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The electronic band structure of InN, InAs and InSb compounds

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Abstract The electronic band structure of InN, InAs and InSb has been investigated by ETB. The ETB method has been formulated for sp^3d^2 basis and nearest neighbor interactions of the compounds and its energy parameters have been derived from the results of the present first principles calculations carried on InN, InAs and InSb. It has been found that the present ETB parameters can produce the band structure of the compounds successfully.

Introduction

There is currently considerable interest in compounds of In with Nitrogen, Arsenic and Antimony, because of their optical and high temperature device applications. Among these compounds, InN is a highly potential material for the fabrication of high speed heterojunction transistors [1] and low cost solar cells with high efficiency [2]. Pure InN was predicted to have the lowest effective mass for electrons in all the III-nitride semiconductors [1] which lead to high mobility and high saturation velocity. Recently, several groups have grown high quality hexagonal (w-InN) and zinc-blende (c-InN) structural InN films by modern growth techniques, such as metal organic chemical vapor deposition (MOVPE) and plasma-assisted molecular beam epitaxy (MBE) [3–8]. The w-InN and c-InN films have been mostly grown on sapphire and GaAs (or Si, GaP) substrates, respectively. In these works [3–7], a buffer layer, particularly, AlN or InAs has been usually grown on the substrate to improve the quality of the InN films. In a very recent work [8], the c-InN has been grown on r-plane sapphire successfully without the use of additional buffer layer. The growth of w-InN and c-InN films have been characterized by many techniques such as, X-ray diffraction, Raman spectra, reflection high-energy electron diffraction (RHEED). The photoluminescence (PL) spectra of high quality w-InN films have illustrated that the band gap energy of InN is smaller than the commonly accepted value of 1.9 eV [9]; it is a round 0.65–0.90 eV [3, 4]. The recent experiment works on c-InN have mainly focused on the characterization of the films [5–8]. The band gap energy of c-InN films has not been reported experimentally, but it has been found around 0.44–0.74 eV by the results of ab-initio calculations [10, 11]. These newly reported values of w-InN and c-InN are compatible with the wavelength of the optical fiber. Therefore, the w-InN and c-InN films will have very important potential to fabricate high speed laser diodes (LDs) and photodiodes (PDs) in the optical communication system.

The other two compounds of In, InAs and InSb are interesting narrow gap semiconductors from the point of view of optical spectroscopy and optoelectronic applications [12]. Since InAs has a high electron mobility it may prove an important material for use in high speed electronics [13, 14]. The high quality InAs material has been grown with certain advantages by different growth techniques such as liquid phase epitaxy (LPE) [15], MBE [15–18], and MOCVD [15, 19]. The quality of grown doped [15] and undoped [15–19] InAs materials has been appraised by mainly PL spectroscopy [15–23] at different

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