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HIGHLY DOPED NANOWIRE ARRAY FOR USE IN HYBRID SILICON/POLYMER JUNCTION SOLAR CELLS.

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The use of silicon nanowire arrays (SiNWA) and conjugated polymers to form organic-inorganic hybrid structures have emerged as a promising technology in the solar cell industry. In this approach the nanostructured silicon offers a large surface area and a direct path for charge transport for increased efficiency while the conducting polymer layer offers a cheap alternative to epitaxial re-growth techniques. We propose a Si nanowire array (SiNWA) pn-junction where the space between the nanowires is filled with p-type conjugated polymer (see Fig.1). The main carrier extraction path is via the Si while the beneficial exciton generation region is also along the length of the NWs.

We have simulated this structure based on the commercial simulation suite TCAD Sentaurus. The simulator solves the drift-diffusion transport equations coupled to the Poisson equation. However, for organic materials, the electrical conduction process is different from crystal lattice semiconductors such as silicon. As such, the physical models used for the simulation process were modified to account for this [2]. Firstly, Poole-Frenkel mobility model – dependent on the electric field and temperature – is used to model the hopping mechanism of carrier transport. Furthermore, to give a better representation of the effective density of states for both carrier types, a Gaussian density-of-states (DOS) has been introduced for the organic regions of the structure. To model the optics (e.g. generation, diffusion, recombination, and radiative decay of singlet excitons) in organic semiconductors, the singlet exciton equation is also incorporated into the simulation. During the process simulation, the device geometry was specified, including an impurity diffusion model and material growth during thermal annealing. Furthermore, the material parameters for poly(3-hexythiophene) (P3HT) were added. Typical values of χ = 3.2 eV and E_g = 1.80 eV are chosen for the energy levels, whilst the effective density of states is set to 10^{21} cm^{-3} and carrier concentration to $10^{16}cm^{-3}$ [3].

We explore different designs by changing the filling ratio and doping profile of the SiNWA and investigate their impact on optical and IV characteristics. A 3D model of the simulated device is given in Fig. 2.

The device is fabricated using a single step metal assisted chemical etch process [1] to form the nanowire array (see Fig 3). The NWA is filled with P3HT – a p-type conjugated polymer. Indium Tin Oxide (ITO) and Titanium (Ti) are used for the front and back contact respectively. Optical and electrical characterization is carried out on the fabricated devices.

References

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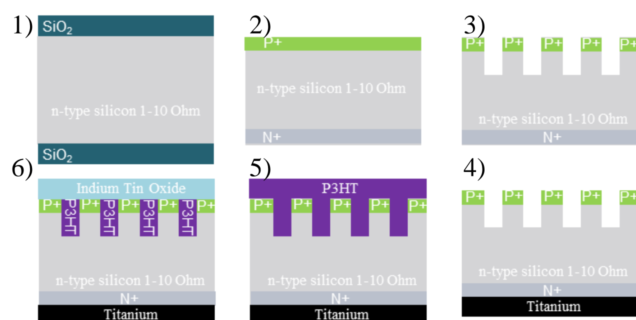

Figure 1: Process Flow
1) Thermal oxidation of the silicon wafer. 2) spin-on-doping and diffusion. 3) metal assisted chemical etching [1] of the pn NW junctions. 4) Ti back contact. 5) P3HT filling. 6) Plasma etching to remove the top layer of polymer, followed by an ITO contact.

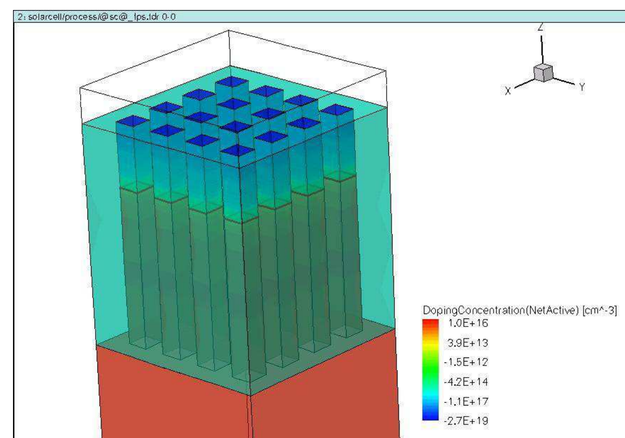

Figure 2: Device Structure on Sentaurus
The process simulation of the device. Simulations include oxidation and resist deposition, as well as thermal annealing, masking, and etching.

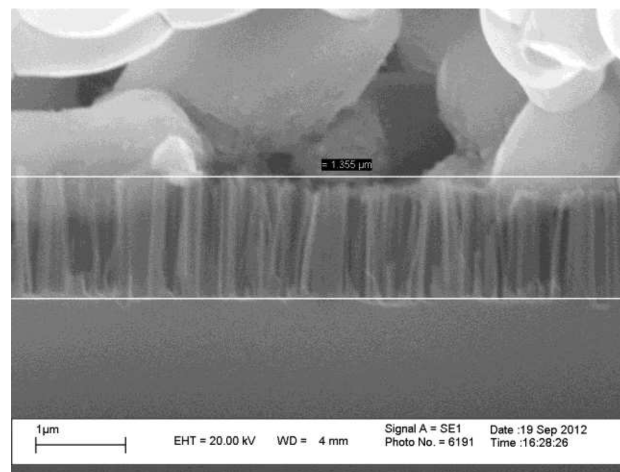

Figure 3: 1.3um length SiNWA
Scanning electron micrograph of a SiNWA etched using a single step etch process in $AgN0_3$/HF solution. The Ag dendrites can be seen deposited above – this is removed by using nitric acid.