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Interface properties determined the performance of thermally grown GaN/Si heterojunction solar cells

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Abstract

We report the fabrication of heterojunction solar cells via the thermal chemical vapor deposition (CVD) of gallium nitride (GaN) nanostructures on clean Si substrates. GaN epitaxial layers were synthesized via the direct reaction of Ga vapor and NH_3 solution at 1050 °C. The structural and optical characteristics of the as-grown GaN layers were investigated. The effects of Si orientation (100 vs 111) and doping type (n- vs p-) on the structural and optical properties of the deposited GaN nanostructures and solar cell performance were explored. The fabricated GaN nanostructures exhibited p-type behavior at the GaN/Si interface as revealed from the Hall-effect measurements. The *J–V* characteristics showed rectifying behavior for the GaN/n-Si junction and Ohmic behavior for the GaN/p-Si junction. Upon illumination (30 mW/cm^2), the as-deposited heterojunction solar cell devices showed conversion efficiencies of 6.18% and 3.69% for GaN/n-Si (1 1 1) and GaN/n-Si (1 0 0) heterojunctions, respectively. The growth of GaN on Si substrates in the presence of NH_3 solution has strong effect on the morphological, optical and electrical properties and consequently on the efficiency of the solar cell devices made of such substrates.

Keywords: GaN; Si; Heterostructure; Chemical vapor deposition; Solar cell; Hall measurement

1. Introduction

Recently, heterojunction solar cells involving a wide band gap semiconductor on a single crystalline silicon substrate have attracted considerable interests due to their excellent blue response, simple processing steps, and low processing cost (Chou et al., 2012; Razykov et al., 2011; Salman et al., 2011; Tseng and Lee, 2013; Yamaguchi et al., 2008). To this end, GaN is one of those materials that is of considerable interest not only because of its ability to capture visible short-wavelength and UV light but also because of its high heat tolerance (Yang et al., 2000). Also, the growth of GaN-based opto-electronic devices has extensively been investigated (Calarco et al., 2007; Saron et al., 2013). In addition, the integration of well-established Si electronics with GaN-based photonic devices (optoelectronic integrated circuits, (OEICs)) has also proven lucrative in the manufacturing industry (Peng et al., 2005). Recently, Toshiba began mass production of white LEDs on 200-mm silicon wafers. The epitaxial growth of GaN is highly desirable for the Si-based electronic industry, because it is a promising route for large-scale, low-cost mass production of GaN-based photovoltaic (PV) technology (Asgari and Khalili, 2011; Saron et al., 2013; Tang et al., 2008). GaN has a unique physical

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properties such as high bandgap (3.4 eV), high refractive index ($n = 2.4$), tunable conductivity from 10^{-11} to 10^{-3} S cm^{-1}, high chemical, mechanical, thermal stability, and high breakdown field. Its relatively stable physical properties even under harsh environments make it the material of favor for optoelectronic applications such as field-emission diodes, light-emitting diodes, short-wavelength optical devices and energy conversion solar cells (Kang et al., 2012; Reshak et al., 2013; Tseng and Lee, 2013). Due to the large lattice and thermal mismatches between the GaN and Si, a thin crystalline Si_3N_4 or AlN buffer layer is often deposited to reduce defect formation and alleviate strain relaxation, thus improving the transport properties of the junction (Reichertz et al., 2009; Wei et al., 2006). Tang et al. reported the fabrication of p-GaN nanorods on n-Si single junction solar cell (Tang et al., 2008). Reichertz et al. reported the growth of p- and n-type GaN dual junction solar cell on a standard n-type Si wafer with a thin AlN buffer layer using molecular beam epitaxy (MBE) (Reichertz et al., 2009). The p-type behavior was related to the Al diffusion into the silicon substrate during growth (Ager III et al., 2009) with low series resistance at the nitride/silicon heterojunction (Reichertz et al., 2009). However, the insulating properties of AlN led to a deleterious effect on the transport properties of the junctions (Ager III et al., 2009). Yamamoto et al. (1994) deposited InN and InGaN on p-type Si (1 1 1) by plasma assisted molecular-beam epitaxy (PA-MBE) and observed the rectifying behavior of the junctions whereas Xu et al. (2011) studied n-GaN/p-Si junction but observed no rectifying property, probably due to charge accumulation at the interface layers. Alternatively, one may resort to a metallic surfactant layer or some novel buffer techniques (Hu et al., 2006). Although these techniques are said to improve epitaxial films, their superiority in photovoltaic applications remains to be demonstrated.

Herein, we present a simple and low cost thermal chemical vapor deposition (TCVD) method to fabricate GaN nanostructures single junction on Si substrates. In this work, GaN nanostructures were gown on clean Si substrates through the direct reaction between vaporized gallium (Ga) and gaseous ammonia (NH_3) solution. Also, the first demonstration of GaN/Si heterojunction solar cell performance is investigated. In the light of the obtained results, a mechanism of GaN growth and the effect of the growth process on the performance of PV GaN/Si device are proposed.

2. Experimental procedure

Using a conventional TCVD system, GaN nanostructures were synthesized through a vapor phase transport at 1050 °C on three silicon n-(1 1 1), p-(1 1 1) and n-(1 0 0) substrates via direct reaction of Ga with NH_3. The growth details were reported elsewhere (Saron and Hashim, 2013b). We used metallic gallium (0.2 mg), NH_3 solution as reactant source material, and N_2 as carrier gas. The cleaned silicon substrates and alumina boat contained Ga metal were transferred into horizontal tube furnace (HTF). The distance between the material source and substrate was adjusted to 15 cm. Then, the furnace was heated to 1050 °C at the rate of 15 °C/min under N_2 atmosphere (with the flow rate of 3 L/min). When the temperature was about 1050 °C, NH_3 was introduced into the HTF using N_2 gas with the flow rate of 2 L/min flowing through a flask containing NH_3 solution at room temperature (*RT*). After allowing the reaction to proceed for 40 min, the NH_3 source was turned-off, while furnace was cooled to ambient temperature under N_2 with the flow rate of 3 L/min. The yellow layer-like product collected on bare Si substrates were characterized by using scanning electron microscopy (SEM) and energy-dispersive X-ray spectrometer (EDX) attached to the SEM (JOEL JSM-6460LV performed at 10 kV) and X-ray diffraction (XRD) using Cu Kα1 radiation source ($\lambda = 1.5406$ Å). The optical reflectance spectra were obtained using an optical reflectometer (Filmetrics, F20, USA). Photoluminescence (PL) was measured at *RT* using a He–Cd laser (325 nm) as the excitation source. The carrier concentration and mobility of the GaN nanostructures grown on Si substrates were obtained by performing the Hall measurements at *RT*. Finally, p–n heterostructure diodes fabrication was completed by depositing Ag/Al and Al ohmic contacts (thickness ~ 250 nm) on top of the GaN NWs and at the back of Si substrate, respectively. Contacts were annealed at 450 °C for 10 min. Current density–Voltage (*J–V*) characteristics measurements were performed in dark and under illumination using a computer-controlled Keithley 2400 Source Meter and solar performance was measured under 30 mW/cm^2 illumination from a solar simulator. The light intensity was calibrated using a standard silicon solar cell.

3. Results and discussion

3.1. Morphological and structural characterization

Fig. 1 shows the top-view SEM micrographs and their corresponding EDX spectra of the GaN nanostructures grown on the n-Si (1 1 1), p-Si (1 1 1) and n-Si (1 0 0) substrates at 1050 °C. Fig. 1a shows the successful growth of highly dense randomly oriented GaN nanorods (NWs) on n-Si (1 1 1) substrate. The formed NWs are about 300 nm in diameter and several microns in length. Fig. 1b indicates that the fabricated NWs are denser on p-Si (1 1 1) substrate. The typical diameters of these NWs are in the range of 130–200 nm, and their lengths are in order of several micrometers. By choosing n-Si (1 0 0) as the substrate, a nanostructure like island-shaped GaN surface structure was formed on the surface of Si substrate, as it can be seen in Fig. 1c. The average size of these nanostructures was approximately 150–250 nm. These findings highlight the effect of crystal orientation of substrate on the morphology and density of the resulted GaN nanoarchitectures. Fig. 1 shows a representative EDX spectrum of GaN deposited