Semi-conductivity Transition in Silicon Nanowires by Hole Transport Layer

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TOC

Abstract

Nanowires surface is a source of interest mainly for electrical prospects. Thus, different surface chemical treatments were carried to develop recipes to control the surface effect. In this work, we succeed to shift and tune the semi-conductivity of Si nanowire based device from n- to p-type. This accomplished by generating hole transport layer at the surface by using an electrochemical reaction-based non-equilibrium position to enhance the impact of the surface charge transfer. This completed by applying different annealing pulses at low temperature (below 400 °C) to reserve the hydrogen bonds at the surface. After each annealing pules, the surface characterized by XPS, Kelvin Probe measurements and conductivity measured by FET based single Si NW. the mechanism and conclusion were supported experimentally and theoretically. To this end, this strategy has been demonstrated as an essential tool which could pave a new road for regulating the semi-conductivity and for other low-dimensional nano-materials.

Keywords

Silicon nanowire, Surface doping, Enhanced surface reaction, Hole transport layer, Semi-conductivity transition.

Semi-conductors with n and/or p types are the basis of semi-conductive devices that build the whole electronic industry.¹ The conventional strategy to control the semi-conductive types, i.e., n type (electron mobility) and p type (hole mobility), is doping the intrinsic semi-conductor with heterogeneous elements which contain different valence electrons. For example, Si doped with P and B, GaN doped with Si and Mg, etc., in nature, which is the regulation of defects and insertion of doping energy levels in the intrinsic band gap of body semi-conductors.^{2,3} When the semi-conductors come into nanoscale, this process is also influenced and/or amplified by surfaces as another kind of ultra-important defects in nano-materials, has dramatically different properties comparing with bulk materials, however, rare to be reported directly regulating the semi-conductive types.^{4,5}

An effective strategy to realize this process is based on surface charge transfer doping (SCTD) which terminate the surface with atoms/molecules producing a transport layer at the surface.⁶⁻⁸ To this end, we are able to tune not only the doping profile but also the surface potential and band bending.^{1,8-11} To date, these surface modifications were performed under equilibrium reaction conditions which could limit the electron withdrawing or donating by the grafted atoms/molecules.¹²⁻¹⁴ However, here we applied annealing pulses to disturb the equilibrium reaction, simulating the Haber–Bosch process but at the nano scale. According to le Chatelier principle, when an equilibrium is perturbed, the equilibrium position moves to counteract the perturbation and, in this way, we expect that electrons withdrawing/donating can be enhanced.

We illustrate this idea on the silicon nanowires (SiNWs), because the one-dimensional channel is suitable for carriers' mobility while the optical absorption cross-section provides a strong resonant field enhancement of the impinging illumination^{15,16}. Various thermal oxidation surfaces with different coverages and thickness, are greatly important in traditional surface passivation

process commonly employed in the semiconductor industry for minimizing the surface affects, Inc., surface states and dangling bonds (reported densities about 10^{10} cm^{-3}). Usually, the annealing temperature in these procedures was chosen to be high (more than 600°C) in order to achieve a direct interaction between the Si dangling bond with the ionized oxygen from the ambient and to decrease fixed charge density.¹⁷ However, in our case, we chose an annealing temperature less than 400°C (440°C is needed to break Si-H bond). Therefore, we force the oxidation mechanism of the Si NWs to rely on Si-H bond and O_2 molecules to go through a redox couple reaction controlled by SCTD, avoiding producing a fixed charge (e.g. producing Si-O^+ complexes) which is an additional advantage of this technique. As a result, the semi-conductivity of silicon NWs were able to be tuned between n and p semi-conductive types due to the charge transfer process.

In this paper we show the transition between n and p semi-conductive types have been successfully achieved by disturbing the reaction equilibrium on the Si NWs surface through a simple pulse annealing approach. Their mechanisms are well studied theoretically and experimentally. This strategy has been demonstrated as an essential tool when the Si based electronic device goes to nanoscale, which could pave a new road for regulating the semi-conductive types and for other low-dimensional nano-materials.

The Si NWs are single crystalline, exhibiting $[112]$ and were grown by the VLS method with an average length and diameters of $3.51 \pm 0.26 \mu\text{m}$ and $65 \pm 25\text{nm}$, respectively (See Supplementary Information, SI). To start with identical surfaces after each (non)equilibrium step, a full Si-H monolayer (ML) on the VLS grown Si NWs surfaces was produced by immersing the Si NWs samples in buffered HF solution ($\text{pH} = 5$) for 30sec (See SI). Afterwards, we applied a series of annealing pulses (4 cycles with temperatures ranging from 100°C to 400°C , See SI and **Figure 1a**). These conditions are and limited by the stability of the Si-H bonds (up to 440°C). As

reference data, we also obtained the same ML(1 monolayer of oxide is define when the emission ratio between the SiOx and Si2p in XPS equal to 0.21)¹⁸ intensity under equilibrium reaction conditions. Compared to the composition of the oxide layer (at ML<1), the SiO₂ content increased to 66.97% while the sub-oxide content decreased to 27.3% at ML>1.

Figure 1. (a) is a schematic diagram for the annealed pulses process along the different stages from ML = 0, to ML <1 and ML >1. (b – f) Left hand Normalized current values (current value/ I_{on}) for 0.6, 1.35, 2, 2.7 and 4.6 oxide ML, respectively. The Hysteresis were measured on single Si NWs based FET, the right hand is the actual current, the blue arrows represent the direction of the voltage change.

To reveal the electrical properties of the Si NWs after the annealing pulses, a current-voltage diagram was used (see **Figure 1b-f**), measurement conducted in vacuum condition. A single Si NW was used as the conductive channel of a Field Effect Transistor (FET) between two gold electrodes representing the source and drain. The interface composes of Si/SiO_x/Ti/Au producing Schottky barrier, therefore, the charge extraction process takes place in the electrodes (see SI)¹⁹. Two main results were clearly observed: (i) hysteresis loop, which decreases with increasing the

perturbation pulses (**Figure 1b-f**), and (ii) a transition from n-type conductivity to p-type conductivity after forming a full monolayer. Therefore, a hole accumulation layer is produced at the surface and a dynamical surface states appeared during the surface modification.

The transition in the conductivity from n-type to p-type is attributed mainly to two processes: first, SCTD via the redox reaction, second, the perturbation of the reaction equilibrium. The relation between these two processes is shown by the redox couple based chemical reaction ($\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightleftharpoons 2\text{H}_2\text{O}$, $V = -5.1\text{eV}$). To this end, the Si-H consumes one electron to produce one water molecule¹² and goes through a transition state that can trap electrons. Evaporating the produced water molecules from the surface leaves vacancies at the Si surface with a lack of an electron, and as a result, a hole transport layer is produced at the surface. Thus, P-type doping is occurring and p conductivity can be detected and a change in the current value by 3 orders of magnitude was found as shown in **Figure 1**, for carrier concentration see table S1 in SI. It is worth to mention that by etching the surface again, the conductivity and the fermi level back to the same initial position, in addition, stability measurement at ambient condition has been conducted, see supporting information. Alternatively, when maintaining the equilibrium conditions, electrons can transfer from the Si surface to the water molecule and vice versa, as a result, no net charge transfer is occurring and a constant fermi level can be detected (**Figure 3c**). Thus, the reaction kinetics is attributed to the production of surface transport layer that controls the overall behavior of the device. With this mind, the raising of temporary dynamical surface states that can be charged and discharged under an applied bias can explain the observed hysteresis.^{20,21} To explain the hysteresis, a First principles calculation has been employed (see SI) based on density functional theory (DFT) using the climbing-image nudged elastic band (NEB). This method was used to assess the difference in the charging and discharging processes of the trap center to explain the physical

mechanism behind the observed hysteresis loops. The formation energy for neutral, positive and negative transition states was calculated as a function of the Fermi level. In minimal energy configuration, the hydrogen trap in the neutral state is localized at the center of an interstitial void. In the positively charged state, hydrogen is coordinated with an oxygen atom, while in the negatively charged state, the hydrogen atom is bound to a Si atom. A nonsymmetrical barrier was found, with the transition state along the energy pathway in between Si-H states (**Figure 2a**), with a reaction coordinate equal to 0.5, and Si-OH⁺, with a reaction coordinate equal to 1, which can be overcome via an applied bias. The formation energy is written as $E_f = E_{TOT} - (E_{UNP} + E_{H2}/2) - n\mu$, where E_{TOT} and E_{UNP} are the total energies of the system with a hydrogen trap and the unperturbed system without a trap, respectively, and E_{H2} is the total energy of the isolated hydrogen molecule, with $n = 0$ for a neutral system and $n = +1$ and -1 for negatively and positively charged systems respectively (**Figure 2b**). The electron Fermi level μ is related to the valence-band edge E_V in the unperturbed system according to the equation $\mu = E_V + \Delta V + x$, where x varies from the valence ($x = 0$ eV) to the conduction ($x = 5.6$ eV) band edge and ΔV accounts for the shift of the average potential of the system with the trap relative to the unperturbed system. It was calculated that the production of two states of opposite charge in the middle of the gap (when they have the same formation energy) corresponds to a gain of energy of $2E_{+/-} = 2.7$ eV. The formation energy of the positive state is lower than the formation energy of the negative state when the Fermi level is above $\chi_{+/-} = 2.8$ eV. In addition, at a Fermi level above 4.2 eV, the formation energy of the negative state becomes greater than 0, i.e. formation of the negative state is not favorable based on thermodynamic rules. This reasoning indicates that the only states that can appear in our system above 4.2 eV (binding energy of 99.6 eV, corresponding to 0.88 eV in as explained later **Figure 3b**) are the neutral (Si-H) and positive (Si-OH⁺) states (**Figure 2a&b**). This result emphasizes that

the transition from a positive to a neutral state and vice versa is responsible for the hysteresis loop as expected (the Fermi level in our system changes from 4.2 to 4.4 eV, **Figure 2b**). Specifically, the neutral-state to positive-state barrier is approximately 0.82 eV, whereas the opposite barrier (from positive to neutral) is 0.89 eV (**Figure 2a**). These energy barriers are much lower than those calculated for H bridge defects and comparable to those calculated for hydroxyl- E' defects for the transition from neutral to positively charged states in amorphous silicon oxide.²² Calculated differences in energy barriers (0.07 eV), represent the difference in the charging and discharging processes, and lead to hysteresis loops in the I-V graph, as shown in **Figure 1b-e**.

Figure 2. Charge trap states at the surface. (a) Calculated Energy pathways between negative and neutral and between neutral and positive states of charge of the hydrogen trap in the silicon oxide, where the energy of the states (black squares) is interpolated as the blue curve for visualization purposes. Yellow spheres are Si, white spheres are H, and red spheres are O atoms. (b) Formation energy for different charge states as a function of the Fermi level (the red line is the formation energy of Si-H⁻, the blue line is the formation energy of Si-OH⁺, the black dotted line is the formation energy of the neutral H trap, and the blue arrows track the minimal formation energy path).

To investigate the fermi level of the surface we measured the XPS after each annealing pulse. Interestingly, the Si2p_{3/2} emissions shifted to a lower binding energy, indicating for increase in the positive charge of the Si atoms, as illustrated in **Figure 3a&b**. It's worth to mention, continuing the oxidation process (above 4.6 ML) will lead to surface charging (See SI) and an increase in the

binding energy will occur, thus, we stop the oxidation process at 4.6 ML, this value presents the upper limit of such surface doping. This unforeseen shift suggests that the surface chemistry proceeds via the suggested mechanism and affects the electronic properties.

Figure 3. (a) Si2p_{3/2} emission of the Si NW surface measured by XPS, which shifted to a lower binding energy by the annealing pulses. The x100 represents 100-time magnification of the oxide emission indicating the formation of sub-oxides. (b) Si2p_{3/2} binding energies measured relative to the Fermi level and converted to the SFL position with respect to the valence band edge E_V of Si. The Si2p emission, (left) is the corresponding SFL according to our model, the insight is the band diagram of the emission. (c) Si2p_{3/2} binding energy with and without annealing pulses. The red line represents the Si2p_{3/2} binding energy position without annealing (red line). The black line represents the Si2p_{3/2} binding energy position after annealing pulses. The transparent light blue represents ML > 1.

To measure this shift precisely, we aligned the Si2p_{3/2} emission with the Surface Fermi Level (SFL). At first step, we extract the Si2p_{3/2} emission from the Si2p emission by splitting into Si2p_{1/2} and Si2p_{3/2} emissions (**Figure 3a**). Then based on the fact that Si2p has a constant binding energy relative to the valence band, the measured difference between the obtained SFL and energy of the valence-band maximum ($E_V - E_F$; when p⁺⁺ used) and conduction band minimum (E_C ; when n⁺⁺ used) were 98.72 ± 0.02 eV and 99.84 ± 0.02 eV respectively. These values agree for bulk Si as previously published by our group, Ristein and Himpsel.^{7,9,23,24} The difference between the SFL in the two samples, (p⁺⁺ & n⁺⁺), equals 1.1 ± 0.04 eV, which is the difference between E_C and E_V and represents the energy gap and midgap is at 99.31 ± 0.03 eV (**Figure 3b**). Anticipating the corresponding edge values of the E_C , E_V and midgap with the relevant Si2p_{3/2} positions, it is possible to align the binding energy with the SFL scales and the shift direction. We can infer that the Si2p_{3/2} of the freshly etched sample (i.e. Si-H surface) is n-type with a binding energy of 99.6 ± 0.02 eV,

which corresponds to the SFL of 0.88 eV above the valence band. In the equilibrium regime, the SFL maintains its value without any shift (**Figure 3c**). However, as the annealing pulses start (from 100°C to 400 °C), the equilibrium is perturbed on the VLS-grown Si NWs, and a gradual shift of the SFL is observed from 99.62 ± 0.02 eV to 99.42 ± 0.02 eV (Fig. 3b). Note that since the Si2p_{3/2} signal is an average of the Si-Si bonds at the surface and Si-Si bonds of the bulk, due to the sampling depth for 3nm, the total shift, 200 meV, can be higher showing an inversion from n-type to p-type. As the shift is to lower binding energy, this indicates for a positive charge accumulation at the Si surface i.e. more p-type character as was shown in the conductivity measurements, in addition, etching the oxide layer that produced in non-equilibrium condition take us back to the initial Si2p emission and n-type conductivity.

To further assist this conclusion, we measured the work function (Φ) *in-situ* using a μ -KP in the Si2p_{3/2} emission area, to have a schematic study for the same spot that was measured by XPS. The surface electron affinity (χ) was calculated by $\chi = \Phi - E_g + (E_F - E_V)$, where E_g is the band gap (1.12 eV), E_F is the SFL and E_V is the valence band maximum.¹¹ As illustrated in **Figure 3c**, the higher the perturbation (annealing pulses), the more oxide layer grows, the higher Φ and χ are, and the lower the SFL is. Specifically, prior to oxide thickness of ML < 1, slight increases were observed in Φ ($\Delta\Phi \sim 0.1 \pm 0.02$) and χ ($\Delta\chi \sim 0.11 \pm 0.02$ eV) and a marginal change in the SFL position (< 20 meV). However, after perturbing the reaction equilibrium beyond ML > 1, Φ and χ increases by 0.65 ± 0.03 eV and 0.47 ± 0.03 eV, respectively, and the SFL notably decreases by 200 ± 0.02 meV (**Figure 3c**). The nonsymmetrical increase in the χ and Φ , indicates again our conclusion from the hysteresis and the theoretical calculation that we have a charge transfer and as $\Delta\Phi > \Delta\chi$ we have an electron depletion i.e. SCTD process.

In summary, we demonstrate that pulse annealing approach for disturbing the reaction equilibrium on the SiNW surface has been successfully applied. The switch of n and p semi-conductive types is achieved, and its mechanism are well studied theoretically and experimentally. The investigation by first principles calculations revealed that Si-O-Si, Si-H and (Si-OH)⁺ surface functionalization is present on the surface at the initial stage of oxidation and that the traps charge/discharge process can explain the hysteresis loops observed in the I-V plots. The reported results quantify the significant role of surface chemistry kinetics in nano-regime on the electronic properties of nanomaterials and illustrate important insights into the impact of surface properties for integrating nano-semiconductor based devices into nanotechnology research and industry.

Supporting Information

The Supporting Information is available free of charge via the internet at <http://pubs.acs.org>.

Synthesis of Si NWs, Si NWs hydrogen termination, Oxide states growth on H-Si NWs, Device Fabrication, Density functional theory calculations, Characterization of Si NWs, Work function measurements by the Kelvin probe method, Electron Hole concentration calculation, Stability of the Si NW in ambient condition and Surface charging.

Notes

The authors declare no competing financial interest.

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