Absorption in and scattering from single horizontal Au-contacted InAs/InP heterostructure nanowires

Steven Limpert, Stephen Bremner, Gavin Conibeer School of Photovoltaic and Renewable Energy Eng. University of New South Wales Sydney, Australia Steven.Limpert@unsw.edu.au

Abstract—Finite element modelling (FEM) is used to show that the addition of Au contacts to a single horizontal InAs/InP heterostructure nanowire substantially alters the nanowire's optical properties in comparison to the uncontacted case. It is found that the addition of contacts can increase absorption efficiency, decrease scattering efficiency and shift the location of absorption within the nanowire. Localized surface plasmon resonances are found to develop at nanowire/contact interfaces at infrared wavelengths and contribute to the alteration of the optical response of the nanowire.

Keywords—nanowires; photonics; plasmonics; absorption efficiency

I. INTRODUCTION

Due to their quasi-1D geometry, semiconductor nanowires are a unique platform for optoelectronic device development. Their high aspect ratio and subwavelength dimensions give rise to optical effects not present in other geometries. For this reason, the optical properties of semiconductor nanowires have been a topic of intense study and many novel variants on conventional optoelectronic devices have been made using semiconductor nanowires. The polarization dependence of absorption by single horizontal InP nanowires has been studied by photoluminescence [1]. The absorption cross-section dependence on Ge nanowire radius has been studied using photoconductive detectors [2]. Vertical array nanowire p-i-n diode solar cells have been shown to exceed the ray optics limit [3] and filter-free color-imaging sensors have been constructed from vertical nanowire arrays of p-i-n diode nanowires of different radii [4].

The theoretical studies executed in support of and in response to such experimental demonstrations have been extensive and have explored the absorption and scattering properties of both single horizontal nanowires and vertical nanowire arrays. The effects of radius, length, inter-nanowire spacing [5], [6] and multiple material layers [7] have been investigated. However, the topic of metal-contacted, single horizontal heterostructure nanowires has not received attention.

This topic requires attention for two reasons. Firstly, Ohmic contacts must be made to optoelectronic devices to connect them to a circuit for measurement and for integration into electronic systems. Although there are alternatives, contacting

Nicklas Anttu and Heiner Linke NanoLund and Solid State Physics Lund University Lund, Sweden <u>Nicklas.Anttu@ftf.lth.se</u>, <u>Heiner.Linke@ftf.lth.se</u>

with a metal is a simple way to accomplish this. As the size of the metal contacts may be comparable to (or larger than) the nanowire itself, it is important to know how their introduction will affect the optical properties of the nano-optoelectronic device. Furthermore, the topic of heterostructure nanowires is an important one as the ability to grow a wide variety of heterostructures without defects in nanowires is one of their fundamental physical advantages [8].

In this paper, results are presented from COMSOL wave optic simulation of absorption in and scattering from single uncontacted and Au-contacted horizontal InAs/InP heterostructure nanowires. Uncontacted and Au-contacted results are compared so that the effect of the addition of the contacts can be determined. Solutions to Maxwell's equations are obtained throughout the 3D domain of the nanowire, contacts and SiO₂ substrate for wavelengths from 500 nm to 1800 nm in steps of 10 nm for two orthogonal linear polarizations of light, transverse electric (TE) and transverse magnetic (TM) - transverse referring to the orientation of the specified field with respect to the nanowire axis (Fig. 1). Results from solutions for these two orthogonal linear polarizations are averaged to obtain results for randomly polarized light and spline interpolation is employed to connect data points.



Fig. 1 (a) Transverse electric (TE) and (b) transverse magnetic (TM) linear polarizations defined with respect to the nanowire axis. A 1.5 μ m long InAs nanowire with radius of 30 nm on a 250 nm thick SiO₂ substrate is shown. This simulation domain is surrounded by perfectly matched layers in order to absorb outgoing, scattered light.

It is found that the addition of Au contacts to a single horizontal heterostructure nanowire dramatically alters the optical properties of the nanowire. This suggests that a more holistic approach to single nanowire optoelectronic device design is required in which contacts are not placed on the device merely out of electrical necessity, but rather are integrated into the optical design of the device.

Specifically, it is found that the addition of Au contacts to a single horizontal heterostructure nanowire can 1) increase absorption efficiency, 2) decrease scattering efficiency and 3) significantly alter electric field distributions within the wire resulting in a repositioning of the locations of strong absorption within the nanowire in comparison to the uncontacted case. Physical explanations for these results are that in the visible range, contacts affect the excitation of waveguide modes in the nanowire and how they interfere, and in the infrared range, localized surface plasmonic resonances develop at nanowire/contact interfaces.

II. RESULTS

A. Enhancement of Absorption and Suppression of Scattering

Calculation of the absorption and scattering efficiencies of an uncontacted 1.5 μ m long InAs/InP heterostructure nanowire with radius of 26.5 nm on a 250 nm thick SiO₂ substrate (Fig. 2a) shows that the wire is a better scatterer of light than it is an absorber of it for wavelengths less than 1 μ m (Fig. 2b). Additionally, a Fano-like resonance of undetermined origin is found to be present in both the absorption and scattering response of the wire at approximately 600 nm (Fig. 2b). The polarization-specific absorption efficiencies of the uncontacted nanowire (Fig. 2c) reveal that the Fano-resonance is present only for TM-polarized light and that the nanowire is a very poor absorber of TE-polarized light.



Fig. 2 (a) 1.5 μ m long InAs/InP nanowire with radius of 26.5 nm on a 250 nm thick SiO₂. InAs segments are grey and InP segments purple. (b) Scattering (purple) and absorption (green) efficiency of the nanowire in (a). (c) Absorption efficiency for TE (red) and TM (blue) linearly polarized light of the nanowire in (a). (d) 1.5 μ m long InAs/InP nanowire with radius of 26.5 nm on a 250 nm thick SiO₂ with 200 nm wide Au contacts placed 400 nm apart across the nanowire. InAs segments are grey, InP purple and the Au contacts yellow. (e) Scattering (purple) and absorption (green) efficiency of the nanowire in (d). (f)

Absorption efficiency for TE (red) and TM (blue) linearly polarized light of nanowire in (d).

For comparison, the absorption and scattering efficiencies of an identical wire with two 200 nm wide Au-contacts placed 400 nm apart (Fig. 2d) are computed. The contacts are found to dramatically alter the absorption and scattering properties of the wire, increasing absorption cross-section, decreasing scattering cross-section and eliminating the Fano-like resonance seen at 600 nm in the uncontacted case (Fig. 2d). The polarization-specific absorption efficiencies of the contacted nanowire (Fig. 2f) reveal that the contacts substantially enhance absorption of TM-polarized light for wavelengths less than 800 nm and enhance absorption of TEpolarized light across all wavelengths investigated. Two broad oscillations of unknown origin are found to be present in the TE absorption efficiency response of the contacted nanowire with peaks at approximately 1.05 μ m and 1.65 μ m.

B. Absorption Rate Densities

Across all wavelengths, the addition of the contacts is found to alter the electric field within the nanowire resulting in a repositioning of the locations of absorption in comparison to the uncontacted case. In the visible range, the field distributions shift within the "bulk" of the nanowire, and in the infrared range, the field becomes concentrated at the nanowire/contact interfaces where the conditions necessary for localized surface plasmon resonances are met.

More broadly, these results indicate that the locations into which photons are concentrated in a semiconductor nanostructure and at which photons are absorbed by the electrons therein can be manipulated by the addition of metal contacts to the nanostructure.

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