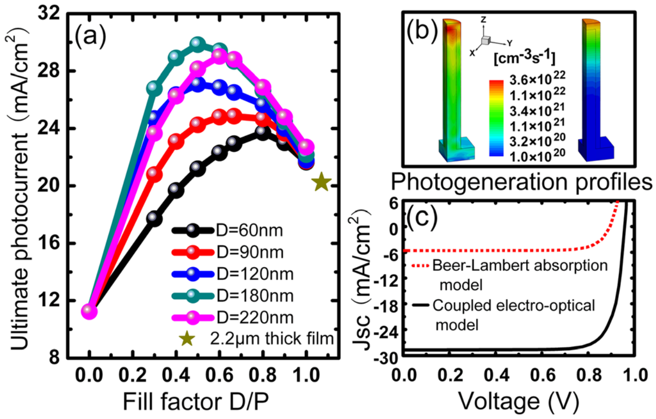

FIG. 3. (Color online) (a) Short-circuit current of GaAs NWA for various diameters at various fill factors. (b) Photogeneration profiles simulated by FDTD (left) and simple optical model (right) in a quarter of the core-shell NWA solar cells. (c) Current-voltage characteristics of NWA solar cells with different photogeneration models.

Further studies will focus on the investigation of the potential photovoltaic efficiency gains stemming from light trapping schemes. Previously simulated 3D photogeneration profiles are then incorporated into the electrical tool[16] to calculate the terminal current-voltage characteristics of GaAs core-shell p-n junction NWA solar cells. The AM1.5G spectrum is divided into 58 discrete wavelength intervals, from 310 to 880 nm. Based on the prementioned optical simulation output, the total optical generation under AM1.5G illumination can be modeled by superimposing the spectrally resolved single wavelength photogeneration rates. The photogeneration profile of the optimized NWA solar cells is shown in Fig. 3(b) (left). The structure is a 180 nm diameter nanowire with a p-type inner core and n-type outer shell of 30 nm thickness in radial direction, 100 nm thickness in axis direction. The ohmic contacts are added on the top of NW and back of the substrate to complete the device. A standard SRV of 10^7 cm/s was assumed for the contacts. Electrical simulation takes into account doping dependent mobility, Auger, radiative, and Shockly-Reed-Hall (SRH) recombination. SRH recombination lifetime was assumed to be 1 ns throughout the simulation. The nominal donor and acceptor doping concentration of the nanowire was $N_a = N_d = 5 \times 10^{18}\,cm^{-3}$.

The simulated current-voltage behavior of the GaAs NWA solar cells is shown in Fig. 3(c) (solid curve). The cell exhibits photovoltaic characteristics with an open-circuit voltage of 0.96 V, a short-circuit current (J_{sc}) of 28.7 mA/cm^2, and a photovoltaic efficiency of 22.3%. Considering the filling ratio of 0.196, our simulation indicates the occurrence of optical concentration and underlines the necessity of a wave optics approach. For illustration purposes only, we compared our coupled electro-optical model with a conventional optical model which based on the Beer's absorption law.[9,17,18] The resulting photogeneration profile is depicted in Fig. 3(b) (right). This model did not take into account the optical effects of the NWA, yielding an extremely low total-area short-circuit current of 5.6 mA/cm^2, which is depicted in Fig. 3(c) (dash curve). When the calculated current is normalized to the nanowire cross-sectional area rather than the substrate area, the conventional optical model give a current of 28.5 mA/cm^2. In contrast, our coupled model exhibits a short-circuit current of 146 mA/cm^2. The results imply that, the optimized NWA structure could absorb 500% more photons per unit volume material. Because of the incredible light trapping schemes, the incident sunlight can be efficiently coupled into a single nanowire, resulting in a high optical concentration.

In summary, simulations were used to evaluate the efficiency limits of GaAs nanowire array solar cells and determine the optical designs requirements for improving the efficiency. The study reveals that an optimized geometry design would absorb 90% of above-bandgap sunlight despite the low volume filling ratio. The combined optoelectronic simulation results reveal that optimization of optical geometry can lead to an attainable photovoltaic efficiency of 22%. The results presented here are expected to shed some light on the fabrication of high-efficiency GaAs nanowire array solar cells.

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