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Sustainability Analysis of Silicon Nanowire Fabrication for High Performance Lithium Ion Battery Anode

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Abstract

Silicon nanowires (SiNWs) are synthesized by two-step metal-assisted chemical etching (MACE) using different etching parameters including $AgNO_3$ concentrations (5/20/50 mM) and H_2O_2 concentrations (0.03/0.1/0.3 M). Diameter distributions of synthesized SiNWs with different parameters are analyzed. Gas emissions and nanoparticle wastes in SiNWs synthesis process are theoretically calculated and experimentally tested. The effects of etching parameters on etching rate are investigated.

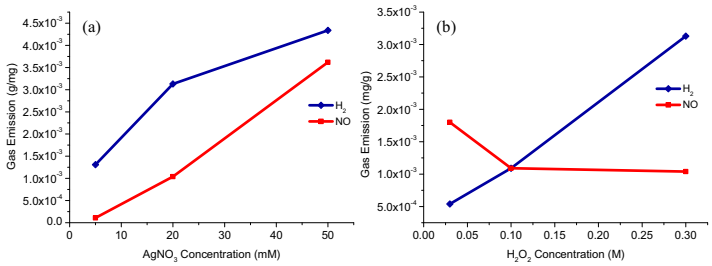

Fig. A.. Gas emissions with different etching conditions. (a) H_2O_2 0.3 M with variable $AgNO_3$ concentrations (5/20/50 mM); (b) $AgNO_3$ 20 mM with variable H_2O_2 concentrations (0.03/0.1/0.3 M).

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1. Introduction

Silicon has a high theoretical specific capacity (4200 mAh/g) and has been widely recognized as the ideal anode material for lithium ion batteries (LIBs). However, bulk Si used in LIBs suffers from substantial volume change during the charging/discharging which leads to structural cracking and even pulverization [1]. Nanostructured Si has been investigated as a possible solution to this issue. In particular, silicon nanowires (SiNWs) are widely studied as a promising anode material for high-capacity LIBs.

A variety of methods have been explored for fabrication of SiNWs, including chemical vapour deposition (CVD) [2], thermal evaporation [3], chemical etching [4], laser ablation [5], molecular beam epitaxy [6], etc. However, these methods are with grave concerns on their sustainability performance, due to the high energy consumptions, toxic chemicals utilizations, gas and nanoparticle emissions from these processing techniques.

Among these methods, metal-assisted chemical etching (MACE) is one of popular methods for fabricating SiNWs due to its low cost, low energy consumption, and simple processing procedure. In general, MACE can be classified into two types, involving one-step (MACE-I) and two-step (MACE-II) reactions. In the one-step process, the SiNWs are produced by immersing Si wafer into an HF/$AgNO_3$ aqueous solution of a given concentration for an appropriate time. In the two-step process, silicon wafer is first immersed in HF/$AgNO_3$ solution to deposit metal catalyst, and then the wafer is transferred to HF/H_2O_2 solution for nanowire formation.

In this paper, two-step MACE of Si wafer is used to synthesize SiNWs with different etching parameters including $AgNO_3$ concentrations (5/20/50 mM) and H_2O_2 concentrations (0.03/0.1/0.3 M). Diameter distributions of the synthesized SiNWs with different parameters are analyzed. Gas emissions and nanoparticle distributions in SiNWs synthesis processes are theoretically calculated and experimentally tested. The effects of etching parameters on etching rate are investigated as well. This study can be helpful in understanding the potential environmental impacts of the SiNWs fabrication process and aid in control of the process emissions for reducing its potential impacts on both the environment and occupational health in future.

2. Experiment

Chemicals used in the experiment: acetone (Sigma-Aldrich, ACS reagent 99.5%), ethanol (Sigma-Aldrich, ACS reagent 99.5%), $AgNO_3$ (Sigma-Aldrich, ACS reagent 99.0%), hydrofluoric acid (HF, Sigma-Aldrich, 40%-45%), H_2O_2 (30%), nitric acid (HNO_3, 70%).

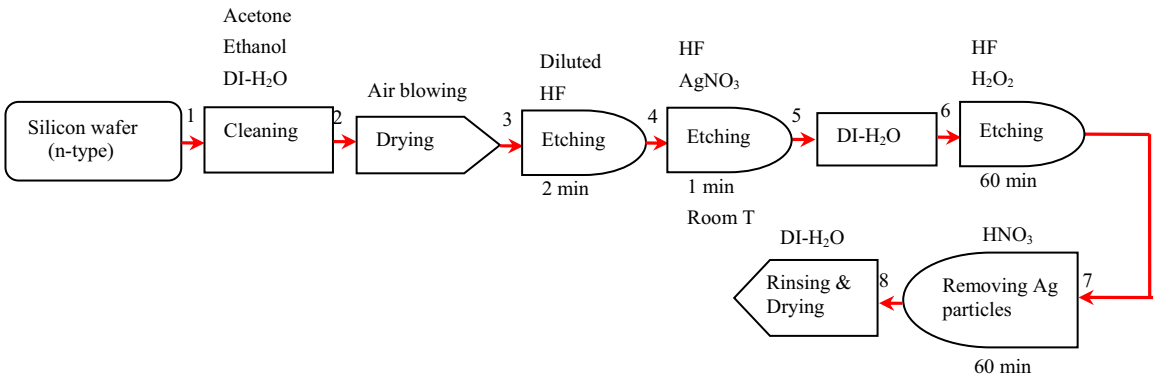

Fig. 1. Experimental flow chart for synthesis of SiNWs using Si wafer.