One-dimensional Electrical Modeling of Axial p-i-n Junction InP Nanowire Array Solar Cells

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***Abstract*—We demonstrate one-dimensional (1D) electrical modeling of InP nanowire array solar cells. This 1D modeling gives accurate description of the current voltage response even at high surface recombination velocity. The 1D electrical model decreases the simulation time by 3 orders of magnitude compared to a full three-dimensional (3D) model.**

***Index Terms*—Nanowire array, solar cell, electrical modeling, p-i-n junction.**

I. Introduction

Photovoltaics, which transforms the solar energy directly to electrical power, has been realized for example in semiconductor planar and nanostructure p-i-n junction solar cells [1, 2]. Nanostructures, such as nanowire arrays, can achieve comparable absorption as their counterpart planar structure, but at a lower material consumption [3, 4]. Due to a broad band absorption, nanowire arrays have attracted attention in both experimental [2, 5–7] and theoretical studies [8–11].

In simulations, the computational time is an important factor that tends to limit the possibilities for optimizing device design. For instance, full 3D opto-electrical simulation of a single GaAs nanowire with diameter of 400 nm and length of 2 micrometers took 500 core hours [10].

In this study, we develop and test a 1D electrical model for an axial p-i-n junction nanowire array solar cell to reduce the simulation time. We express the surface recombination as an effective bulk recombination and transformed the 3D optical generation rate into a 1D profile. In this way, we obtain good agreement between 1D and 3D drift diffusion modeling under both low and high surface recombination velocity. Such 1D electrical modeling reduce the computation time by 3 orders of magnitude.

II. Method description

Our nanowire array solar cell modeling consists of optics and electrical modeling, which are both performed in Comsol Multiphysics. First, we solve the 3D Maxwell equations and calculate the optical generation rate as a function of spatial position by

$$G(\boldsymbol{r}) = \int_{280nm}^{\lambda_{bandgap}} \frac{A_e(\boldsymbol{r}, \lambda)}{E_{photon}} d\lambda, \tag{1}$$

Here A_e is the absorbed energy density at position $\boldsymbol{r}$ for incident light with wavelength λ.

With this optical generation function, we carry out a 3D electrical modeling by solving drift-diffusion equations [12]. In the bulk of the nanowire, we include Shockley-Read-Hall(SRH), radiative and Auger recombination. Surface recombination is included at the surface of nanowire through the surface recombination velocity V_{sr} [11, 12].

For the 1D electrical modeling, we average the 3D optical generation rate into an average value in cross section of the nanowire and solve 1D drift diffusion equations for the resulting 1D, axially dependent, photogeneration profile. SRH, radiative and Auger recombination with same recombination parameters as in the 3D model are used in the 1D model. In addition, we transferred the surface recombination to a SRH-like bulk recombination with an effective recombination parameter:

$$A_{eff} = \beta_1^2 \frac{D}{R^2}. \tag{2}$$

where β_m is defined by the solution of the following Bessel transcendental equation

$$\beta J_1(\beta) = \frac{R V_{sr}}{D} J_0(\beta), \tag{3}$$

Here $J_{0/1}$ is the zeroth/first order Bessel function of the first kind, R is the radius of nanowire and D is the diffusion constant. The solution of equation 3 gives a list of $\beta_m(m = 1, 2, ...)$ which we order in increasing order of β_m.

Alternatively, we can write A_{eff} as a fitting equation:

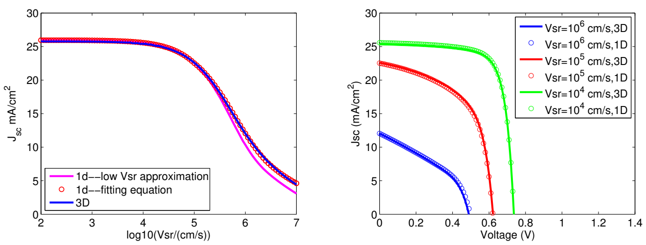
$$A_{eff} = A_0 \frac{V_{sr}}{R} \tag{4}$$

$$A_0 = min[\frac{1}{2} log_{10}(\frac{V_0}{V_{sr}}), 2], \tag{5}$$

where V_0 is a parameter that depends on the mobility of carrier and the nanowire radius. This parameter can be calculated either through extraction from Eq. 2 or through numerical fitting between 1D and 3D modeling. For InP nanowires of 90 nm in radius and 5400 (200) $cm^2V^{-1}s^{-1}$ in mobility of electrons (holes), we suggest the value $V_0 = 10^7 m/s$. For varying nanowire radius and surface recombination velocity, this parameter can be calculated by the following fitting equations:

$$V_0 = (\frac{R}{90nm})^{-log_2(10)} \frac{\mu}{\mu_{InP}} \times 10^7 m/s, \tag{6}$$

III. Results and discussions



(a) (b)

Fig. 1. InP nanowire array with diameter of 180 nm, pitch of 330 nm and length of 1400nm without contact layer under AM 1.5D spectrum. (a) Short-circuit current of an InP nanowire array solar cell as a function of surface recombination velocities. (b) Voltage-Current response of nanowire array solar cells with different surface recombination velocity in both 1D and 3D modeling.

In Figure 1 (a), we plot the current as a function of surface recombination velocity. We find that 3D and 1D modeling results agree well. The error in the current density in the approximate 1D modeling is less than 0.2 mA/cm^2 for surface recombination velocity up to 10^7 cm/s. We also show the result from previous study which is valid at low V_{sr} with the assumption of $V_0 = 2$ [13]. Then, the error in short-circuit current density increases with increasing V_{sr} beyond $10^5 cm/s$ with an error of 1.4 mA/cm^2 at 10^7 cm/s.

We note that the short-circuit current density starts to drop at a surface recombination velocity of about $10^4 cm/s$. At this surface recombination velocity, the corresponding recombination parameter A_{eff} is $2.8 \times 10^9 s^{-1}$ and it indicates a surface recombination carrier life time of 360 picoseconds. The corresponding hole diffusion length of InP is 430 nm and electron diffusion length is 2200 nm. Thus, when the surface recombination velocity starts to affect the short-circuit current, the electron and hole diffusion lengths are comparable to the nanowire length, 1400 nm.

In Figure 1(b), we further illustrate the accuracy of 1D modeling by current-voltage response. We calculated up to $V_{sr} = 10^6$ cm/s which is the level of unpassivated GaAs. The error in V_{oc}, compared to 3D modeling, is less than 0.01 V and in fill factor less than one percent. These results illustrate the applicability of 1D modeling for electrical analysis of p-i-n junction nanowires.

Thus, with the approximation in Eqs. 4 and 5 for the surface recombination in the 1D model, the simulation time decreases by 3 orders of magnitude with a similar accuracy as in the 3D modeling.

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References

1 M. Green, K. Emery, Y. Hishikawa, W. Warta, E. Dunlop, D. Levi and A. Ho-Baillie, 'Solar cell efficiency tables (version 49)', Prog. Photovolt. Res. Appl., vol. 25, pp. 3-13, November 2016.

2 I. berg, G. Vescovi, D. Asoli, U. Naseem, J. Gilboy, C. Sundvall, A. Dahlgren, K. Svensson, N. Anttu, M. Bjrk and L. Samuelson, 'A GaAs Nanowire Array Solar Cell With 15.3 Efficiency at 1 Sun', IEEE J. Photovolt., vol. 6, pp. 185-190, October 2015.

3 L. Hu and G. Chen, 'Analysis of optical absorption in silicon nanowire arrays for photovoltaic applications', Nano Lett., vol. 11, pp. 3249-3252, October 2007.

4 M. Kelzenberg, S. Boettcher, J. Petykiewicz, D. Turner-Evans, M. Putnam, E. Warren, J. Spurgeon, R. Briggs, N. Lewis and H. Atwater, 'Enhanced absorption and carrier collection in Si wire arrays for photovoltaic applications', Nat. Mater. vol. 9, pp. 239-244, February 2010.

5 G. Mariani, Z. Zhou, A. Scofield and D. Huffaker, 'Direct-Bandgap Epitaxial CoreMultishell Nanopillar Photovoltaics Featuring Subwavelength Optical Concentrators', Nano Lett., vol. 13, pp. 1632-1637, March 2013.

6 J.Wallentin, N. Anttu, D. Asoli, M. Huffman, I. berg, M. Magnusson, G. Siefer, P. Fuss-Kailuweit, F. Dimroth, B. Witzigmann, H. Xu, L. Samuelson, K. Deppert and M. Borgstrm, Science, vol. 339, pp. 1057-1060, March, 2013.

7 M. Yao, S. Cong, S. Arab, N. Huang, M. Povinelli, S. Cronin, P. Dapkus and C. Zhou, Nano Lett., vol. 15, pp.7217-7224, October 2015.

8 N. Anttu and H. Xu, 'Efficient light management in vertical nanowire arrays for photovoltaics', Opt. Express, vol. 21, pp. A558-A575, May 2013.

9 B. Wang and P. Leu, 'Tunable and selective resonant absorption in vertical nanowires', Opt. Lett., vol. 37, pp. 3756-3758, September 2012.

10 X. Wang, M Khan, M. Lundstrom and P. Bermel, 'Performance-limiting factors for GaAs-based single nanowire photovoltaics', Opt. Express, vol. 22, pp. A344-A358, February 2014.

11 S. Yu, F. Roemer and B. Witzigmann, 'Analysis of surface recombination in nanowire array solar cells', J. Photon. ENERGY, vol. 2 pp. 028002-1-9, September 2012.

12 Y. Chen, P. Kivisaari, M. Pistol and N. Anttu, 'Optimization of the short-circuit current in an InP nanowire array solar cell through opto-electronic modeling', Nanotechnology, vol. 27 pp. 435404-1-9, September 2016.

13 Y. Dan, K. Seo, K. Takei, J. Meza, A. Javey and K. Crozier, 'Dramatic Reduction of Surface Recombination by in Situ Surface Passivation of Silicon Nanowires', Nano Lett., vol. 11 pp. 2527-2532, May 2011.