Journal of
NANOSTRUCTURES
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Study of System Pressure Dependence on n-TiO_2/p-Si Hetrostructure for Photovoltaic Applications

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Article history:
Received 3/12/2014
Accepted 9/02/2015
Published online 1/03/2015

Keywords:
TiO_2 nanowires
System pressure
I-V characteristics
Hetrojunction

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Abstract

This study reports the fabrication of n-TiO_2/p-Si hetrojunction by deposition of TiO_2 nanowires on p-Si substrate. The effect of system pressure and the current-voltage (I-V) characteristics of n-TiO_2/p-si hetrojunction were studied. The morphology of the samples was investigated by Field Emission Scanning Electron Microscopy (FESEM) which confirms formation of TiO_2 nanowires that their diameters increase with increasing the pressure of system. The I-V characteristics were measured to investigate the hetrojunction effects of under forward and reverse biases at different system pressure by sweeping in the voltage from 0 to +6 V, then to -6 V, and finally reaching 0 V. TiO_2/Si diodes in the system pressure 60 mbar and 30 mbar indicated that a p-n junction formed in the n-TiO2/p-Si hetrojunction. But as the system pressure increased to 1000 mbar, the I-V characteristics became inversed. This treatment can be scribed by the change of the energy band structure of TiO_2.

1. Introduction

Nanowires are crystalline fibers about one thousandth the width of human hair. Small volumes of nanowires make them extremely sensitive photodetectors- much more sensitive than larger photodetecors made from the same materials. Titanium dioxide is a promising oxide for various kinds of industrial application such as gas sensors [1], electronic devices [2-6] and solar cells [7]. photodetectors are important device that have a range of commercial research and military application. When nanoscale materials are utilized, the hetrojunction effect are magnified and become even more critical. A heterostructures device is formed by deposition a wide band gap semiconductor film on a narrow band gap [8]. Semiconductor hetrojunctions can be absorbed a different region of the solar spectrum. With deposition of TiO_2 nanowires on p-Si structures n-TiO_2/p-Si heterojunction photodiodes could be synthesized, that are useful to the performance of photoelectrice detectors. There are some reports on structure and optical properties rutile TiO_2 nanowires grown on Si substrate [9-17]. But to date there have been a few results on the hetrojunction effect and photodiode behavior of TiO_2 nanowires. Therefore, more studies in this field are necessary, especially in nanostructure system. Wang et al. reported that n-TiO_2/C hetrojunction could increase absorption in the visible region and exhibit a higher photocatalytic activity [18].

In this study, n-TiO_2 nanowires were prepared by a thermal evaporation on silicon substrate at 850°C for 1h in horizontal furnace, and the hetrojunction effect under forward and reverse biases at different system pressure was investigated.

2. Experimental procedure

With the use of thermal evaporation method, TiO_2 nanowires were successfully synthesized on p-type silicon as substrate for the n-TiO_2/p-Si heterojunction. Si wafers were ultrasonically cleaned using acetone and ethanol for 10 min. then were coated with a Ti buffer layer with a thickness of 50 nm by the e-beam evaporation technique evaporation rate under the pressure of 10^{-5} mbar. In this step, voltage and current was held to be 4 kV and 100 mA, respectively. A gold thin film was then deposited as a catalyst on the Ti layer by a sputtering system. A mixture of Ti and graphite powder with the ratio of 1:1 was placed in a quartz boat as the source material. The boat was located at the center of a horizontal tube furnace, and the Si substrate was placed over the quartz boat in the low-temperature zone (800-850°C). The tube was heated with the heating rate of 20°C/min up to the temperature 1050°C, and then, held for 1h at the same temperature Then, the substrate was cooled down to room temperature naturally. In the other experiments, with other parameters (i.e. reaction time, heating and cooling rate, deposition temperature, etc.) unchanged, the system pressure was varied from 1000 mbar to 30 mbar by a rotary pump. Thereafter, the samples were taken out for characterization. The structure and morphology of the samples were analyzed by Field Emission Scanning Electron Microscope (FESEM: S-4166, Hitachi) and X-Ray diffraction (XRD: JEOL JDX-8030). To provide a lower contact resistance of electrode, 0.5 mm-diameter Ag dot of circle form was contacted on to TiO_2 surface. In the same manner, a contact was made onto backside of Si wafers. The I-V characteristics were measured in air at room temperature by sweeping in the voltage from 0 to +6 V, then to -6 V, and finally reaching 0 V.

3. Results and discussion

To obtain detailed information regarding the crystallinity, morphology and growth plans of as-synthesized 1D nanostructure, XRD diffraction pattern analyses were performed and representative results are discussed as follows. Figure 1 shows typical XRD patterns of TiO_2 nanowires grown on Si substrate at different system pressure. All the samples indicate that the TiO_2 nanowires are mainly composed of rutile phase, where reflection (101) is the most predominant. Our morphological studies suggested that as the system pressure decreases, the full-width at half-maximum of (101) increases and the intensity become lower. In general, the smaller the FWHM lead to the higher the crystalline, when oxygen environment increases the defects (oxygen vacancies and titanium interstitials) decrease and nearly stoichiometric films are obtained.

Decreasing the system pressure from 1000 mbar to 30 mbar makes a low oxygen environment therefore less crystallinity produce. The unit cell constants, full-width at half-maximum (FWHM) and percentage of crystalline of TiO_2 nanowires listed in table1.

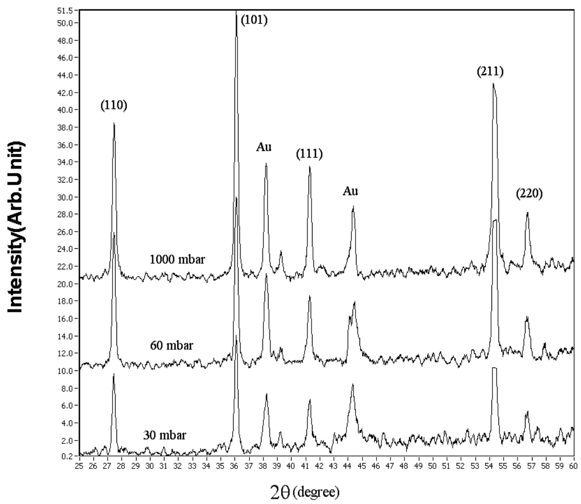

Fig.1 X-ray diffraction pattern of TiO_2 nanowires at different system pressure. It can be seen that TiO_2 nanowires are rutile phase with a dominate reflectance of the (101) plan

Table 1. Unit cell constants and FWHM nanowires at different system pressure

System pressure(mbar)	FWHM	percentage crystalline	a(Å)=b(Å)	c(Å)
1000	0.19	44%	4.586	2.959
60	0.21	37.6%	4.598	2.956
30	0.22	33%	4.593	2.955

The Field Emission Scanning Electron Microscope (FESEM) images of the TiO_2 nanowires at different system pressure have been represented in Fig 2. Fig 2(a) shows the nanowires with a diameter of around 60-120 nm. As the system pressure decreases the nanowires become thinner, so that in the system pressure 60 mbar the nanowire of diameter is 60-100 nm (Fig 2(b)) and in the system pressure 30 mbar the diameter of nanowires decreases to 40-100 nm (Fig 2(c)). The advantage of using low pressure in the fabrication 1D nanostructures can be understood from the fact that lowering the system pressure increases the mean free path and as a result the gas phase transfer to deposition surface is facilitated. Also a low pressure system is beneficial to establish the desired degree of supersaturating for 1D nanostructure.

I-V characteristics of the three n-TiO_2/p-Si diodes are presented in Fig.3. The rectified current characteristic in the system pressure 60 mbar (Fig.3b) and the system pressure 30 mbar (Fig.3c) indicates that a p-n junction formed in the n-TiO2/p-Si nanowires. But as the system pressure increases to 1000 mbar, the I-V characteristics become inversed. This treatment can be scribed by the change of the energy band structure of TiO_2.Oxygen pressure affects the defect densities during deposition. In lower system pressure (30-60 mbar) more oxygen vacancies and Ti interstitials are formed during deposition, which are donors. So the reverse current is small and is almost similar to a common n-p junction. However, the TiO_2 nanowires grown at higher system pressure (1000 mbar) have more acceptors (Ti vacancies and oxygen interstitials). In this case Fermi level must move away from the bottom of conduction band and an energy spike appears at interface between Ti and Si. So that under forward bias electron transfer don not take place and forward current is small. This result is useful for design of photodiodes that reverse current need to be small.

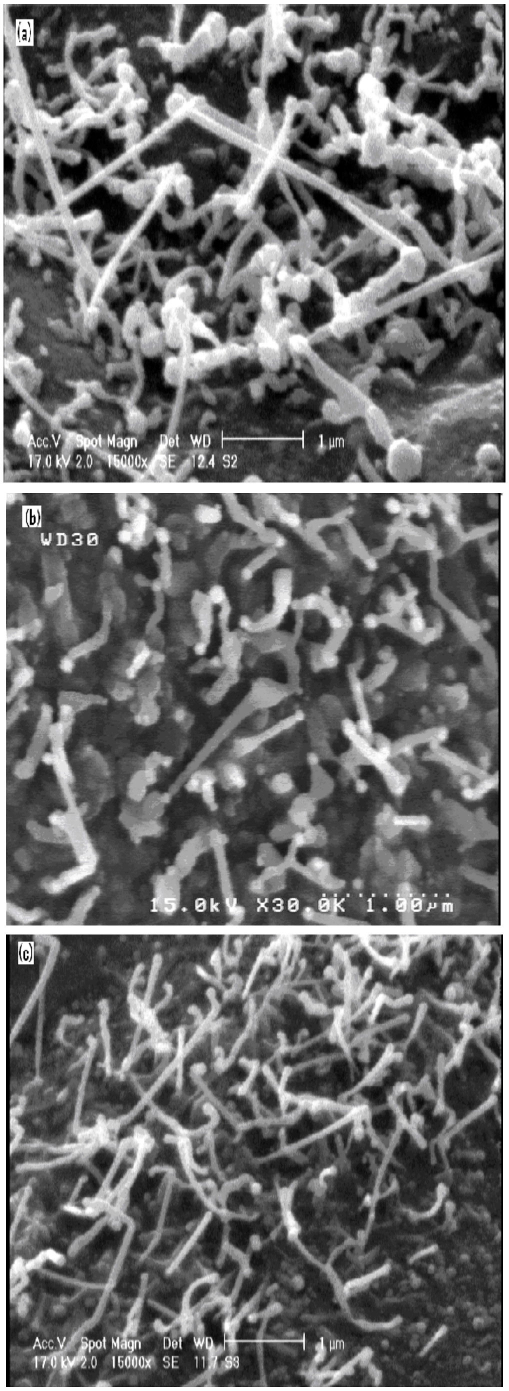

Fig.2. SEM images of as synthesized TiO_2 nanowires at different system pressure: (a) system pressure 1000 mbar; (b) system pressure 60 mbar; (c) system pressure 30 mbar. Scale bar isµ 1 μ m.

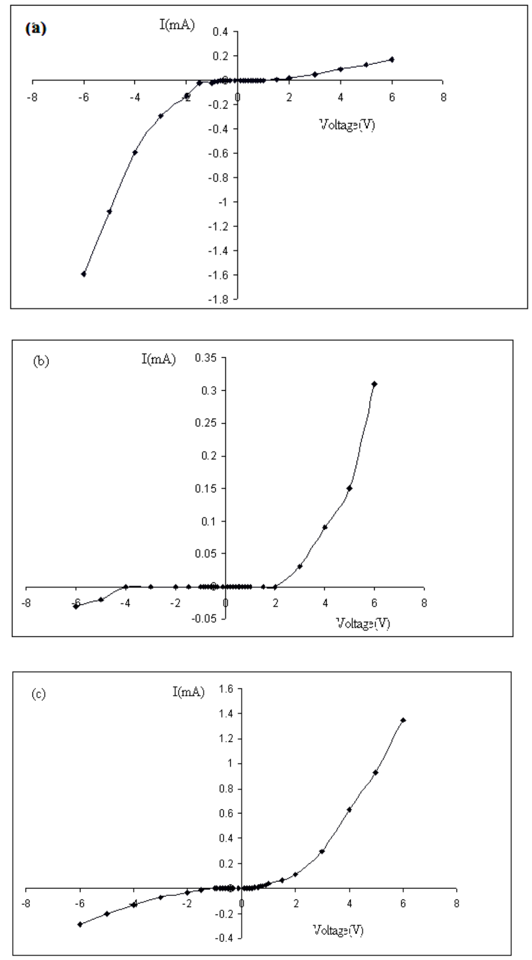

Fig.3. The I-V Curves of the heterojunction:(a) system pressure 1000 mbar; (b) system pressure 60 mbar; (c) system pressure 30 mbar.

4. Conclusion

TiO_2 nanowires were grown by thermal evaporation on a silicon substrate coated with a catalytic Au-coated Ti layer substrate under different system pressure. The rectified current characteristic in the system pressure 60 mbar and the system pressure 30 mbar indicates that a p-n junction formed in the n-TiO2/p-Si nanowires. But as the system pressure increases to 1000 mbar, the I-V characteristics become inversed. This treatment can be scribed by the change of the energy band structure of TiO_2.

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