# Laser Induced Heating of Group IV Nanowires

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## ABSTRACT

Semiconductor nanowires (NWs) are fundamental structures for nanoscale devices. The excitation of NWs with laser beams results in thermal effects that can substantially change the spectral shape of the spectroscopic data. In particular, the interpretation of the Raman spectrum is greatly influenced by excitation induced temperature. A study of the interaction of the NWs with the excitation laser beam is essential to interpret the spectra. We present herein a finite element analysis of the interaction between the laser beam and the NWs. The resultas are applied to the interpretation of the Raman spectrum of bundles of NWs.

## INTRODUCTION

Semiconductor NWs are promising structures for advanced nanodevices, due to their unique optical and electrical properties [1]. One of the main issues regarding these nanostructures is the thermal transport. In spite of the lower power supply required for driving the nanodevices the heat per unit area dissipated is still very high. Optical characterization of semiconductors, and in particular of NWs, is necessary for the understanding the properties of the NWs, in order to develop performing and reliable devices. The optical characterization is usually carried out under excitation with laser beams focused through microscope lenses, e.g. microRaman (μ-R) spectroscopy, and microphotoluminescence (μ-PL). The NW diameters range from a few nm to a hundred nms; these sizes are below the diffraction limit; therefore, one does not know the exact position of the NWs inside the laser beam, which is not uniform but has a gaussian power distribution. Generally, the measurements are carried out with bundles of NWs, which can have different dimensions; therefore, the spectroscopic analysis is done on the basis of averaging over a certain number of NWs, or using complex size distribution functions (2,3).. Therefore, the excitation conditions are uncertain in both Raman and PL measurements, because of the non ability to localize the NWs with respect to the laser beam. On the other hand, NWs are systems with reduced thermal conductivity, orders of magnitude below the bulk thermal conductivity (4,5); furthermore, they stand in air, which makes very difficult the evacuation of heat, which is extensible to devices under operation. NWs under the excitation with a focused laser beam can reach non negligible temperatures, which is crucial for interpreting the Raman and PL spectra (6, 7). These techniques can be used as contact less probes for measuring the thermal thermal conductivity of NWs; X.F.Liu et al measured the thermal conductivity of CdS NWs using microPL spectroscopy (8), and M. Soini et al. measured the thermal conductivity of GaAs NWs using micro-Raman spectroscopy (9). Therefore, the study of the interaction between NWs and laser beams, is crucial, to interpret the spectroscopic data recorded on NWs under laser beam excitation, and to support the study of the thermal conductivity of NWs. We present herein a finite element analysis of the interaction between a laser beam and Si NWs of different dimensions. We will show that the temperature reached by the NWs depends on different intrinsic (thermal conductivity, NW dimensions..), and extrinsic (laser power, relative position with respect the laser beam, surrounding media..) factors, which have to be considered in order to interpret the spectroscopic experimental data.

## EXPERIMENTAL AND METHODS

Si NWs were grown by the vapor liquid solid (VLS) method in a low pressure chemical vapor deposition (LPCVD) reactor on (100) Si substrates. $Si_2H_6$ was the precursor gas (10 sccms). Au particles (30 nm in diameter) from a colloidal suspension were used as the catalysts. The dimensions of the typical NWs grown by this method are diameters ranging from 10 to 200 nm and several μms length.

The Raman spectra were acquired with a Labram UV-HR 800 Raman spectrometer (Jobin Yvon). The excitation was done with an Ar+ laser (514.5 nm), 80 μW power in the focal plane; because of the Gaussian distribution and the small dimension of the objects it does not make sense to give the power density as the excitation data. The diameter of the laser beam spot at the focus plane is ≅ 1 μm, more than one order of magnitude larger than the NWs diameters. Individual NWs were detached from the substrate by sonication in methanol suspension and dropped on an electron microscope grid holder for the measurement of the Raman spectrum in individual NWs.

The NWs are overheated under the local heat source generated by the absorption of the laser beam, which should determine the shape of the Raman spectra. The NW overheating analysis is carried out by a finite element method (fem) for solving the heat transfer equation inside a NW of predefined dimensions.

## RESULTS AND DISCUSSION

The laser beam absorption by the NWs constitutes a local heat source, which, because of the poor thermal conductivity of the NWs and the reduced heat dissipation can induce non negligible heating of the NWs, which can get a few hundred ºC, depending on the excitation conditions. Fig. 1 shows the Raman spectra obtained on a bundle of NWs, and on an individual NW ($\phi \approx 30$nm) respectively; one observes an anomalous broadening of the phonon bands especially for the bundle of NWs, which can even split the Raman band (spectrum A in Fig.1). The laser beam spot focused by a microscope objective is diffraction limited; therefore, it is modelled by a Gaussian power profile. The effective laser energy absorption depends on the laser wavelength, but also on the NW geometry (10). Therefore, one needs estimating the absorption efficiency, $Q_a$, which was calculated according to the procedure reported in (10, 11). Because the NW diameter is smaller than the laser wavelength, Qa is modulated at determined wavelength by the diameter of the NW, resulting in a series of resonances, Fig.2, which determines the energy absorbed by the NWs as a function of their diameter.

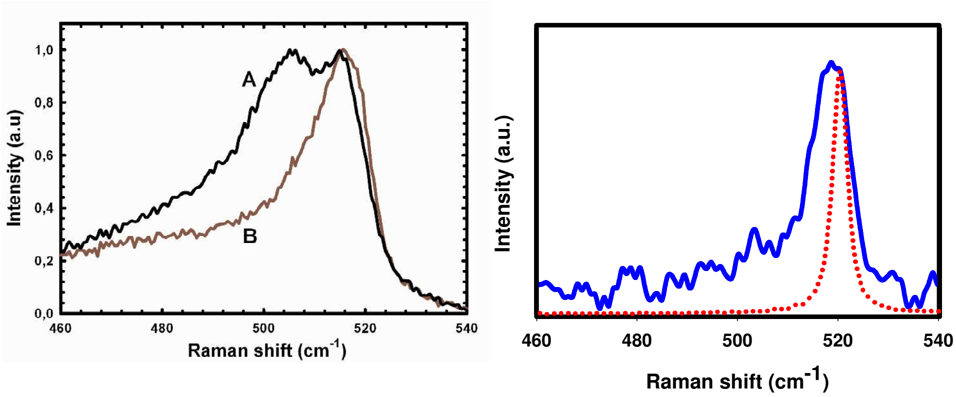


**Figure.1**. Left) Raman spectra of bundles of NWs measured for two positions of the laser beam, spectra A, and B respectively. Right) Raman spectrum of an individual Si NW (ϕ≈30 nm) (solid), and Raman spectrum of a control Si substrate (dotted)

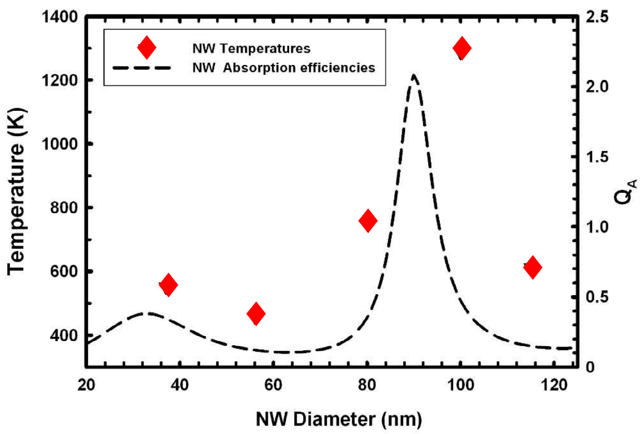


**Figure 2**. Absorption efficiency for λ=514.5 nm calculated as a function of the NWs diameter (dashed line). Temperatures calculated for NWs of different diameters excited with the 514.5 nm of an Ar laser (red diamonds).

On the other hand, the thermal conductivity of NWs depends on the NW diameter as well. The measurement of the thermal conductivity of NWs is a complex exercise, which makes the experimental data about the thermal conductivity of Si NWs only available for a few diameters (4).

When studying the NW heating induced by the laser beam, one has to consider both the laser energy absorbed, and the thermal conductivity; therefore one expects that the NW dimensions, both diameter and length, but also the excitation conditions, e.g. the part of the NW excited by the laser beam, and the relative position of the NW with respect to the laser beam spot, are the factors determining the thermal behavior of the NW under the laser beam.

The NW diameter is very important, as it determines the absorbed energy, through the volume exposed to the laser beam, but also through the dependence of the absorption efficiency, Qa, which gives the results shown in Fig.2; the temperatures reached by NWs of different diameters are superposed to the absorption efficiency, showing that the NW temperature roughly follows the dependence with the diameter of the absorption efficiency. This means that the temperature reached by the NWs depends in a great amount of the total absorbed energy, which is primarily determined by the NW diameter, and the laser wavelength.

The influence of the NW length is shown in Fig.3, where the temperature reached by a NW with 37 nm diameter, one choses this diameter because of the availability of thermal conductivity data, as a function of the NW length is represented when the laser impacts on the center of the NW. One observes that the temperature has a strong dependence with the NW length.

The temperature distribution inside the NW depends on the length and the zone of the NW where the laser impacts, see in Fig.4 the temperature distribution inside a NW 5 μm long, and 37 nm diameter, when the laser impacts on one of the ends, or in the center of the NW. The temperature is higher when the laser impacts close to the ends, while it is lower when the laser impacts on the medium region of the laser. The temperature distribution inside the NW is mainly determined by the thermal conductivity. An

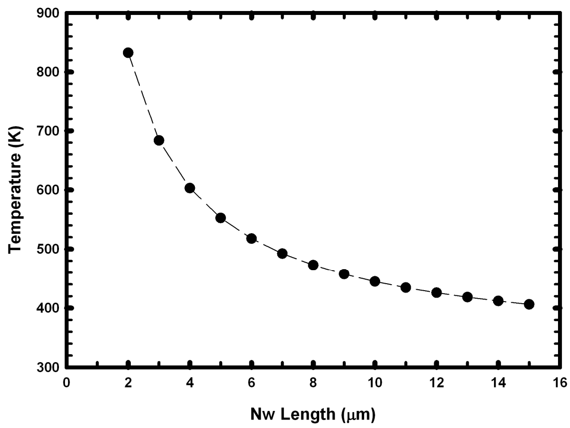


**Figure 3**. NW temperature as a function of the NW length. Note that this is the temperature at the zone of impact of the laser beam on the NW.

important observation concerns the temperature gradient inside the zone of the NW under excitation, which is no more than a few degrees per μm, contrarily to what has been claimed for describing the Raman spectrum of Si NWs (2).

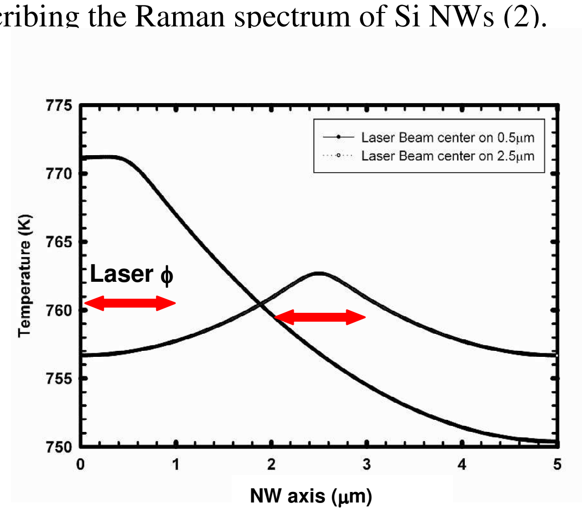


**Figure 4**. Temperature distribution along a NW 5μm long, and 37 nm diameter, for two different impact positions of the laser beam, an end and the center of the NW respectively

As mentioned above the laser beam presents a Gaussian power distribution, while the NWs have diameters at least one order of magnitude smaller than the beam diameter, which mean that the effective excitation of the NW is greatly dependent on the position inside the laser spot. Fig.5 shows the temperature reached in a Si NW ($\phi$=37 nm) as function of the position of the NW with respect to the laser beam center. A large temperature change is observed depending between the NW excited in the center of the laser beam, or excited in the periphery of the laser beam.

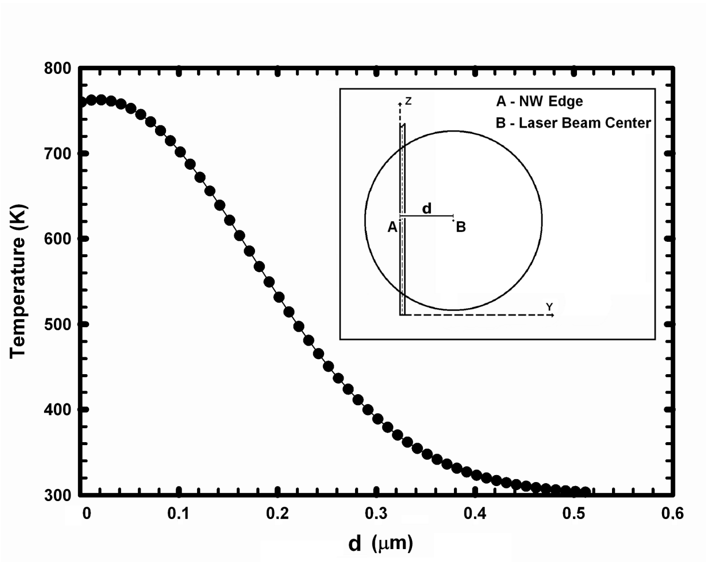


**Figure 5**. NW temperature depending on its position with respect to the beam center, see the insert scheme

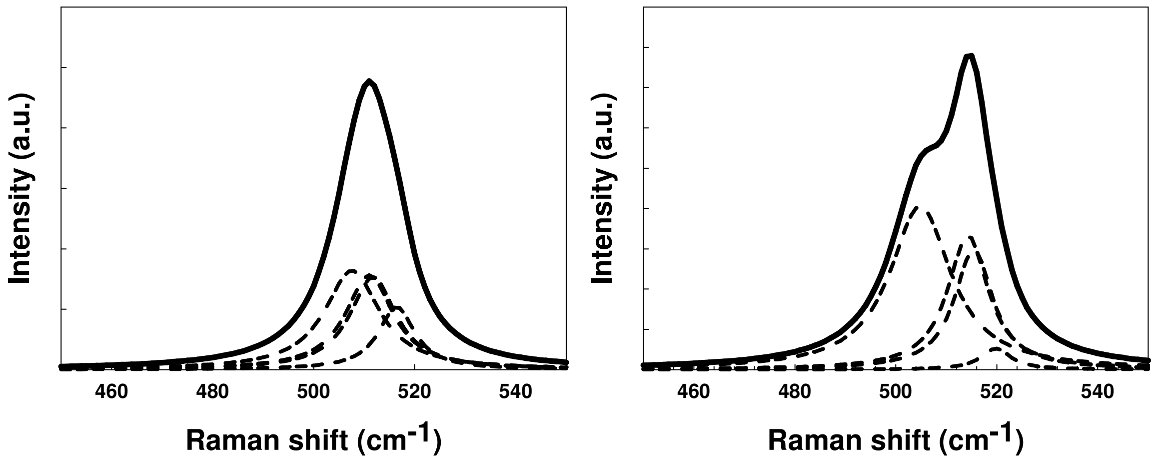


**Figure 6.** Raman spectra calculated for each of the four NWs ( dashed lines), and the convolved global spectrum NWs (solid lines), for two different positions of the four NWs inside the laser beam spot. Showing how the same NWs can give very different spectra depending on the NW distribution inside the laser beam

According to this, when several NWs are exited simultaneously, one has to consider the relative positions of the NWs inside the laser beam spot, but this position cannot be determined in an optical microscope. We have simulated the Raman spectrum of a bundle of four NWs with the same diameter, 37 nm, but placed in different positions of the laser beam spot. First, we have calculated the temperature of each NW under the laser excitation; then we have calculated the corresponding Raman spectrum, and the spectra arising from the four NWs have been convolved taking account of the weight of each one to the global spectrum. The resulting spectra for different configurations of the four NWs inside the laser beam spot are shown in Fig.6, showing very different shapes of the global spectrum, which is due to the differences in the temperatures of the NWs being probed by the laser beam, which depends on the position of the NWs inside the laser beam. These spectra qualitatively reproduce the experimental Raman spectra measured on bundles of NWs, Fig.1, for different positions of the laser beam spot.

## CONCLUSION

The study of the interaction between Si NWs and the laser beam is crucial for a reliable interpretation of the optical spectroscopy data. In particular, we have calculated the temperature induced by the laser beam on Si NWs, as a function of the dimensions of the NWs, and we have applied these results to the interpretation of the Raman spectrum of bundles of NWs.

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## REFERENCES

1. Y.Cui, C.M.Lieber ; Science 291, 851 (2001).
2. S. Bhattacharya, S.Samui ; Appl. Phys. Lett. 84, 1564 ( 2004)
3. S. R. Gupta, Q. Xiong, C. K. Adu, U. J. Kim, P. C. Eklund; Nano Lett. 3, 627 (2003).
4. D.Li, Y.Wu, P.Kim, L.Shi, P.Yang, A.Majumdar; Appl. Phys. Lett. 83, 2934 (2003).
5. M. Kazan, G.Guisbiers, S.Pereira, M.R.Correia, P. Masri, A.Bruyant, S.Volz, P.Royer; J. Appl. Phys. 107, 083503 (2010)
6. H. Scheel, S. Reich, A.C. Ferrari, M. Cantoro, A. Colli, C. Thomsen; Appl. Phys. Lett. 88, 233114 (2006)
7. Torres, A. Martín-Martín, O. Martínez, A.C. Prieto, V. Hortelano, J. Jiménez, A. Rodríguez, J. Sangrador, T. Rodríguez; Appl. Phys. Lett 96, 011904 (2010)
8. X.F.Liu, R.Wang, Y.P.Jiang, Q.Zhang, X.Y.Shan, X.H.Qiu; J. Appl. Phys. 108, 054310 (2010)
9. M.Soini, I.Zardo, E.Uccelli, S.Funk, G.Koblmuller, A.Fontcuberta i Morral, G. Abstreiter; Appl. Phys. Lett. 97, 263107 (2010)
10. B. K. Sun, X. Zhang, C. P. Grigoropoulos; Int. J. Heat Mass Transfer 40, 1591 (1997).
11. G.S.Doerk, C.Carraro, R.Maboudian; ACS Nano 4, 4908 (2010)