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NANOSCALE JOULE HEATING ALONG SILICON NANOWIRE AND ITS NANOSCALE HEATER APPLICATION

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ABSTRACT

In this paper, we present numerical and experimental studies on the nanoscale Joule heating along the single crystalline silicon nanowires. 50-100nm wide single crystalline silicon nanowires are heated via Joule heating by applying an electrical potential across them. Numerical simulation result predicts an extremely localized temperature field by resistive heating of silicon nanowire. We experimentally verified this highly localized heating of silicon nanowires by AFM imaging of localized thermal ablation of polytetrafluoroethylene (PTFE) thin film. This result implies potential applications of silicon nanowires as nanoscale heaters for the generation of highly localized temperature fields

INTRODUCTION

Nanowires are wires with diameters in the nanometer range and high aspect ratio (length/width). Their lateral dimensions are usually constrained to 1 to a few 100's nm while the longitudinal dimensions are unconstrained. Because of their dimensions, they exhibit distinct electronic properties (eg. quantum confinement [1]), thermal properties (decreased thermal conductivity by boundary scattering [2]), etc. compared to the bulk materials. Due to these interesting properties, they are drawing a great attention in various fields including nanoscale electronics [3-5], biotechnology [6-9], and energy generation technology [10, 11]. For example, single crystalline silicon nanowires synthesized by vapor-liquid-solid growth method were used as field effect transistors with performance comparable to state-of-the-art planar MOSFET devices [3]. Accordingly, extensive studies on the electronic properties of nanowires have been conducted [4, 5]. According to the quasi-one dimensional geometry of nanowire, the electrical transport is greatly affected by the surface conditions (roughness, defects, surface charges, etc.). A number of field-effect transistor-type biosensors based upon the surface charge effects have been developed for the detection of bio-molecules such as DNA [6, 7] and protein molecules [8, 9]. Also, the mechanical vibration of piezoelectric zinc oxide (ZnO) nanowires by external waves has been transformed into electrical energy for the nanoscale energy scavenging [11].

Herein we are introducing a new application of silicon nanowires (SiNW) as nanoscale heaters with highly localized temperature field with huge temperature gradient. The thermal and electronic properties of SiNW can be easily modulated by adjusting the concentration of doping impurities [5]. Since they can function as ohmic electrical resistors, one can utilize them as resistive heaters. The resistive heating performance strongly depends upon the electrical and thermal properties of the heater materials. Thermal conductance of SiNW is known to be much smaller than that of bulk silicon by several factors [2], which may facilitate more effective Joule heating along the SiNW. Also, due to their nanoscale dimensions, they can be used for the applications where highly localized heating is required. We first describe the finite element analysis (FEA) simulation results of resistive heating along SiNWs. Then, highly localized nanoscale heating of SiNWs is visually verified by ex-situ AFM imaging of localized thermal ablation of thin polymer layer (PTFE) initially coated on the SiNWs. Finally, we propose a few possible applications of nanoscale Joule heating along SiNWs, with an example of localized surface functionalization of SiNW-based biosensors for enhancement of sensor sensitivity and detection limit.

NUMERICAL ANALYSIS AND EXPERIMENT

We performed a FEA simulation of resistive heating along SiNW and its surrounding areas. Accurate computation of nanoscale heat transfer in nanowires requires extensive modeling based upon molecular dynamics [12]. One-dimensional structures like nanowires have distinctive thermal and electric properties than bulk materials. According to the literature [13], these distinctions stem from several mechanisms such as quantum confinement, sharp features of one-dimensional density of states [14], increased boundary scattering of electrons and phonons [15], and modified electron-phonon and phonon-phonon scattering [16,17]. Most of the research on the heat transfer along the nanowires has been focused on the investigation of their thermal properties (eg. conductivity). For example, theoretical and experimental studies of heat transport along silicon nanowires have been done [2, 16-18]. Temperature and size dependency of thermal conductivity of silicon nanowires and Si / SiGe superlattice nanowire was investigated by using suspended microscale heating elements [17, 18]. From this study, thermal conductivity of nanowires was observed two orders of magnitude lower than the bulk value due to characteristic phenomena such as phonon-boundary scattering and phonon spectrum modification. Numerical approaches such as Monte Carlo method [17] have been employed for the estimation of thermal properties of silicon nanowires. However, this molecular dynamics simulation involves a very complicated and time-consuming computation although it may provide only a limited accuracy due to many uncertainties and unknowns. Furthermore, thermophysical properties of silicon in nanoscale are lacking especially in the high temperature regime (>500K) while most of the nanoscale thermal properties have been studied in low temperature regime. The purpose of our numerical analysis is to obtain a first-order approximation of temperature distribution in the resistive heating of silicon nanowires. For simplicity of the analysis, we have run the numerical simulation based upon macroscale heat transfer models (eg. Fourier law for heat conduction, Newton's law of convective cooling, Stefan-Boltzmann law of radiation, etc.), but with thermal conductivity of SiNW 1-100 times smaller than those of bulk Si. Even though this macroscale-based heat transfer model may be different from reality, this simplified analysis should provide general trends of nanoscale Joule heating by SiNW and estimate rough temperature distribution around SiNWs.

In Figure 1 is given a two-dimensional model used in the numerical simulation (FEMLAB Multiphysics® module) of resistive heating of SiNW. An array of ten single crystalline p-type SiNWs (100nm height, 100nm width, 200nm pitch) is located above 400nm thick silicon oxide (SiO_2) thin film thermally grown on p-type Si wafer. SiNW are assumed to be uniformly doped with boron at $5 \times 10^{18} / cm^3$ concentration. The cross-sections of SiNWs are in square geometry because they are made by top-down method (electron beam lithography followed by reactive ion etching) on silicon-on-insulator (SOI) substrates. A thin polymer layer (polytetrafluoroethylene; PTFE) is deposited on the SiNW array in order to experimentally visualize the localized Joule heating along SiNW. Heat generated by SiNW is dissipated by thermal conduction to underlying SiO_2 insulation layer and thin polymer layer, radiation to neighboring SiNW, and convection and radiation to the surrounding environment at room temperature (300K). Electrical bias is applied across either single nanowire (eg. wire #1) or multiple nanowires (eg. wire #1,4,7,10).

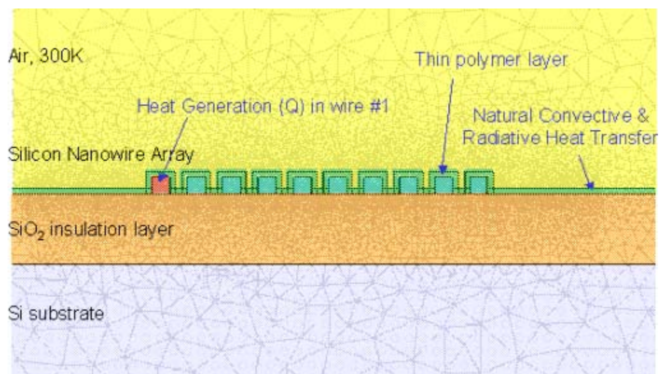


Figure 1. Numerical simulation model for resistive heating of silicon nanowires (SiNW) array. Nanowires with 100nm height / width and 200nm pitch are heated by applying an electrical bias across the wires. In this case, only NW #1 is heated.

For the experimental verification, we have fabricated single crystalline silicon nanowires by top-down approach. Silicon on insulator (SOI) wafer (Soitec, France) with a silicon (Si) device layer thickness of 1000Å and buried oxide layer of 3800 Å was used as a substrate for the device fabrication. SiO_2 layer (1100 Å) was thermally grown on the Si device layer to reduce the silicon device layer down to 500 Å. Then, Si device layer was doped with boron (B) by ion implantation (35keV, 7° tilt, dose=1.20 × 10^{14}/cm^2) and rapid thermal annealing at 1025°C for 60 seconds. The silicon nanowire pattern was defined by electron beam lithography system and transferred to underlying Si device layer by Cr lift-off and reactive ion etching processes (CHF_3+O_2 for SiO_2 etching and HBr for Si etching). (See Figure 2) To decrease the density of surface dangling bonds on Si surface and increase the electrical stability of the nanowire a high quality 3nm SiO_2 layer was grown on Si nanowire surfaces at 925°C for 1 minute in O_2 environment. After selectively etching contact area between Si nanowire and metal interconnect with buffered oxide etchant (HF: NH_4F=1:10), Al interconnect pattern was defined by photolithography and lift-off process. Electrical bias was applied across silicon nanowires by HP4145B semiconductor parameter analyzer for the localized Joule heating of silicon nanowire.

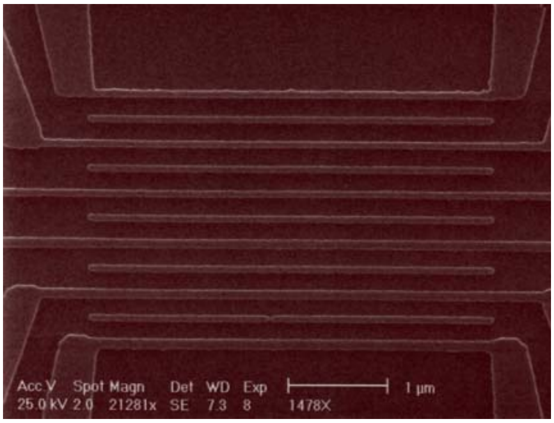


Figure 2. Array of eleven SiNWs (50-150nm width and 50nm height) fabricated by electron beam lithography and reactive ion etching of thin device layer silicon on insulator (SOI) wafer.

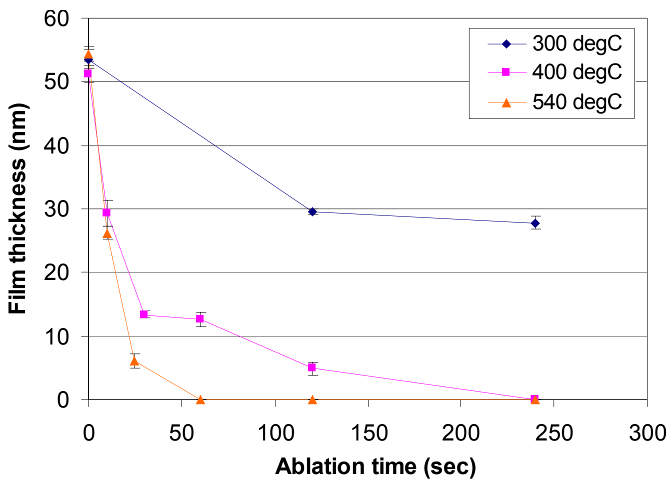


Figure 3. Removal of PTFE thin film by heating at different temperatures (300-540 ºC) measured by surface profilometry

The imaging of temperature field in nanoscale resolution still remains very challenging due to current technical limitations. Conventional temperature measurement techniques such as thermocouples, thermistors, infrared imaging, laser reflectance imaging, etc. cannot provide nanoscale spatial resolutions. Although scanning thermal microscopy (SThM) has been developed for the nanoscale mapping of temperature fields, the resolution is currently limited to 100-200nm [19]. Therefore, the accurate temperature imaging during nanoscale Joule heating of SiNW is currently impossible. For the verification of highly localized heating, we have chosen a novel alternative approach – ablation of thin polymer films around SiNW by SiNW heating and its ex-situ imaging by microscopy techniques such as scanning electron microscopy (SEM) and/or atomic force microscopy (AFM). We have chosen polytetrafluoroethylene (PTFE) as a ablated polymer material. PTFE is a synthetic thermoplastic fluoropolymer polymer. It does not become fluid at moderate heating temperatures (eg. 300 ºC), but thermally decompose at above 400 ºC [20, 21]. (See thermal ablation of PTFE thin film at different temperatures in Figure 3.) Therefore, ablation of PTFE can function as a proof of temperature rise above 400 ºC by Joule heating of SiNW. Approximately 35-40nm thick PTFE layer was deposited by vapor-based deposition system (STS plasma etching system). The ablation of PTFE film by SiNW Joule heating was done in atmospheric air environment. The locally ablated nanowires were observed by SEM and AFM for topological analysis.

RESULTS AND DISCUSSION

In Figure 4 is shown a numerical simulation result when only nanowire #1 was heated by electrical bias of 2.5V/μm (i.e. 10V applied on 4μm long SiNW). The maximum temperature of SiNW #1 reached 599.5K. A very steep temperature distribution is observed. Temperatures for wire # 1, 2, and 3 are 599.5K, 413.2K, and 354.9K, respectively. This high temperature gradient is attributed to small size of heat source (SiNW) and thermal insulation by underlying SiO_2 layer and air environment. The dependence of maximum temperature of SiNW on the applied voltage for 4μm long SiNW is given in Figure 5. The maximum temperature increase is proportional to the square of applied voltage. For example, 4μm long SiNW is heated to 347.9K, 491.5K, and 1069.9K for 4V, 8V, and 16V of bias, respectively. Also, the maximum temperature increase is inversely proportional to the length of the SiNW. For example, when 16V of bias is applied, the maximum temperatures of SiNW are 1069.9K, 640.7K, 491.7K, and 422.9K for 4μm, 6μm, 8μm, and 10μm of lengths, respectively.

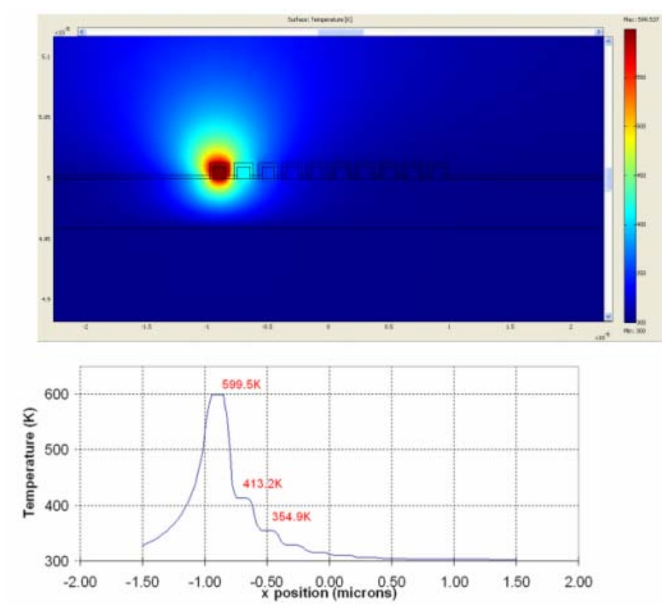


Figure 4. Numerical simulation of Joule heating of single SiNW (NW #1) by 10V bias. Highly localized temperature distribution is generated.

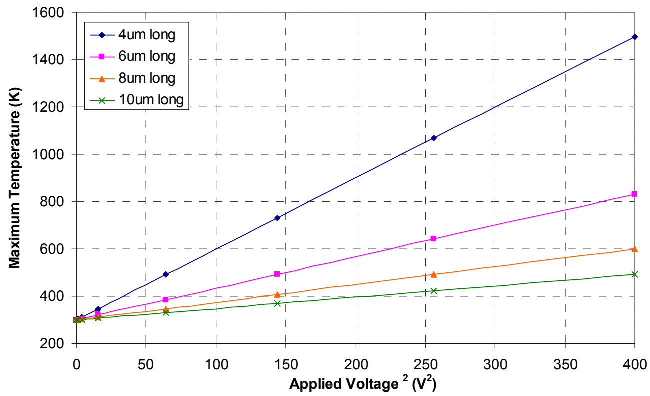


Figure 5. Estimation of maximum temperature of SiNW by resistive heating depending on the applied voltage and length of SiNW by numerical simulation

When the electrical bias is applied on the nanowire #1, 4, 7, and 10, the temperature distribution is also localized on these nanowires as shown in Fig.6. The temperatures of these nanowires are increased up to 812.1K. Although the temperatures of the neighboring nanowires increase, their temperatures are maintained below 600K, low for the ablation of the PTFE layer. Therefore, PTFE is thermally ablated only along nanowire #1, 4, 7, and 10, while other remaining nanowires are covered with PTFE layers. Since this simulation has excluded the possibilities of nanoscale heat transfer phenomena [2,17,22], there could possibly be a considerable discrepancy from the real experimental results. If the thickness of the silicon thin film becomes smaller than 100 nm level, the effect of phonon scattering at the film boundaries cannot be ignored since the mean free path of phonon is in the order of ~100nm [22]. Due to the boundary phonon scattering effect, the effective thermal conductivity of silicon can be significantly reduced for a nanowire of 100nm thickness and width [13, 17, 22]. When we consider this thermal conductivity reduction in the numerical simulation, the temperatures of nanowires by Joule heating actually shows a slight increase of temperature (820K for 30% of conductivity reduction) for nanowire #1. For more accurate estimation of temperature distribution, further detailed heat transfer modeling with nanoscale heat transfer phenomena in the thermal conduction, convection, and radiation should be used. However, the numerical analysis conducted in this paper will provide useful first order estimation.

In Figure 7 is shown the AFM scanning image of single SiNW with PTFE thin film coating before and after Joule heating along SiNW. A high bias voltage (30V) was applied across SiNW in order to increase the temperature of SiNW above 400 ºC for the ablation of PTFE film. The ablation of PTFE film occurred only in a very close vicinity of the SiNW while the surrounding regions were not affected. Detailed AFM image at the center of the SiNW (Figure 7(b)) clearly shows the local ablation of PTFE film along the SiNW. This result verifies that a highly localized heating occurred by the Joule heating of SiNW.

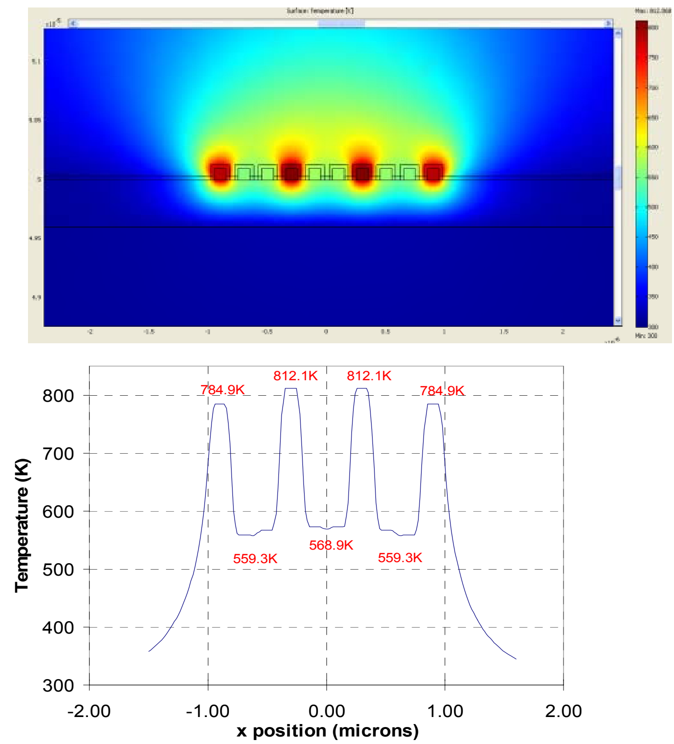


Figure 6. Numerical simulation of Joule heating of multiple SiNWs (wire #1,4,7,10) by 12V bias. Highly localized temperature distribution is generated.

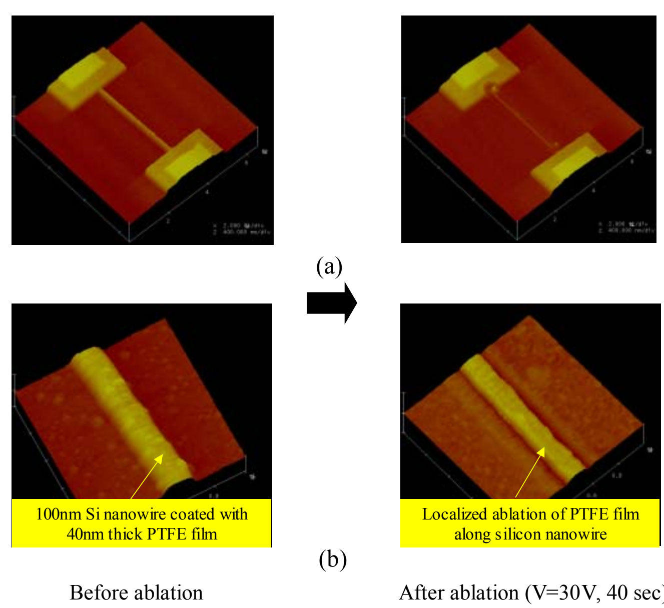


Figure 7. AFM scanning image of localized ablation of PTFE thin film by nanoscale Joule heating along single SiNW (100nm width, 50nm height)

The comparison of cross-sectional images before and after the SiNW Joule heating (Figure 8) provides quantitative information about the PTFE film ablation. In Figure 8, blue dotted line and white solid line represent the original profile of SiNW covered with PTFE film (before Joule heating) and new profile of SiNW (after Joule heating), respectively. The difference of these two profiles indicates the area of PTFE ablation. From these profiles, it appears that the ablation of PTFE occurred nonuniformly around the perimeter of SiNW. Step height reduction by 40nm indicates complete ablation of PTFE film. The width reduction by ~23nm along the sidewalls of SiNW, which is smaller than 40nm reduction on the vertical direction may be due to either thickness nonuniformity of deposited PTFE film or less temperature rise in the horizontal direction. The lateral range of PTFE ablation is measured as 253.9nm. This indicates that the temperature rise occurred only close to the SiNW. If we lower the applied bias voltage, we could lower the temperature rise of SiNW and decrease the range of thermal ablation of PTFE as a consequence.

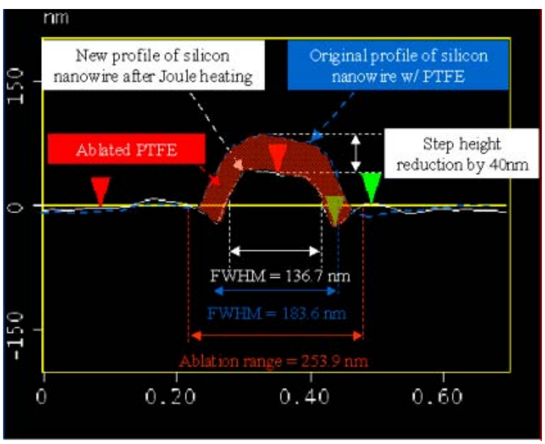


Figure 8. Cross-sectional profiles of SiNW before and after PTFE ablation by SiNW Joule heating. The discrepancy between two profiles indicates ablation of PTFE film by SiNW Joule heating.

Nanoscale Joule heating was also demonstrated in a high density array of SiNW shown in Figure 9. An array of eleven SiNW (50nm width, 250nm pitch) was fabricated and coated with 50nm thick PTFE film. A bias voltage of 30V was applied only on SiNW #1, 3, 5, 7, 9, and 11. The AFM image and cross-sectional profile of SiNW array shows that the ablation of PTFE occurred only along SiNWs on which an electrical bias was applied without affecting the neighboring SiNWs. The heights of SiNWs #1, 3, 5, 7, 9, and 11 were decreased while those of SiNWs #2, 4, 6, 8, and 10 were maintained the same. This proves that the temperature rise by SiNW Joule heating happens in a highly localized manner. Only along and in close vicinity of resistively heated SiNW exhibit high temperature rise, while the surrounding areas still remain to be much less heated. As mentioned above with numerical simulation results, highly localized temperature distribution by nanoscale Joule heating of SiNW is due to small size of heat source (SiNW) and efficient thermal insulation by underlying SiO_2 layer and air environment. The macroscale thermal conductivities of SiO_2 and air at room temperature are ~1.4W/m·K and 0.03W/m·K, respectively. These values are lower than the thermal conductivity of single crystalline silicon by several factors. The thermal insulation across the SiO_2 and air prevents the heat dissipation from SiNW to the surrounding regions, facilitating high temperature rise of SiNW and steep temperature drop in the surrounding areas. Consequently, a very localized nanoscale temperature field with high temperature gradient (>1.5 ºC/nm from numerical simulation) is created by nanoscale Joule heating of SiNW.

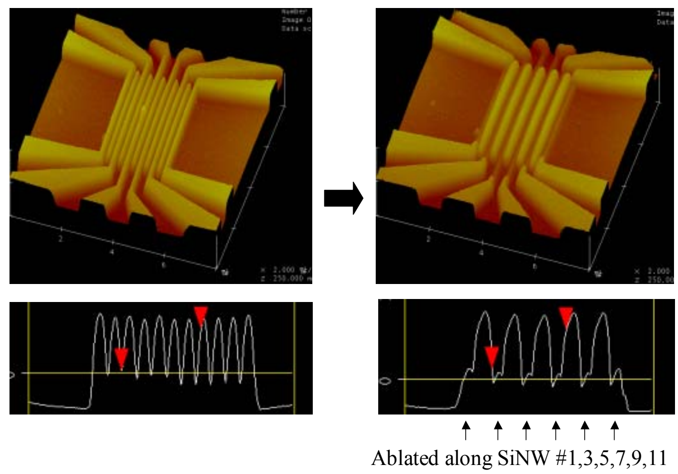
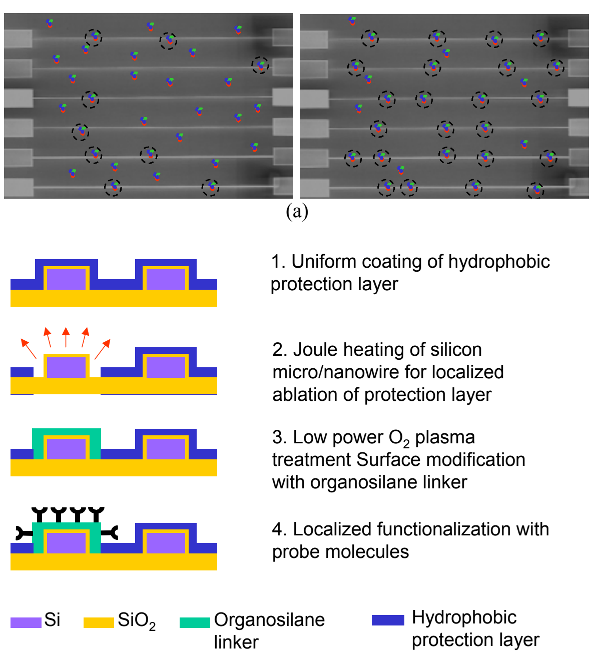


Figure 9. Joule heating along high density SiNW arrays (50nm width, 250nm pitch). Joule heating along SiNW #1,3,5,7,9,11 did not affect unheated SiNW #2,4,6,8,10.

There could be many possible applications of this localized temperature field by SiNW Joule heating. We have applied this localized Joule heating to the selective surface functionalization of SiNW in the SiNW-based biosensors [23]. In SiNW sensor device, the active sensing component (SiNW) has a thin native SiO_2 surface for the binding of biomolecules. Unfortunately, the surrounding regions are also silicon-based materials such as SiO_2 or Si_3N_4. Therefore probe molecules get bound not only to the active sensing area (SiNW) but also to the surrounding areas. Therefore, only a small portion of target molecules will be actually detected by active sensing region (SiNW) while the majority will be wasted by binding to the surrounding region as shown in Figure 10 (a). This will not only reduce the sensitivity and raise the detection limit of the sensor, but also introduce sensing noise, which will be very critical in the in-vitro detection from individual cells with extremely small number of target molecules for detection. Selective surface functionalization only along SiNW surface will improve sensor sensitivity and detection limit. By coating SiNW with protective layer (PTFE) and selectively ablating this layer by nanoscale Joule heating of SiNW, only the surface of SiNW becomes available for the surface functionalization and biomolecule immobilization. By subsequent oxygen plasma treatment and vapor phase deposition of chemical linkers (eg. 3-mercaptopropyltrimethoxysilane or aminopropyltriethoxy-silane), we were able to achieve a localized surface functionalization in a nanoscale resolution [23]. This method is very simple to implement and does not require any difficult alignment process in nanoscale accuracy. The detailed mechanism of the selective surface functionalization is shown in Figure 10 (b).

Another possible applications of SiNW-based nanoscale heating are nanoscale biology or chemistry, where nanoscale temperature distribution is critical for the biochemical or chemical reaction. For example, if the chemical reaction is endothermic (requires thermal energy), the reaction can occur only in the vicinity of the SiNW heaters. Thereby, extremely high gradient of the chemical reaction can be created by the localized heating of SiNW. Also, localized heating by SiNW could potentially help local treatment of biological tissues.



(b)

Figure 10. (a) Conceptual image for the comparison between global and localized functionalization of SiNW. (b) Operational principle of thermally assisted selective surface funtionalization of silicon nanowire.

CONCLUSION

We have investigated a localized heating by nanoscale Joule heating of silicon nanowire (SiNW). numerical analysis shows that highly localized temperature field with extremely high temperature gradient is created by SiNW Joule heating. Also, localized thermal ablation of PTFE coating on SiNW verified the localized temperature rise by nanoscale SiNW Joule heating. SiNW nanoheater would have a number of potential applications as self-aligned selective surface functionalization of SiNW based sensor, creation of high chemical gradient, biological tissue treatment, etc.

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