Carbon-Conducting nanostructures to promote high density Si nanowires growth

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Due to the critical demand for high-energy, compact Li-ion batteries are increasingly driven by technologic industry for the operation of multiple telecommunications, computer and entertainment devices, as well as clean transportation vehicles [1]. Nowadays, a point of great interest is to find an alternative material with a Li storage capacity higher than that of graphite (372 mAh g⁻¹) that is the actual common commercial anode-material. Among the several candidates, silicon has much research attention because it exhibits the highest known theoretical capacity, i.e., 4200 mAh g⁻¹ [2]. The ultrahigh capacity of silicon stems from the fact that in the electrochemical reaction 4.4 Li atoms are incorporated by each Si atom, compared with the insertion mechanism of graphite. However, incorporating a huge amount of Li⁺ inevitably causes gigantic changes in volume and an intense lattice strain; consequently, particles are pulverized and electrical connections are lost. Another limitation to the high performance of silicon comes from its semiconductive character that hinders the electrode redox process and electronic diffusion, compared with the good conductivity of the graphite.

In this study, we present a simple procedure to avoid both difficulties that are present when silicon is used as anode material. By one hand, instead of bulk silicon, Si nanowires (SiNWs) are synthesized because of the 1-D nanostructures can better accommodate the changes in volume and mechanic strain thanks to their large elasticity. On the other hand, electronic conduction can be improved by the addition of different carbon-conductive nanostructures on the anode electrode. Herein, we report the use of carbon nanostructures as supporting material in the synthesis of SiNWs that promotes a high density of nanowires growth.

We use crystalline Si (100) and other substrates, covered by the nanostructures and a thin film of gold. The silicon nanowires were synthesized by thermal treatment (900 °C) at ambient conditions with a flux of hydrogen and argon during 30 min. The details of this method have recently been reported [3]. It is necessary for the nanowire growth that the substrate has an adequate roughness; in this way, during the thermal treatment, the gold film becomes nanoparticles which catalyze the nanowires formation.

For this purpose, silica nanospheres were the first nanomaterial used as supporting for the synthesis of SiNWs. The silica nanospheres were fabricated by controlled hydrolysis of alkyl following the Stöber-Fink-Bohn method [4]. The curved surface of these nanostructures makes gold film agglomerates in particles of nanometric size by superficial stresses and these nanoparticles catalyze the nanowires growth following a vapor-liquid-solid (VLS) process (Fig. 1). In light of these positive results, we introduced a new improvement, changing silica nanospheres by carbon spheres that were synthesized according to a process of dehydration and condensation of sugar [5]. Due to the low conductivity of the SiNWs, the introduction of a conductive material on the interface of silicon nanowires would allow the electron transfer during the charge/discharge cycles.

From the viewpoint of electronic conduction, we moved in the direction to include graphene and carbon nanofibers as supporting material for the SiNWs synthesis process. These materials are massless charge carriers with high mobility. The results obtained were successful and a high density of SiNws was obtained by using these carbon-conducting materials onto the substrates (Fig. 2).

A full characterization has been performed with the synthesized SiNWs, which includes Atomic Force Microscopy (AFM), field emission scanning electron microscopy (FESEM), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS).

The results of this work demonstrate the favorable role of inclusion carbon-conducting nanostructures in the substrates for SiNWs growth. We show the improvement of them for silicon nanowire synthesis, as well as the good electron conductivity of the electrode.

References

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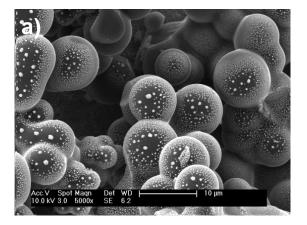
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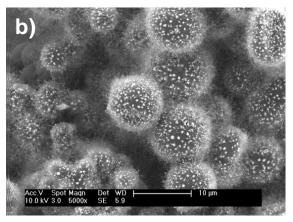
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Figure 1

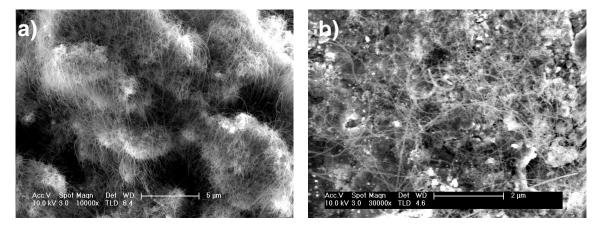




FESEM images of carbon spheres after a thermal treatment at 900℃ by using 5 nm of Au as catalyst.

- a) Au nanoparticles formation in absence of H_2 gas
- b) SiNWs synthesis from Au nanoparticles

Figure 2



FESEM images of SiNWs growth on Si substrates using carbon-conducting nanomaterials as supports:

a) Carbon nanofibers

b) Graphene