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The Role of Aluminum Catalyst Atoms in Shaping the Structural and Electrical Properties of Epitaxial Silicon Nanowires

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1. Introduction

Silicon nanowires (SiNWs) have been attracting a great deal of attention as important components for future electronic, optoelectronic, photovoltaic and sensor nanodevices [1]. So far Au has dominated as the catalyst for growing silicon nanowires via the vapor-liquid-solid mechanism [2]. Unfortunately, Au is a deep level dopant, which traps charge carriers and poses serious contamination problems for Si-based devices processing. Al is by far more attractive as catalyst to grow SiNWs compatible with CMOS requirements. A first demonstration of the growth of monocrystalline silicon nanowires catalyzed by Al (Al-SiNWs) was reported recently by our group [3]. In this paper, we will show that Al-SiNWs exhibit superior structural and electrical properties compared to the widely investigated gold-catalyzed Si nanowires (Au-SiNWs) [4]. Indeed, we found that that the use of Al as a catalyst leads to atomically smooth SiNWs in contrast to rough {112}-type sidewalls observed in Au-catalyzed SiNWs. We found that the stabilizing effect of Al plays the key role in the observed nanowire surface morphology. Additionally, in spite of using temperatures of 110-170 K below the eutectic point of Al-Si system, we found that the incorporation of Al into the growing nanowires is sufficient to induce an effective p-type doping of SiNWs. Besides circumventing the detrimental deep level doping, the use of Al as a catalyst yields SiNWs with superior structural properties.

In order to elucidate the role of Al catalyst atoms in the observed distinct structural properties of Al-SiNWs we combined high-resolution cross-sectional transmission electron microscopy (HRXTEM), spot-profile-analyzing low-energy electron diffraction (SPA-LEED) and scanning tunneling microscopy (STM). The electrical properties of individual as-grown nanowires were characterized using conductive atomic force microscopy. The exact amount and distribution of Al catalyst atoms within a single nanowire were obtained using 3D Local Electrode Atom Probe Tomography (3D-LEAP). Details of LEAP tomographic sample preparation using the focused-ion beam liftout technique will be presented and a method to circumvent Ga ion-induced radiation damage will be discussed

2. Low Temperature Growth of Al-SiNWs

SiNWs growth experiments were carried out in an ultrahigh vacuum chemical vapor deposition reactor (UHV-CVD) with a background pressure of $< 1.0 \times 10^{-10}$ mbar. Phosphorous- and boron-doped Si(111) wafers were used as substrates in our experiments. The substrates surface was conditioned by a standard wet chemical cleaning followed by a dip in 2% hydrofluorid acid to hydrogen-passivate the surface. The wafers were immediately transferred into the UHV-CVD reactor. A 1 nm-thick Al film was then deposited *in situ* onto the substrate by a thermal evaporation source. Immediately after Al deposition, the substrate was annealed for 30 min at 600 ºC. The growth of Al-SiNWs was accomplished by using monosilane (diluted to 5% in argon). The partial pressure of the silane was kept below 0.15 mbar.

3. Structural Properties of Al-SiNWs

Figure 1 displays a scanning electron microscopy (SEM) image of Al-SiNWs grown at 410 ^{o}C. The grown nanowires display a high density and good uniformity with an average diameter and height of 35 nm and 300 nm, respectively. The growth at higher temperature was found to lead to slightly tapered nanowires as demonstrated in Fig. 2 showing a XTEM of Al-SiNWs grown at ~470 ºC. The interesting observation here is the absence of rough sidewalls previously reported for SiNWs grown using Au as catalyst. Indeed, Al-SiNWs were found to display atomically smooth sidewalls surface (Fig. 3). Using SPA-LEED and STM, we found that the observed surface morphology is attributed to the Al stabilizing effect of Si(112) surfaces (making the nanowire sidewall), which manifests by revoking the reconstruction along the $[\bar{1}\,\bar{1}\,2]$ direction leading to equivalent adjacent step edges and flat surfaces. Our finding suggests that the Al density on the nanowire surface is at least 2 atom/nm^2. Owing to the high surface-to-volume ratio, the surface structure and morphology define the nanowire transport properties[18,19]. Thus improved charge carrier transport should be expected for smooth nanowires due to the weak surface scattering as compared to rough surfaces. Similarly, the reduced phonon scattering at smooth surfaces can lead to higher thermal conductivity, which is suitable to manage the heat in SiNW-based devices. Smooth surfaces are also convenient for the growth of nanowire heterostructures such as core-shell *p*-*n* junctions.

3. Electrical Properties of Al-SiNWs

Besides the aforementioned influence of Al on the structural and morphological properties of Al-SiNW surface, the incorporation of Al into the growing nanowires is expected to yield *p*-type doping [6]. We exploited this phenomenon to implement a device made of an array of vertically aligned as-grown Al-SiNWs grown on *n*-type Si(111) as schematically illustrated in Fig. 4a. We found that this device behaves as a well-defined *p*-*n* junction (Fig. 4).

More details on the doping level as well as Al distribution within a single nanowire will be presented.

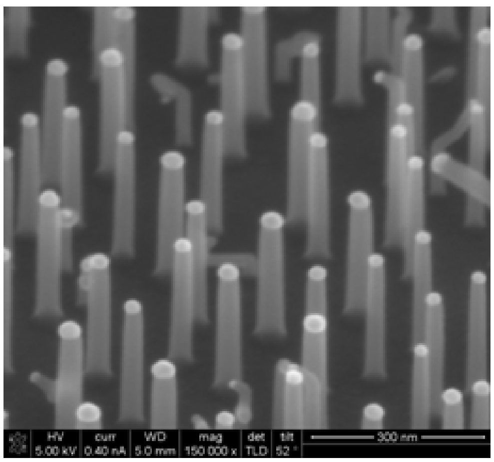

Fig. 1 A SEM image of Si nanowires synthesized in a UHV-CVD reactor at a temperature of ~400 ºC using Al as catalyst.

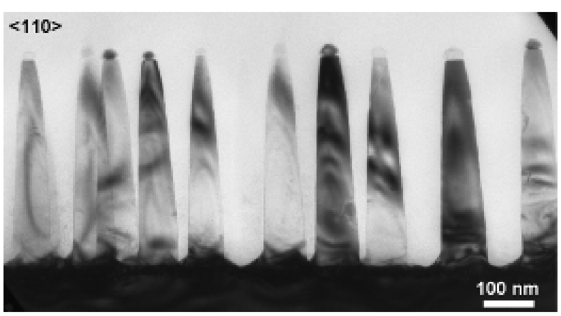

Fig. 2 XTEM image along the <110> direction of Al-SiNWs grown at 470 ºC. The letter “F” indicates the nanowires with faceted catalyst nanoparticles.

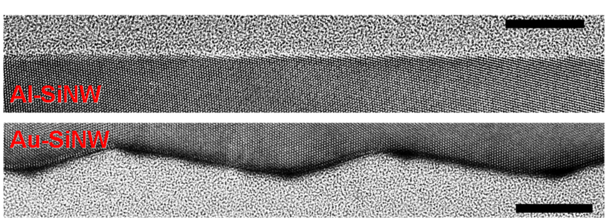

Fig. 3 HRXTEM images of sidewalls of Al-SiNW (top) and Au-SiNW (bottom) grown at similar temperatures. Note that Au-SiNW sidewall surface is rough with well-defined facets, whereas Al-SiNW sidewall is atomically smooth. The scale bar denotes 10 nm.

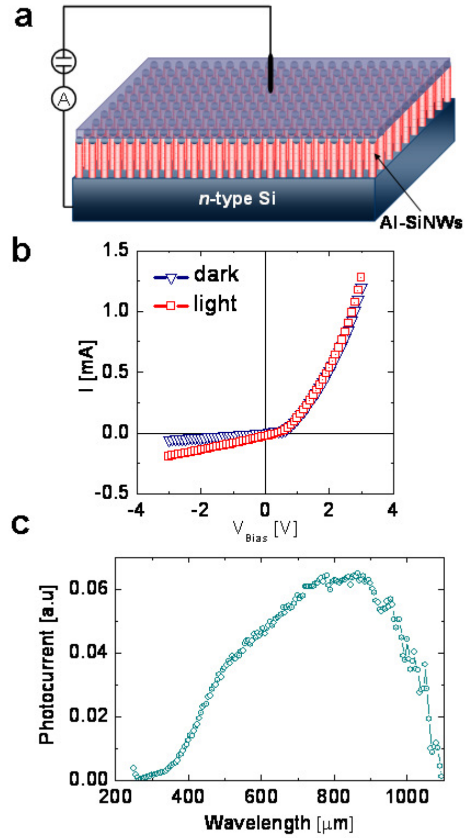

Fig. 4 **a**, Schematic illustration of a device made of an array of Al-SiNWs vertically aligned on *n*-type Si(111). For the fabrication of the device, as-grown Al-SiNWs were first capped in a polymer. By using reactive ion-etching, the deposited polymer cap was partially etched until the tips of the nanowires emerge. Afterwards, a metal contact was deposited by evaporation on area containing up to ~9×10^4 nanowires. **b**, The dark and under illumination *I*-*V* characteristic curves of the device described in **a**. **c**, The spectral distribution of the generated photo-current in the device described in **a**.

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