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Numerical simulation of planar BaSi₂ based Schottky junction solar cells toward high efficiency

Lian Chen^a, Hai Chen^a, Quanrong Deng^{a,b*}, Geming Wang^a, Shenggao Wang^a

^a Hubei Key Laboratory of Plasma Chemistry and Advanced Materials, Wuhan Institute of Technology, Wuhan, 430205, China

^b State Centre for International Cooperation on Designer Low-Carbon and Environmental Materials, Zhengzhou University, Zhengzhou 450001, China

Abstract

The theoretical and experimental studies on BaSi₂/Si heterojunction solar cells have demonstrated the great potential in utilization of BaSi₂ material as light absorption layer for developing high efficiency solar cells with low cost. In addition to BaSi₂/Si heterojunction solar cells, BaSi₂ based Schottky junction solar cells could also be achieved by coupling n-type or p-type BaSi₂ with suitable metal electrode. In this work, BaSi₂ based Schottky junction solar cells were simulated with the program AMPS (analysis of microelectronic and photonic structures)-1D in order to thoroughly understand the mechanism for further improvement in conversion efficiency. Simulation results demonstrated that a simpler structure of metal/n-BaSi₂ Schottky junction solar cell with thickness of 2000 nm can reach high conversion efficiency up to 24.12% and 25.28% for $N_D=1\times10^{15}\text{ cm}^{-3}$ and $N_D=1\times10^{18}\text{ cm}^{-3}$ respectively, being comparable to BaSi₂/Si heterojunction solar cell. Contact barrier height, illumination condition, as well as defect level of metal/n-BaSi₂ Schottky junction solar cell were also identified to significantly influence the device performance.

Keywords: Schottky junction solar cells; BaSi₂; AMPS; Device simulation

1. Introduction

Solar energy harvesting and utilization has been proven to be one of the most feasible solutions to resolve worldwide energy crisis and associated environmental problems brought by fossil fuel. In order to achieve cost-effective photovoltaic systems instead of crystal Si solar cells, researchers around the world have begun to search for new semiconducting materials with high optical absorption coefficients, suitable band gap and photoelectronic properties. Semiconducting material BaSi₂ is recognized as a potential alternative due to its high absorption coefficient over $3\times10^4\text{ cm}^{-1}$ at 1.5 eV as compared with c-Si [1,2,3,4], and suitable band gap of 1.3 eV [3,5] close to the optimum band gap of 1.4 eV to match the spectrum of solar illumination [5,6]. Besides, BaSi₂ is non-toxic and rich in the earth's crust, together with its narrow band gap and high absorption coefficient, making it a promising candidate for low cost and environmental friendly thin film solar cells. Orthorhombic crystal structure BaSi₂ thin films have been successively fabricated on Si substrates using molecular beam epitaxy (MBE) [7,8,9,10], radio-frequency magnetron sputtering [11] and vacuum evaporation [12]. The undoped BaSi₂ is an n-type semiconductor with electron concentration of approximately $5\times10^{15}\text{ cm}^{-3}$ [5, 13], long minority-carrier diffusion length reaching 10 μm and long lifetime greater than 10 μs [14,15,16]. Through Sb, Ga or Cu doping, the electron concentration of n-type BaSi₂ could reach $10^{16}\sim10^{20}$

* Corresponding author. E-mail address: quanrongdeng@wit.edu.cn

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