Solar Energy 142 (2017) 231–242

Contents lists available at ScienceDirect

Solar Energy

journal homepage: www.elsevier.com/locate/solener

Quantum confinement effect on the electronic and optical features of InGaN-based solar cells with InGaN/GaN superlattices as the absorption layers

A. Laref [a,b,*], A. Altujar [a], S. Laref [c], S.J. Luo [d]

[a] Department of Physics and Astronomy, College of Science, King Saud University, Riyadh 11451, Saudi Arabia
[b] Department of Physics, National Taiwan University, Taipei 106, Taiwan
[c] Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Str., D-35032 Marburg, Germany
[d] School of Science, Hubei University of Automotive Technology, China

ARTICLE INFO

Article history:
Received 29 January 2016
Accepted 6 December 2016

Keywords:
GaN-InN solar cell based material
Photo-voltaic materials
Optoelectronic

ABSTRACT

The short period group III-V nitrides superlattices (SLs), have turned out contemporary in the technology of optoelectronics and solar cell applications. Our theoretical simulation is carried out by means of first-principles full potential linearized augmented plane waves (FP-LAPW) methodology within generalized gradient approximations (GGA) in conjunction with the modified Becke–Johnson (mBJ) potential. In this respect, a comprehensive study for the electronic structures and optical aspects of $(In_xGa_{1-x}N)_n/(GaN)_n$ (0 0 1) zinc-blende superlattices (SLs) (x = 0.5 and n = 3–4), is carried out. Specifically, the electronic band structure calculations and their related features, like the absorption coefficient, reflectivity, refractive index and electron energy loss function spectra of these systems are computed over a wide photon energy scale up to 25 eV. The effect of periodicity layer numbers and In composition (x = 50%) on the band gaps of $(In_xGa_{1-x}N)_n/(GaN)_n$ SLs is examined. The tailoring of the underlying energy band gap relies on the In content and the periodicity of the superlattices. All these ultrathin superlattices (n = 3–4) possess a direct energy band gap. The InGaN layers have immense prominence in ascertaining the underlying energy gap of these superlattice because of the distinctive quantum confinement impact. Furthermore, the flexible energy gap of these ultrathin-period SLs leads to the alteration of the absorption coefficients and static refractive indices. It is viable to attain InGaN solar cells possessing high efficiencies since the energy gap covers all the spectrum optical regime. Predominantly, it is feasible to tune the optical characteristics of these short-period SLs and provide plausible results for the optoelectronic devices applications.

1. Introduction

The advent of III-Nitride materials have manifested because of the opto-electronic applications and solar cell technology of GaN and $In_xGa_{1-x}N$ in many areas such as, laser diodes, blue light-emitting diodes (LEDs), long wave length emitters, photodetectors, photovoltaics, heterojunction transistors and solar water splitter (Yoshimoto et al., 1991). It has been testified that since 2002, the mixture between GaN and InN compounds could extend the opportunity of InGaN systems for engineering the energy gap over the full-solar-spectrum spectrum and this is due to the fact that InN possesses an energy band gap close to 0.7 eV (Nakamura and Mukai, 1992; Nakamura et al., 2000; Silveira et al., 2008; Pereira et al., 2006). InGaN and InAlN ternary materials (Novikov et al., 2008; Nagatomo et al., 1989) envelop a large regime of the optical spectrum between the ultraviolet and infrared as well as between the infrared and the deep ultraviolet. Importantly, the energy band gap of blended InGaN would be flexible with a particular wavelength for emitting light.

The emergence of InGaN alloys is owed to their tunable energy band gaps and they have shown their capability as novel solar cell systems enveloping roughly the entire solar spectrum and superior photovoltaic aspects (direct energy gap in the entire alloy span, drift velocity, high carrier mobility and optical absorption of $\sim 10^5$ cm^{-1} close to the band edge) (Jani et al., 2007b; Neufeld et al., 2008). In this respect, it is viable to optimize and design theoretically tandem photovoltaic (PV) devices, while the optimal band gaps absorbing photon energy operates from 0.7 eV of infra-

* Corresponding author at: Department of Physics, National Taiwan University, Taipei 106, Taiwan.
E-mail address: amel_la06@yahoo.fr (A. Laref).

http://dx.doi.org/10.1016/j.solener.2016.12.009
0038-092X/

red to 3.4 eV of ultraviolet regimes by the mutual $In_xGa_{1-x}N$ ternary alloys. The valuable dissimilarities in the underlying energy gaps of GaN and InN could permit to tailor the energy band gap along a large regime between 0.7 and 3.4 eV by combining their corresponding alloying. This is the easiest method for engineering the electronic and optical features of the materials. The characteristics of ultrahigh-efficiency multi-junction tandem solar cells will be gained in a single epitaxy system. Accordingly, the growth of thickness maximum of fairly good-crystallinity of $In_xGa_{1-x}N$ epitaxial layers over GaN requires merely hundreds of nanometers. This situation is owed to the sizeable lattice mismatched between GaN and $In_xGa_{1-x}N$, exclusively for large indium composition materials (Jani et al., 2007a; Tabata et al., 2002; Hsu et al., 2010; Kuykendall et al., 2007; Yam and Hassan, 2008; Iwanaga et al., 2005; Kawakami et al., 2006). Hence, the main confront is to attain $In_xGa_{1-x}N$ absorption layers having wide thickness and small energy band gap under 2.0 eV. InGaN ternary alloys possess convenient electronic and optical aspects as it was exposed in the light-emitting applications.

From the experimental perspective, InGaN systems have been proved to be the most appropriate for photovoltaic applications, whilst the indium content is sweeping between 0 and 50% (Frankowsky et al., 1996; Wierer et al., 2004; Im et al., 1998; Scholz et al., 2009; Rumyantsev et al., 2006). In this regard, the necessity of the band gap for the highest cell should be around 2.4 eV for these structures. The III-Nitride semiconductors involving GaN, InN and their mutual alloys support the thorough band gaps demanded to produce solar cells with response over 2.4 eV. One of the essential demand to attain solar cell conversion efficiencies bigger than that of 50% represents a photovoltaic device which has an energy band gap about 2.4 eV or bigger. Interestingly, $In_xGa_{1-x}N$ systems belongs to the minor alloys which fulfil this fundamental prerequisite (see reference Jani et al. (2007b) and references therein). The realistic optical features were detected in the narrow band gap of InN (Jani et al., 2007a; Tabata et al., 2002) which was conform with the reports on In-rich InGaN (Senda et al., 2009; Fujiyama et al., 2010; Damilano et al., 1999; Hangleiter et al., 2005). Few statements on InGaN based solar cells have been pointed out, even though these systems proposed promising usage for space and terrestrial photovoltaic applications. Additionally, the most recorded InGaN solar cells possess band gap approximately 3 eV, while the In composition is inferior than 15%. However, these systems can handle reduced quantum efficiency at wave lengths longer than 420 nm (Jani et al., 2007b; Neufeld et al., 2008). A prior theoretical determination has suggested that the necessity of active materials to procure solar cells with a solar energy conversion efficiency bigger than 50%, would be accomplished in InGaN (for In composition about 40%) (De Vos, 1992).

Applications of III-nitrides in the visible light region of electromagnetic spectrum demand to lower the band gap of GaN (3.4 eV), frequently via the growth of InGaN layers. By the realization of the growth of GaN layers on sapphire, trial growing InGaN layers on sapphire substrates provided unsatisfactory crystalline quality (Araujo et al., 2013a; Van Den Broeck et al., 2014; Fadil et al., 2014; Park et al., 2011). The first accomplishment was yielding a high-quality InGaN layer on thick GaN buffer layer grown on sapphire (Jeong et al., 2015; Yeh et al., 2012; Tu et al., 2014; Araujo et al., 2013b; Dahal et al., 2009; Ul Haq et al., 2009; Schubert et al., 2007; Tabata et al., 2002; Yu and Cardona, 2001; King et al., 2008). Such layers are determined to possess strong band-to-band emissions at different indium compositions. It has been suggested that InGaN/GaN multi-quantum wells with quite good crystalline quality may be grown consistently on moderately relaxed GaN layer regardless the sizeable lattice mismatch and thermal inconsistency with the basic substrate. Using the photoluminescence measurements, narrow and bright band edge suggested good crystalline quality of InGaN/GaN SL structures. The realization of high brightness (HB) blue InGaN *LEDs* has essentially drive to a revolution in *LED* technology and opened up immense new markets that were inaccessible before. Also the InGaN material systems offer a valuable potential to develop high efficiency solar cells. Moreover, III-Nitride multi-junction solar cells having nearby perfect band gap with maximal solar energy conversion efficiency should include InGaN layers with larger In composition or inferior energy gaps.

The main challenge is to realize high crystalline quality InGaN films across the thorough concentration span. One of the major complexity is related to the sizeable lattice mismatch between the two constitutes such as, GaN and InN stemming in lesser phase separation and solubility (Karpov, 1998). The greatest In composition is needed for efficient conversion of inferior energy photon. This could restrict the maximum thickness of this layer with the diminution of its light absorption. Later, it has been displayed that InGaN alloys would be grown with the embedded layer of InGaN/GaN double hetero-structures (Hangleiter et al., 2005; De Vos, 1992; Araujo et al., 2013a, 2013b; Van Den Broeck et al., 2014; Fadil et al., 2014; Park et al., 2011; Jeong et al., 2015; Yeh et al., 2012; Tu et al., 2014; Dahal et al., 2009; Ul Haq et al., 2009; Schubert et al., 2007) along the full concentration regime. It was stated previously (Kawakami et al., 2006; Frankowsky et al., 1996; Wierer et al., 2004; Im et al., 1998; Scholz et al., 2009; Rumyantsev et al., 2006) that the characterization and fabrication of InGaN solar cells could be performed, while the inclusion of InN fractions is varying from 30% to 40%. This could be accomplished for $In_xGa_{1-x}N$/GaN MQWs with the endeavor to alleviate to some level of the phase separation issue and establish solar cell operation in wavelengths longer than that of earlier attainments. Further benefits involve high optical absorption, low effective mass of holes and electrons and high mobilities. From practical point of view, the large dislocation concentration and strong polarization in InGaN alloys represent the two significant difficulties accompanied with the amelioration of the luminescence efficiency. Various resolutions have been suggested to acquire optical activity with InGaN alloys. Among the appealing systems to attain this aim is inevitably InGaN based InGaN/GaN SL's. This kind of structure leads to the minimization of lattice mismatch and the outcome piezoelectric effects. Moreover, the viability for confining the electrons turns out a realism. This confinement carries alterations in the electronic structure of these SL's, which in turn varies their optical characteristics. Interestingly, the short-period InGaN/GaN exhibit novel physical aspects, for instance the decrease of the energy gap with In-rich composition in InGaN layers. Previous theoretical reports have been carried out for studying the electronic structure and optical properties of $(InGaN)_n/(GaN)_n$ zinc-blende SL's grown along (001) direction (n = 1–2) in the framework of FP-LAPW method within mBJ-LDA approximation (Laref et al., 2014). It has been demonstrated that the variation of In-content in InGaN layers can alter the energy gap of these SL's.

Stimulated by all these concerns, we carry out theoretical simulations to explore the alloy composition which mimics the strain effects on the electronic and optical characteristics of these III-nitrides heterostructures. The short-period group III-Nitride superlattices for example, InGaN/GaN gained a special regard (Hangleiter et al., 2005; De Vos, 1992; Araujo et al., 2013a, 2013b; Van Den Broeck et al., 2014; Fadil et al., 2014; Park et al., 2011; Jeong et al., 2015; Yeh et al., 2012; Tu et al., 2014; Dahal et al., 2009; Ul Haq et al., 2009; Schubert et al., 2007), which have proven immense applications in the optoelectronic devices and solar cell technology. Accordingly, a rational and exact reorganization regarding the composition effects on the electronic and optical ingredients is vital for optimizing III-nitride based superlattices. These SLs construction are overall governed by the strain effect