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## CONTROLLING DOPING PROFILES OF SILICON NANOWIRES FOR QUANTUM COMPUTING AND PHOTOVOLTAICS USING MICRO-RAMAN SPECTROSCOPY

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Silicon technology has been the cornerstone for the advance of the current age of information since the inception of the first transistor, due to an exponential development of microelectronics and chip miniaturization. Based on this success, some of the emerging technologies in photovoltaics and quantum computing are being developed using silicon nanowires as a fundamental building block. In the case of photovoltaics, p-n axial and core-shell junctions in Si nanowires allow the integration of silicon technology with other materials and thus a potential larger solar cell efficiency [1]. In quantum computing, silicon nanowires serve as one of the semiconducting platforms for qubit development by controlling the electron spin levels using a tailored selected doping and voltage in gates that split the nanowire into different quantum dots [2]. In both scenarios it is of paramount importance to control several key parameters, among them the dopant concentration in the nanowire, the stress, and the concentration of defects. They can all affect the operation of the corresponding device and result in critical failure or lack of reliability. Accessing these parameters with nanoscale resolution has been a challenge for spectroscopic techniques due to the diffraction limit of currently widespread optical spectroscopy. We present here a characterization using micro-Raman imaging and tip-enhanced Raman spectroscopy (TERS) that shows the potential of these techniques to determine the doping profile of silicon nanowires in both p-n junctions and silicon nanostructures for qubits, and to distinguish doping effects from others such as the presence of strain, crystal grains, and defects. High dopant concentrations lead to Fano asymmetric line shape of the Raman spectrum of silicon with an asymmetry parameter proportional to the dopant concentration and character – p- or n-type doping [3]. Confinement of the electric field due to the nanoscale diameter of the nanowires results in an enhancement of the Raman signal that yields higher resolution than that expected without this antenna effect. This enhancement allows us to employ micro-Raman spectroscopy successfully to distinguish several of the above mentioned effects in nanostructures. In the case of p-n axial junctions in silicon nanowires, we observe an asymmetry with higher spectral weight in the low and high energy side for p-type and n-type doping, respectively, being the effect more pronounced in the case of p-type doping. This effect is more significant for doping concentrations above 10<sup>17</sup> cm<sup>-3</sup>. In the case of nanostructured silicon for qubits we observe residual strain and crystallite grain boundaries close to the nanowire, tentatively attributed to the presence of We analyze the Raman spectra employing several asymmetric functions and compare the results obtained in nanowires with those reported in the literature and achieved in bulk silicon as a function of doping. Finally, we employ TERS to reach nanoscale spatial resolution and compare the accuracy and limitations of micro-Raman in the determination of the doping profile.

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## **FIGURES**



**Figure 1.** (left) Optical microscopy image of a p-n axial junction silicon nanowire (NW). The numbers 1 and 2 denote the n- and p-type sides of the junction. (center) Typical micro-Raman spectrum of the n-type side of the p-n axial junction Si NW fitted with a Fano lineshape. Note the asymmetric broadening towards the high energy side. (right) Typical micro-Raman spectrum of the p-type side of the p-n axial junction Si NW fitted with a Fano lineshape. Note the asymmetric broadening towards the high energy side. Note the asymmetric broadening towards the low energy side.



**Figure 2.** Color map of asymmetry factor q from a modified Fano function [3] fit of the micro-Raman spectra at the *p*-*n* axial junction Si NW shown in Fig. 1. Taken with an excitation laser of 532 nm wavelength, 4.5 mw power and 0.2 s acquisition time. Note the positive and negative values for the asymmetry factor corresponding to *p*- and *n*-type doping edges, respectively.



**Figure 3.** (a) Optical microscopy image of the contacts and Si NW region of a Silicon-on-insulator bottom-up structure for development of Si qubits. Color maps of (b) Raman shift, (c) asymmetry parameter, and (d) full width at half maximum (FWHM) of asymmetric Lorentzian fit to the micro-Raman map of spectra taken with constant step of 0.1 microns and similar wavelength and power than that of Figs. 1 and 2. The small but significant changes in the Raman shift indicate strain induced at the contacts and NW region due to the lithography and etching processing, whereas those of the asymmetric parameter display a combination of the growth of the grain boundaries at the Si NW and the increased doping at that region.