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Comparative studies on photovoltaic performance of InN nanostructures/p-Si(100) heterojunction devices grown by molecular beam epitaxy

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ABSTRACT

Comparative studies have been carried out on the performance of the photovoltaic devices with dissimilar shapes of the InN nanostructures fabricated on p-Si (100). The devices fabricated with the nanodots show a superior performance compared to the devices fabricated with the nanorods. The discussions have been carried out on the superior junction property, larger effective junction area and inherent random pyramidal topographical texture of the cell fabricated with nanodots. Such single junction devices exhibit a promising fill factor and external quantum efficiency of 38% and 27%, respectively, under concentrated AM1.5 illumination.

INTRODUCTION

III-Nitrides attracted tremendous scientific quest in the field of photovoltaics in recent years [1, 2]. Among them indium nitride (InN) exhibits several important attributes, including relatively high absorption coefficient, high carrier mobility, large drift velocity that are required for high efficiency photovoltaics. The revised band gap value of InN[3] has also attracted the scientific attention due to technological opportunities for the implementation of high efficiency InN photovoltaic devices. An energy-conversion efficiency of over 20% is expected for an ideal InN single-junction solar cell [4]. However, InN can be internalized to form heterojuction solar cell or be incorporated as the critical subcell for III-N based full solar spectrum tandem solar cells.

The significant challenge to the device designer is the lack of cheaply available, reasonably lattice matched substrates to grow III-N material system. From this point of view, the Si substrates offer several advantages such as ease of cleaving, availability of conducting substrates in large size wafers at very low cost, suitability in device processing and the growth of InN on Si substrates is of significant academic and commercial interest. However, InN films grown on Si contain relatively high densities of defects or dislocations [3]. Eventually, the exploration of the InN nanostructures on Si substrates is important due to the drastic reduction in the dislocation densities, resulting in the effectual lateral stress relaxation. The additional advantage of devices fabricated with the nanostructures is the increased surface area for enhanced light absorption. However, few reports are evident on the growth of InN nanostructures and layers on Si substrates by molecular beam epitaxy (MBE) [5, 6]. Since the p-type doping of the InN is still a challenge for the scientific community, the heterostructure of InN is gaining equal scientific interest. Recently, Nguyen *et al.* [7] reported on the InN p-i-n nanowire solar cells on n and p type Si substrates.

This report focuses on fabrication of InN nanodots (NDs) as well as nanorods (NRs) on p-Si(100) substrates by MBE and structural characterization of the nanostructures. A detailed analysis on the junction propertis, effective junction area and shape dependence of photovoltaic performance of InN nanostructures/p-Si heterojunctions has also been carried out.

EXPERIMENT

InN nanostructures were directly grown on p-Si(100) substrates by nitrogen plasma assisted molecular beam epitaxy system (PAMBE) to fabricate InN/p-Si heterojunction. Two different types of nanostructures viz. nanodots and nanorods were grown by following two different growth conditions. The general set of growth conditions includes, the beam equivalent pressure (BEP) of Indium, RF- plasma power, were kept at $2X10^{-7}$mbar, 350W, respectively for NDs as well as for NRs. The fabrication of InN NDs consists of a two step growth method. The initial low temperature buffer layer was deposited at 410^oC for 10 min. Further, the substrate temperature was raised to 500˚C to fabricate the nanodots. The duration of ND growth was kept for 60 min. The growth temperature and duration of growth for NRs were kept at, 410^oC and 120min, respectively. The nitrogen flow rate was maintained at 0.5 sccm and 1sccm for the growth of NDs and NRs respectively. The structural evaluation of the as-grown nanostructures was carried out by the scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Aluminum film was thermally evaporated at 10^{-6} Torr with a thickness of ~80 nm as monitored by a quartz crystal thickness monitor. The typical device area used in our experiments was 0.002 cm^2. The photovoltaic performances of the heterojunctions were examined by a solar simulator set up (AM 1.5). The room temperature transport characteristics were studied at dark condition using the probe station attached with the KIETHLY 236 source measure unit.

DISCUSSION

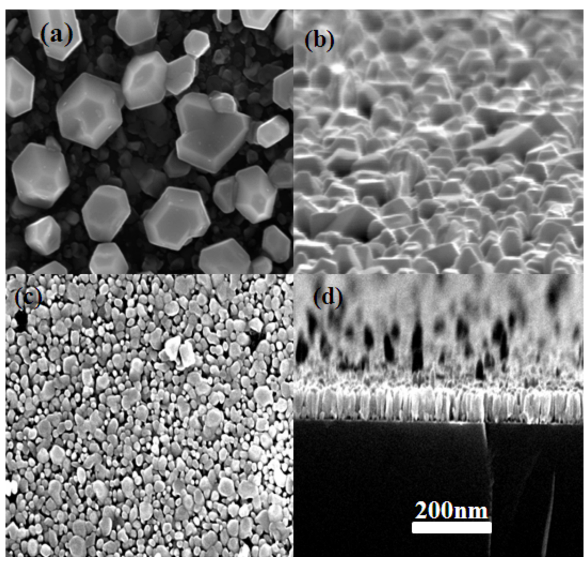

Fig.1 Scanning electron microscope images of NDs and NRs. (a) front view of NDs and (b) tilted view of NDs (c) front view of NRs and (d) tilted view of NRs.

Figure 1shows the top and tilted view SEM images of the InN nanostructures grown on p-Si(100). InN NRs are vertically oriented to the substrate surface as shown in the figure. The average height and diameter of NRs were found to be 100nm and 25nm respectively. NRs were formed of compact arrangement with the columnar structure vertical to the substrate. The NDs are vertically aligned and uniformly grown on the entire substrate. The average height and diameter of these dots were found to be 100nm. From the SEM and TEM (not shown) results, one can conclude that the shape of the NDs corresponds to a perfect hexagon in the film plane and a truncated pyramid in the vertical direction with very clear crystallogaraphic facets of hexagonal structure. It can be described more accurately as a truncated pyramid with hexagonal base with a base diameter few times larger than the height. Such growth behavior is in agreement with that reported earlier [8].

Current density versus voltage characteristics for devices with nanodots and nanorods under AM1.5 equivalent conditions are presented in Fig. 2(a). The measured solar cell parameters for devices fabricated with InN nanodots as well as nanorods are summarized in Table I. The device with nanodots exhibits the superior parameters like, open circuit voltage (V_{OC}) of 0.277 V and fill factor (FF) of 38%. Further, the best stabilized conversion efficiency of 0.41% was achieved without any anti reflection coatings. In the case of devices fabricated with nanodots, a low J_{SC} and high V_{OC} was observed when compared with nanorod devices, resulting due to comparitively high series and shunt resistances, respectively. The absence of local shunting regions is the major reason behind the present behavior of InN nanodot/p-Si devices. The unoptimized diameter distribution of the nanorods results in the regions of local shunting across the cells provides the partial explanation for the reduction of V_{OC}. Spectral responses of both the samples of differing in shapes of InN nanostructures are shown in figure 2(b). The devices fabricated with nanodots demonstrated high peak external quantum efficiency (EQE) (ηe) of 27% at 525 nm and flat quantum efficiency of 24 %. A decline in the EQE was also observed when the morphology of InN surface goes from the random pyramidal surface of NDs to reasonably flat surface of NRs might be due to the enhancement of light trapping in the pyramidal textured NDs (as shown in the tilted view of the surface in figure 1.), Vanecek et al. also observed similar improvement in the performance of their Si solar cells by introducing the nanostructured ZnO layer [9]. Thus random pyramidal layout of the InN surface is a contributing factor to exhibit superior performance when compared to the flat surface and regular pyramid layout [10].

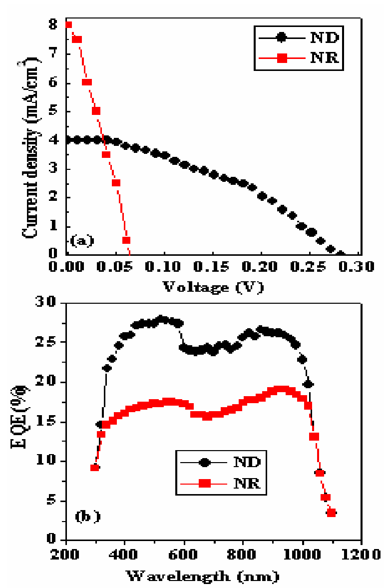

Fig. 2 (a) Typical current density versus voltage characteristics of solar cells fabricated using InN NDs and NRs. (b) External quantum efficiency versus wavelength of solar cells fabricated with InN NDs and NRs.

Device with	V_{OC} (V)	J_{SC}(mA/cm^2)	FF(%)	Conversion Efficiency(%)
Nanorods	0.063	8.21	29	0.15
Nanodots	0.277	3.99	38	0.41

Table I. Measured solar parameters for devices fabricated with NDs and NRs.

Due to the high electron affinity of InN i.e, 5.8 eV when compared to that of Si i.e, 4.05eV, a large conduction band offset is resulted. The resulting schematic energy band alignment diagram under thermal equilibrium is shown in figure 3(a). A type-III band alignment for the InN/p-Si heterojunction has been proposed. The detailed studies on band alignment of InN/p-Si heterojunction can be found elsewhere [11, 12]. Due to the high chemical reactivity of silicon surface with atomic nitrogen, the formation of amorphous silicon nitride interfacial layer during the nucleation stage is expected in both the devices. Zimmler *et. al* [13], also observed such interfacial layers in their GaN single nanowire based light emitting diode structures. By considering the unintentionally formed ultra thin[14] (~1nm) silicon nitride interfacial layer between the InN and Si, the junction properties have been analyzed. Introduction of insulating layer provides an impediment to majority carrier flow (although minority carrier flow is also attenuated) [15]. Also insulating layer acts as buffer and reduces image force effects. Both these effects combine together to increase the short wavelength response of the minority carrier tunnel diode. As Singh *et. al,*[15] described, minority carrier current is dominant in tunnel diode case, which is a favorable condition for photovoltaic purposes. As the diode is forward biased and more semiconductor current is available, there is a point where the magnitude of this current is greater than that which can be supported by the tunneling process and an effective tunnel "series resistance" appears, the thinner the layer the better [16]. Shewchun *et al*. [16] suggests that, for ultrathin (t < 2.8nm) insulating interfacial layer the semiconductor-insulator-semiconductor (SIS) diode is in a non equilibrium mode of operation. Minority carrier nonequilibrium tunnel diodes with the ultra thin insulator layer have properties similar to *p-n* junctions, along with the exhibition of I-V characteristics and photovoltaic energy conversion properties[15, 16]. Hence, the room temperature dark *I-V* characteristics of the InN nanostructures/p-Si heterojunction photovoltaic devices were also measured, as shown in Figure 3(b) and comparatively interpreted. A superior rectifying characteristic was observed for nanodot devices when compared to nanorod devices. The *I-V* curves were fitted by using the standard diode equation,

$$I = I_s \left[\exp\left(\frac{qV}{\eta kT} \right) - 1 \right] \qquad (1)$$

The forward bias *I-V* data showed ideality factors η, 1.04 and 4 for the devices with nanodots and nanorods, respectively. The ideality factors greater than 2 indicate a nonideal nature of the diodes [17]. Further, the high ideality factors were often attributed to the presence of defect states which causes the deep level assisted tunneling[18] or lateral in homogeneities of the barrier height at the interfaces.[19] However, the occurrence of the nonuniform Schottky interface was also concluded in the case of InN nanodot/p-Si heterojunction in our previous report[11]. The drastic reduction in the ideality factor in the case of nanodots might be due to the superiority in the crystallinity and the interface when compared to nanorods which was certainly dependent on the growth procedure as well as on the growth parameters. Thus, the lesser effective junction area due to columnar growth, nonideality of the diode are the important reasons for the poor photovoltaic performance of the device with nanorods when compared to devices with nanodots.

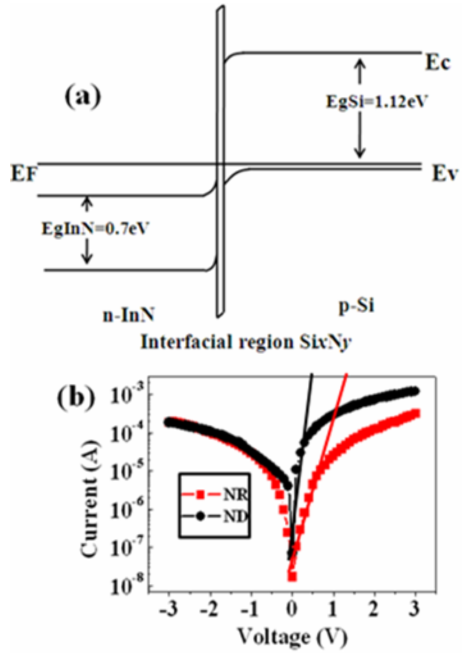

Fig.3. (a) Schematic of energy band diagram of the InN/Si*x*N*y*/p-Si heterojunction tunnel diode under equilibrium. (b) Room temperature I-V characteristic of InN/p-Si heterojunction for both the nanostructures.

The mechanism for the poor device performances of InN nanostructures/p-Si observed has been predicted as follows. Performances of the presently demonstrated InN nanostructure/p-Si solar cells may also be severely limited by the surface electron accumulation of n-type InN and the nonideal carrier transport across the InN/Si misfit interface. Since depletion occurs at both sides of the junction, we could observe the quasi ohmic behavior in InN/p-Si heterojunction under dark conditions. This behavior justifies the presence of the recombination of the electrons accumulated at the heterojunction with the holes in the Si valence band.

CONCLUSIONS

Photovoltaic performances of the InN nanostructures/p-Si heterojunctions fabricated by MBE had been investigated. The electron microscopic studies confirm that, the as-grown NDs and NRs are fairly single crystalline, and are crystallized hexagonally along the [001] direction with uniform geometry. Further demonstrate that the shape of the as grown nanodots corresponds to a perfect hexagon in the film plane and a truncated pyramid in the vertical direction with very clear crystallogaraphic facets of hexagonal structure. The devices fabricated with the nanodots show a superior performance compared to the devices fabricated with the nanorods due to the absence of local shunting, superior junction properties, larger effective junction area along with the contribution from inherent random pyramid texture of the cell. Such single junction devices exhibit a promising fill factor and external quantum efficiency of 38% and 27%, respectively, under concentrated AM1.5 illumination.

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