Numerical simulation study of graphene silicon solar cell with boron diffusion layer

Yawei Kuang^{1,2,3}, Yushen Liu¹, Xifeng Yang¹, Debao Zhang¹, Yulong Ma¹, Xuekun Hong¹, Zhenguang Shao¹, Jinfu Feng¹

 School of Physics and Electronic Engineering, Changshu Institute of Technology, Changshu, 215500, China
Jiangsu Province Cultivation Base for State Key Laboratory of Photovoltaic Science and Technology, Changzhou University, Changzhou, 213164, China
Centre for optical and electromagnetic research, Zhejiang University, Hangzhou, 310058, China

Abstract: Two dimensional model of graphene silicon heterojunction solar cell with an boron doped surface layer is structured using Silvaco TCAD tools by accurate control of diffusion process. The introduction of inverse doped layer obviously improved the efficiency of heterojunction photovoltaic cell.

1. Introduction

Graphene semiconductor schottky solar cell has been received more attention since it could be fabricated at room temperature which shows great potential in light harvesting and conversion application with the advantage of low cost, facile processibility and environmental amity[1,2]. In this structure graphene film not only serves as a transparent electrode for light transmission but also as an active layer for electron/hole separation and carrier transporting medium[3-6]. A mount of experimental work has been done to explore graphene semiconductor junction solar cells while the theoretical simulation on this topic is not enough[7,8].

In this paper, simulation of graphene silicon heterojunction solar cells with a thin inverse doped layer is carried out using Silvaco TCAD tools. The simulation program solves the Poisson, the continuity and the current density equations by using a standard procedure for amorphous materials including the continuous density of state model, schottky and auger recombination mechanisms. The dependence of these parameters of optical parameters with the photon energy has been included, taking into account the energy of diffusion technique, doping concentration and their effect on cell efficiency.

2. Modeling

As mentioned above, Fig.1 shows the cross section of the graphene semiconductor junction solar cell simulated using Technology Computer Aided Design (TCAD) tools. The device consists with three regions which are semiconductor substrate such as silicon, SiO₂ window layer and graphene layer from bottom to the top area respectively. Here the graphene layer with a thickness of 10nm was coated onto the semiconductor substrate with 1 μ m×12 μ m oxide window which could decrease the surface recombination.



Fig.1 Cross section of the graphene silicon junction solar cell with inverse doped surface layer

As can be seen from this graphs, a thin boron doped layer (1e16) located at $0.1 \mu m$ near surface is accurately produced by high temperature diffusion which indicate that the parameters related with the simulation have been appropriately chosen.

3. Figures and tables

3.1 Parameters used in the simulation Table.1 Baseline input parameters used in the simulation

Parameter	Description	Value	
Eg	Silicon band gap	1.08 ev	
Т	Temperature	300K	
ф _G	Graphene work	4.8 ev	
_	function		
Nc	Effective density of	2.8e19 cm ⁻³	
	states in silicon CB		
N _v	Effective density of	1.04e19 cm ⁻³	
	states in silicon VB		
χ	Silicon electron	4.17 ev	
	affinity		
phos.c	n-type concentration	1e12 cm ⁻³	
	of silicon		
L	Thickness of	10µm	
	silicon substrate		

3.2 Hole current density distribution



Fig.2 Hole current density distribution at Y direction of the device: (a) graphene n-type silicon solar cell (b) graphene n-type silicon solar cell with boron doped layer

3.3 I-V performance of the cell with boron doped



Fig.3 IQE of the device under AM1.5 illumination

The boron doped layer yields an obviously increased response at all the range which indicates that the carriers generated in the silicon crystal are collected much more effectively into the heterojunction. Meanwhile the IV curve shows that the increase of open voltage results in an obvious increase of efficiency, as shown in Fig.3 and Fig.4.



Fig.4 IV characteristics of the device under AM1.5 illumination

Table.2 Simulated I-V performance of the graphene silicon solar cell under AM1.5 illumination

Structur	Jsc(mA/	Voc(V	FF(%)	η(%)
e	cm ²))		
Without	10 446	0 1 4 0	43 34	1 936
inverse	10.110	0.110	15.51	1.750
doped layer				
With t	10 684	0 1 6 4	46 56	2 4 8 2
Boron	10.004	0.104	40.50	2.402
doped layer				
1e16 cm ⁻³				

4. Acknowledgements

The project was supported by research fund of Jiangsu Province Cultivation Base for State Key Laboratory of Photovoltaic Science and Technology (No. SKLPSTKF201505), National Natural Science Foundation of China (No.61306122, No.61404012, No.11347021). Thanks are also given to The Shanghai Institute of Technical Physics (SITP) for software support.

5. References

[1] Xinming Li, Hongwei Zhu, Dehai Wu,et al, "Graphene on silicon schottky junction solar cells," Adv.Mater 22,2743-2748 (2010)

[2] YF Li, W Yang, LQ Zhang,et al, "Schottky junction solar cells based on graphene with different numbers of layers," Appl Phys Lett 104, 043903 (2014)

[3] L Lancellotti et al, "Graphene applications in schottky battier solar cells," Thin Solid Films 522, 390-394 (2012)

[4] Dhiraj Sinha and Ji Ung Lee, "Ideal graphene silicon schottky junction diodes," Nano Lett 14, 4660-4664 (2014)

[5] Xie C, Lv P, Nie B, et al. Monolayer graphene film/silicon nanowire array Schottky junction solar cells[J]. Applied Physics Letters, 2011, 99(13): 133113.

[6] Miao J, Hu W, Guo N, et al. High - Responsivity Graphene/InAs Nanowire Heterojunction Near - Infrared Photodetectors with Distinct Photocurrent On/Off Ratios[J]. small, 2015, 11(8): 936-942.

[7] Kuang Y, Liu Y, Ma Y, et al. Theoretical Study on Graphene Silicon Heterojunction Solar Cell[J]. Journal of Nanoelectronics and Optoelectronics, 2015, 10(5): 611-615.

[8] Sanjay KB, Pramila M, Omkar J, et al, "Theoretical simulation of photovoltaic response of graphene on semiconductors," Appl Phys A 111,1159-1163 (2013)