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Water passivation effect on polycrystalline silicon nanowires

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Defects present in the grain boundaries of polycrystalline materials are known to impede carrier transport inside the materials, and the electronic device performance having such materials as active channels will be adversely affected. In this work, dramatic improvement in device performance was observed as field-effect transistors with polycrystalline silicon nanowire (poly-SiNW) channels were exposed to a wet environment. Passivation of defects in the poly-SiNW by H^+ and/or OH^- contained in the aqueous solution is proposed to explain the phenomenon. © 2007 American Institute of Physics. [DOI: 10.1063/1.2814033]

Field-effect transistors (FETs) have been proposed for chemical sensor applications since 1975 by Lundstrom *et al.* who reported a hydrogen-sensitive FETs with palladium as gate metal.¹ In addition to gas detection, FETs can also be used to measure *pH* or ions in aqueous solutions.² In those early works, the test devices adopted a planar structure having a channel exposed to the environment. However, the sensitivity is seriously affected by the leakage current from source to drain through the bulk of the substrate. To address this issue, recently a sensing structure utilizing Si nanowire (SiNW) as the channel was proposed.³ Owing to the high surface-to-volume ratio, the bulk leakage could be effectively suppressed and, thus, the sensitivity is greatly improved. Such SiNW sensors have demonstrated their function in detecting protein,³ DNA,⁴ glucose,⁵ and virus.⁶

The aforementioned works on biological sensing applications employed monocrystalline SiNWs as the channel, enabling a high carrier mobility which is essential for good device performance. Recently, we investigated the use of polycrystalline silicon (poly-Si) NW channels for building electronic devices.^{7,8} The scheme we proposed could greatly simplify the fabrication flow. However, defects contained in the grain boundaries of the poly-Si NW would impede carrier transport and thus degrade the mobility.⁹ For biological sensors, the polycrystalline nature of NWs raises the concern of sensitivity degradation. In this work, we show that such concern could be lifted as long as the measurement is carried out in an aqueous solution.

Here, we briefly describe the fabrication of the poly-Si NW devices. A thermal oxide of 100 nm was first grown on a silicon wafer. Then a 90-nm-thick amorphous silicon film was deposited on the wafer using a low-pressure chemical vapor deposition system. After doping of source/drain (S/D) regions using ion implantation technique, the film was then transformed into polycrystalline via an annealing step per-

formed at 600 °C in nitrogen ambient. The SiNW channels and S/D regions were patterned simultaneously using e-beam lithography and subsequent plasma dry-etch step. Figure 1 shows the scanning electron microscopic (SEM) picture of a device, which contains six NW channels. Afterwards, a passivation oxide was capped on the wafer surface. The SiNW channels were then exposed by removing the covering oxide, and the entire device was then enclosed in a microfluid sample delivery structure with an aim of performing electrical measurements in an aqueous environment. During the measurements the Si substrate itself serves as the gate electrode upon which a bias is applied to modulate the drain current.

Typical characteristics of the NW transistors at room temperature are shown in Fig. 2. First, the measurement was carried out in a dry ambient. Afterwards, de-ionized (DI) water was injected and flowed through the microfluid cavity to immerse the NW channels, and then the same measurement scheme was repeated. Detailed performance parameters are summarized in Table I. Two distinct features are found.

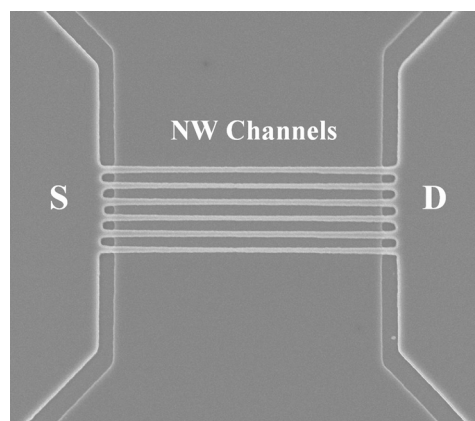


FIG. 1. SEM picture of a device which contains six NW channels. Planar width and thickness of each NW is 70 and 90 nm, respectively.

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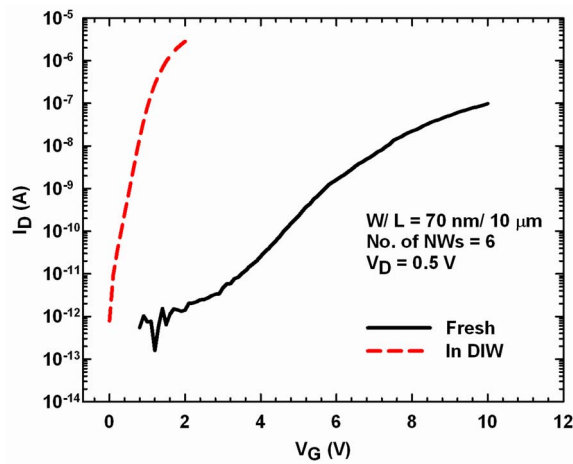


FIG. 2. Transfer characteristics of a device operating in dry and wet (DI water, denoted as DIW) environments.

First, the subthreshold swing (SS) dramatically reduces as the measurement environment becomes wet. Note that the very large SS value recorded in the dry ambient is consistent with the fact that the polycrystalline material used in this study contains a large amount of defects. These defects act as trapping centers for carriers⁹ and tend to slow down the modulation of channel surface potential with increasing gate voltage. Dramatic reduction in SS of the device when operating in a wet environment implies that those trapping sites become ineffective. The other important finding is the significant increase in mobility and the saturation drain current when measured in a wet environment. This again evidences the decrease in the amount of active defects in the channels, which is further confirmed by extracting the trap density (Table I) using the Levinson method.¹⁰ These differences originating from the different measurement environments imply that the ingredients contained in the water play an essential role in modifying the conduction behavior of carriers inside the NW. It is worth noting that when measured in a wet environment, the performance of poly-Si NW devices is almost on a par with that of monocrystalline-Si NW devices.¹¹

Passivation of defects in poly-Si by hydrogen-related species is well-known and has been utilized extensively for improving the device performance of poly-Si thin-film transistors (TFTs). Such treatment is typically done by exposing the devices to an H-containing plasma¹² or via a high-pressure water vapor annealing step.¹³ Since the TFTs are

TABLE I. Comparisons of device performance parameters measured in dry and wet (DI water) environments.

Ambient	Dry	Wet
Threshold voltage (V)	6.8	0.7
Mobility ^a (cm ² /V sec)	75	126
Subthreshold swing (V/decade)	1.1	0.2
Trap density ^b (10 ¹² cm ⁻²)	1.2	0.41

^aThe channel width used in mobility extraction procedure is 70 nm (the planar width of the SiNW) for the case of dry ambient. However, owing to the high dielectric constant of water (~ 80), a gate-all-around operation scheme is assumed for the case of wet ambient. In other words, the effective width is assumed to be 320 nm (the total edge length of the NW's cross section) for the case of wet ambient.

^bTrap density was extracted using the method presented in Ref. 10.

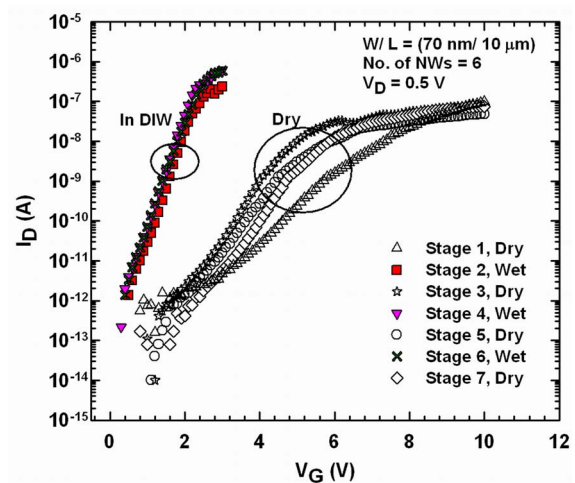


FIG. 3. Transfer characteristics of a device operating in seven stages of alternative dry and wet environments. Period of each stage is about 14 min.

normally capped with a dielectric (typically a silicon oxide layer), these process treatments are usually performed at an elevated temperature to enhance the passivation mechanisms. Among the previously developed techniques, the process ambient of high-pressure vapor anneal contains same ingredients as the wet environment investigated in this work. So we postulate that similar mechanism may occur in our devices. The DI water is neutral with pH value of 7. This means that the concentration of H⁺ (and OH⁻) is 10⁻⁷ mole/L or 6.02 × 10¹³ cm⁻³. This value is actually much higher than ion density in typical H-containing plasmas ($\sim 10^{10}$ cm⁻³).¹² The abundant H⁺ and/or OH⁻ may diffuse into the grain boundaries and terminate on the dangling bonds wherein. As a consequence, the amount of electrically active defects is substantially reduced, resulting in a dramatic improvement of device performance.

To test the reproducibility of the water passivation effect, measurements were repeatedly performed on a device which went through seven stages of exposure to alternate dry and wet environments. Within each stage the device was characterized several times to confirm the stability of device performance, and the representative I - V curves for all stages are shown in Fig. 3. Clearly, the device characteristics recover when the device was switched from wet to dry environment and vice versa. Also worth noting in this figure is that the passivation effect occurs only in water, indicating that the passivation bonds are not stable and could easily be desorbed from the poly-Si NW when the water is pumped away from the microfluid cavity.

The significance of the water passivation effect found in this work is that it can be cleverly used to boost the performance of poly-Si NW devices to a level comparable to the monocrystalline counterparts.¹¹ This scheme is thus suitable for biologic sensing applications, which are usually done in aqueous solutions. Since poly-Si is easier to grow and prepare on a number types of substrates, this finding is attractive for biological sensing device fabrication in terms of lower complexity as well as reduced cost.

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