

Simulation of photovoltaic efficiency of a tandem solar cell on Si with GaN nanowires as an emitter layer

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Abstract. Modeling of photovoltaic properties of multi-junction solar cells integrated on a Si substrate with an array of GaN nanowires as a top emitter has been carried out. Very good antireflection properties of the structure are demonstrated theoretically: the calculated reflectance is lower than 3% for both GaN nanowires/Si and GaN nanowires on GaPN/Si cells. According to our simulations, basic GaN nanowires on Si cell with optimised parameters (doping and NWs morphology) provides energy conversion efficiency of 20%. The approach demonstrates high potential of the GaPN(As)-based multi-junction lattice matched with Si solar cells using an array of GaN nanowires as a top emitter.

1. Introduction

The great interest confined nowadays to the studies in the field of photovoltaics is mainly justified by the inexhaustibility of the solar energy source. The other important reasons for searching the new ways of electrical energy generation are the growing energy consumption firstly caused by the very fast global computing power increase and the irreversible negative impact of hydrocarbons burning on global ecology and their upcoming depletion. That is why researches in the field of sun light energy conversion aimed at development of efficient and green solar cells are considered very important in modern science.

Our letter is dedicated to the integration of lattice-matched heterostructures on a Si substrate with GaN nanowires (NWs) in order to obtain a multi-junction solar cell (SC). We demonstrate theoretically that such a structure possesses several benefits. Firstly, among them we highlight the high energy conversion efficiency. Synthesis of NWs provides very good antireflection and carrier transport properties and allows formation of the wide band gap window. As a side effect, during growth of the NWs the top surface of the SC is being passivated.

It is well known that III-V semiconductor heterostructures provide great optical and electronic properties [1]. That is why integration of Si technology with epitaxial III-V structures is being pursued for the long time. The bottleneck of this problem is a large lattice mismatch between Si and conventional optical III-V materials [2]. NWs seem to be one of the possibilities on this way because



they can be grown epitaxially on mismatched substrates due to a developed surface area [3]. Therefore, quasi one-dimensional semiconductor NWs are one of the most promising building blocks for future nano- and optoelectronic devices [4]. It is worth mentioning that NW morphology and high crystal quality should greatly affect recombination losses as compared to the polycrystalline materials [5]. In our study we have chosen GaN as the material for NWs because of its wide band gap, a high carrier mobility and a large band gap difference with Si [1,2,6].

Recently it's been reported that GaPN(As) materials allow variation of the band gap with simultaneous variation of the lattice constant [7-8] in a wide range and can be lattice-matched with Si. Using the latter materials we can produce a tandem SC with multiple junctions grown epitaxially on a Si substrate with a top emitter formed with an array of GaN NWs. A very important for our investigation property of GaN NWs as compared to other III-V materials (like GaAs, GaP) is the possibility of n-type doping of these structures up to high doping levels. This property together with a relatively high electron affinity (~ 4.1 eV) permits formation of high quality ohmic contacts with metals or transparent conductive coatings as well as good carrier transport. On the other hand, a big gap in the valence band occurs at the interface between GaN and conventional SC materials of Si, GaAs and GaP. Formation of the gap provides good restriction for positive charge carriers' transport.

The method of GaN NWs growth in a molecular-beam epitaxy machine includes deposition of a mask AlN layer on top of the SC base. This layer implements passivation of the SC surface and restricts electrical transport for carriers of both signs along the area free of NWs.

2. Modelling

Simulations of photovoltaic properties of a basic type of the multi-junction SC containing GaN NWs synthesized on a Si substrate have been carried out. In our modeling we considered different morphologies of NWs and doping levels of both semiconductors. In figure 1 you can find the schematic image of the investigated SC and its band diagram. A thin dielectric layer (e.g., SiO₂, polymethyl methacrylate (PMMA) or SU-8) is assumed to cover an unwanted 2D GaN layer (formation of this layer is a side effect of NW growth). We proposed use of conductive transparent indium tin oxide (ITO) or Al-doped zinc oxide (AZO) coating atop NWs in order to obtain good electrical contact. Ohmic losses in the top contact have been neglected.

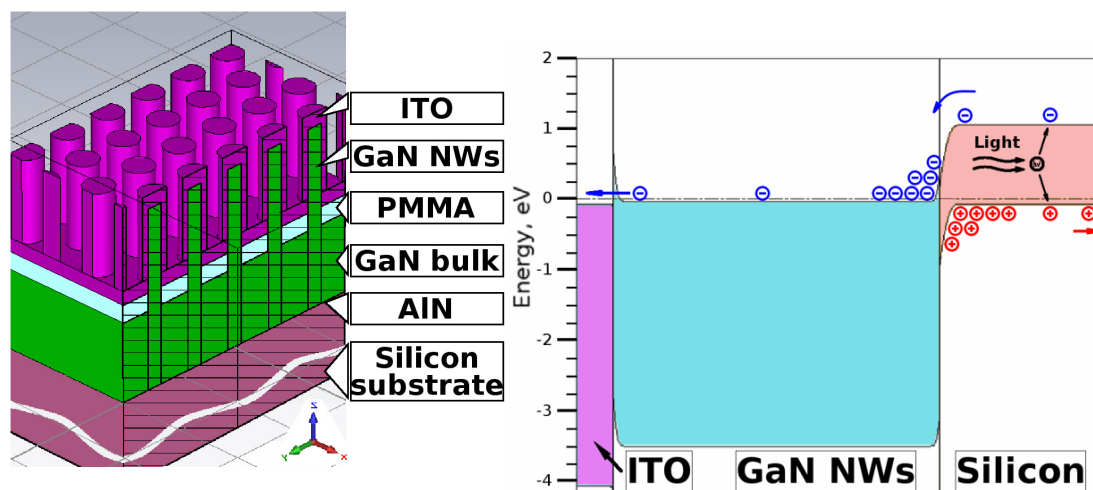


Figure 1. The schematic image of GaN/Si SC and its band diagram

In the first part of our modeling, we studied reflection properties of the structure. We have carried out the variation of nanowire diameters, lengths and surface density in a wide range in order to find the optimal configuration corresponding to minimum reflectance losses. For this purpose, we developed a 3D model of the cell in the “CST Microwave” software package. The model of a NWs

array was introduced with cylindrical nanostructures having the same dimensions with a regular hexagonal position on the substrate surface. The investigated SC model includes a p-type Si substrate, a bulk GaN layer, n-type GaN nanowires, a dielectric layer of PMMA and a top contact in form of ITO layer. The bulk GaN layer thickness was considered half of the GaN NWs length. The dielectric and ITO layer thicknesses were taken as 50 nm and 100 nm, respectively.

We have calculated the model SC integral reflectance over AM1.5D spectrum over a wide range of geometrical parameters. The following steps were taken during the simulations: first, we took arbitrary values of the NWs radius and length and for these values we obtained the optimal distance between NWs (or NWs surface density) corresponding to the lowest value of the structure reflectance; second, we took the same arbitrary value of the NWs length and the optimal wire to wire distance and obtained the optimal NW radius; on the third step by using the optimal values of NW surface density and radius calculated previously, we obtained the optimal length of NWs. We repeated the described sequence, using the estimated parameters until their values converge. By using this calculation technique, we obtained the following geometrical parameters corresponding to the lowest reflectance: wire to wire distance is 540 nm, radius is 120 nm, and length is 1300 nm. According to our simulations, such an array will provide the integral reflectance value of only 3%, which is an order of magnitude less than the reflectance of pure Si. In figure 2 one can see the dependence of antireflection properties on the distance (or period) between NWs at different values of the NWs radius for the fixed optimal NWs length of 1300 nm.

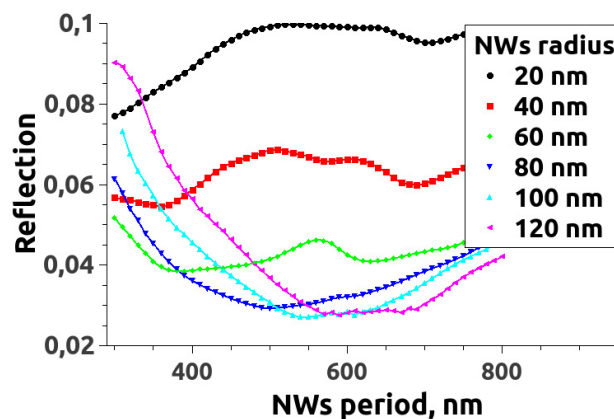


Figure 2. Dependence of antireflection properties on the period and NWs radius for the fixed NWs length

In the second part of our modeling, we studied semiconductor properties of the modeled SC. The optimal doping levels of both a Si substrate and GaN NWs corresponding to the maximum solar energy conversion efficiency were obtained. For this purpose, the Newton method with Fermi statistics was used. We assumed NWs to be defect-free and neglected the influence of the surface states at the sidewalls. The latter allowed us to simplify the problem solution to one-dimensional calculations. In our modeling we substituted the NWs array with a GaN layer which thickness has a value of a minimum travel distance for photogenerated carriers. This is an effective spacing between a Si substrate and an ITO layer which equals the GaN 3D layer thickness plus the dielectric thicknesses multiplied by the ratio of the total SC area to the area covered with NWs. We used the following latter values: the GaN layer and PMMA total thickness equals 700 nm and the area ratio is 8.

In figure 3 (a) one can find the curves representing the calculated dependencies of cell efficiency on the substrate doping level at different levels of NW doping. These graphs possess maxima at the Si acceptor concentration of around $6 \times 10^{17} \text{ cm}^{-3}$. Further increase of the substrate doping level leads to a decrease of both the depletion region and carrier mobility in Si which causes a fall in SC efficiency. The maximum estimated efficiency reaches 20%.

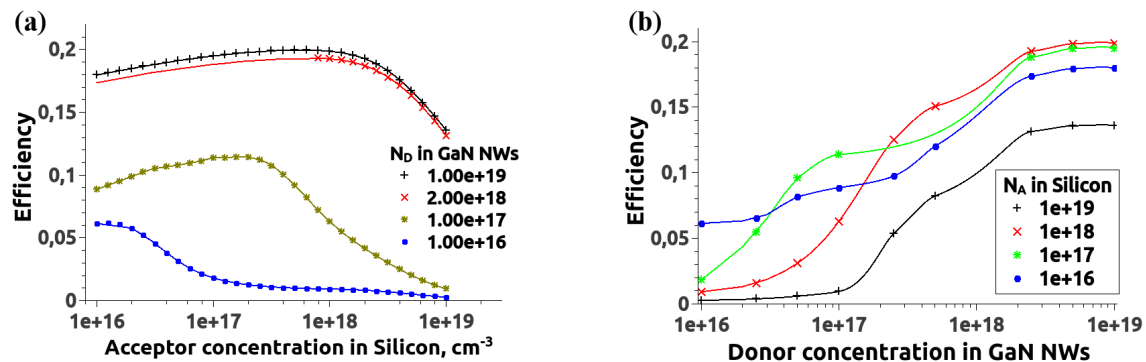


Figure 3. The calculated dependencies of cell efficiency on the substrate (a) and NWs (b) doping levels

In figure 3 (b) one can find the curves representing the calculated dependencies of cell efficiency on the NWs doping level at different levels of the substrate doping. Analysis of the graphs shows that at the donor concentration of around $5\text{e}+18 \text{ cm}^{-3}$ the SC efficiency tends to saturation and further increase of NWs doping would not result in a significant rise in efficiency. At the optimal doping level, VOC is 0.73 V, ISC is 34 mA/cm^2 and fill factor (FF) is 85%.

3. Conclusion

Simulations of the solar cell based on the GaN NWs/Si heterostructure have been carried out. It has been demonstrated theoretically that if the doping levels of Si and GaN NWs have the values of $6\text{e}+17$ and $5\text{e}+18 \text{ cm}^{-3}$, respectively, and the distance between NWs, their diameter and length are 540 nm, 100 nm and 1300 nm, respectively, then reflectance of the solar cell is only 3% while its energy conversion efficiency reaches 20%.

The proposed design of a solar cell represents the basic type of a tandem cell that includes a NW array as an emitter of the top junction. The use of GaN NWs allows to improve light absorption and electrical transport properties of the SC. This approach opens new perspectives for the studies of multi-junction solar cells based on GaPN(As) optical materials lattice-matched to Si substrates.

Acknowledgements

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