

# Numerical simulation of GaAs nanowires with a p-n core-shell structure

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Nanowire p-n core-shell structures have many interesting properties and potential applications, such as sensors, solar cells, and transistors. However, the nanowire dimensions present a challenge to designing pn core-shell structures without a fully, or partially, depleted core and shell layer. When dealing with nanowire carrier transport, surface recombination is also very important due to the large surface to volume ratio. The surface recombination will degrade the current transport when a nanowire is used as a diode, or influence the sensitivity of the nanowire as a sensor, or reduce the electrical conversion efficiency of a nanowire solar cell. Therefore, it is important to consider the surface of the nanowire when designing a pn-junction core-shell nanowire device.

A numerical model is presented to determine the electrical properties of a core-shell nanowire pn-junction. The model is based on a finite element analysis of nanowires that have been grown by molecular beam epitaxy using the vapour-liquid-solid growth technique. As our research has found, the wire geometry is changed when the growth duration of n-doped core to the p-doped shell is altered. In the growth of these nanowires the n-dopant used is Te and the p-dopant is Be. The geometries of the core, the shell, and the film that grows between the wires, for use in the model, were determined by scanning electron microscopy.

The model solves the Poisson equation and the continuity equations for both the electrons and holes. In addition, both drift and diffusion of the carriers are taken into account. We assume a surface mid-gap pinning of the Fermi-level and include bulk and surface recombination. It will be shown that surface depletion, the p-doped shell thickness, and, most interesting, the p-doped film all contribute to the potential of the n-doped core and p-doped shell.

A comparison of the simulation between four samples with different core thickness, core height, shell thickness, and shell height will be shown, and compared against similar structures from experimental data. It will be shown how the p-doped film contributes to the potential variation of the nanowire. As well, an optimized geometry for a nanowire photovoltaic device will be presented based on simulated IV curves when generated electron hole pairs are created in the nanowire structure. The optimized nanowire geometry will be based on a structure that can be realistically grown using the VLS growth method. The optimized core and shell geometry will take into account the thickness and height that can be controlled by the growth temperature and the use of the Te and Be dopant species.

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