

# Nearly free electron model and k-p method calculations of electronic band structure of wurtzite InN

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The theoretical models for calculations of band structure of wurtzite InN have been studied. Several models including nearly free electron model, pseudopotential method, Tight-Binding method and k-p method will be discussed. Currently most InN epitaxial films grown on GaN or sapphire substrate have wurtzite structure. To study the symmetry properties of the electron wave function in wurtzite structure, a nearly free electron model is presented. Based on that, full band structure will be calculated using k-p method.

Indium nitride, as the least studied semiconductor in nitrides family (AlN-GaN-InN), has attracted much interests in recent years. The most interesting and controversially property is the fundamental bandgap of InN. Before 2003, the InN films was mainly grown by sputter techniques and the accepted bandgap measured from absorption edge was around 1.9 eV [1, 2]. Recently high quality InN epitaxial films have been grown by both metal organic chemical vapor deposition (MOCVD) [3, 4] and Molecular Beam Epitaxy (MBE) [5-8], the optical characterizations including photoluminescence and absorption spectrum show that the bandgap of InN is around 0.7 eV [6, 9, 10], which is much smaller than previously reported value. And it is also found that there is no noticeable feature around 1.9 eV.

The origin of this big discrepancy has been explained in many hypotheses. Since InN has a high electron affinity, almost all impurities and defects will act as donors, and thus result in high electron concentration in InN [11]. Even in unintentionally doped InN, the electron concentration was observed in the order of  $\times 10^{17} \sim \times 10^{18} \text{ cm}^{-3}$  [5, 6]. And the Fermi level in InN was believed to be inside the conduction band, and about 180 meV above conduction band edge [12]. This high Fermi level could produce the Burstein-Moss shift, which results in blue shift in absorption edge. Wu et. al has shown that the absorption edge increased with the increasing of electron concentration [13]. The formation of oxidation and precipitation of In clusters could also effect the optical properties of InN [14, 15].

The narrow bandgap of InN opens many opportunities for the application of opto-electronic devices in IR region and high speed electronic devices [16, 17]. InN and high indium composition InGaN could be possible materials for opto-electronic devices IR regions for communication applications. Since the nitrides (AlN, GaN and InN) semiconductor bandgap energy can cover the whole solar spectrum, they can be used for high efficiency photovoltaic application with environment friendly non-toxic elements. Due to the narrow bandgap of InN, a small effective electron mass ( $0.05m_0$ ) has been assigned to InN [18]. As a result, high electron mobility of 14000

$\text{cm}^2/\text{V}\cdot\text{s}$  at room temperature has been predicted by a Monte-Carlo simulation [19]. Thus InN is very attractive for high speed electronic devices. Leary et al. have used a three-valley Monte-Carlo simulate to analysis the steady state and transient electron transport properties in InN [20]. They found that the drift velocity was greatly depends on the band structure such as the bandgap, effective mass and non-parabolic coefficient. Thus to fully understand the band structure of InN is very important to explore its electrical and optical properties and also device performance.

So far many investigations have been carried out on calculating the band structure of InN. Before 2003, due to lack of basic parameters of InN, early theoretical calculations using empirical pseudopotential model predicted the bandgap of wurtzite InN was around 2.0 ~ 2.6 eV [21-23]. One year later, the same group using new InN parameters had calculated the bandgap of 0.79 eV and the electron effective mass of  $0.07m_0$  [24]. Recently, many works have been done using the first principle calculation [25] and *ab initio* calculation [26, 27]. These first-principle pseudopotential method (also known as *ab initio* method) are *self-consistent*: first an atomic pseudopotential and an ionic potential of crystal structure were used as the starting point; then wave functions have been calculated; after that the total one-electron potential was derived from the wave functions and compared with the initial potential. On the other hand, empirical pseudopotential requires experimental inputs such as atomic pseudopotential form factor. However the atomic pseudopotential form factor for one element is *transferable*, which means the atomic pseudopotential form factor of In determined from InP could be used in other In compounds such as InN and InAs. With accurate input, the empirical pseudopotential could give good overall agreement with experimental results. Other calculation like tight-binding method has also been used for band structure of nitrides [28].

Other than pseudopotential and tight-binding methods, k-p method can also to used to extrapolate  $E-k$  dispersion relation. Compare to pseudopotential and tight-binding methods, k-p requires more experimental input

data but provide more accurate results especially near the high symmetric points in Brillouin zone. Substituting the Bloch wavefunction into Schrodinger equation, one can get:

$$\left(\frac{p^2}{2m} + \frac{\hbar\mathbf{k}\cdot\mathbf{p}}{m} + \frac{\hbar^2k^2}{2m} + V\right)u_{nk} = E_{nk}u_{nk}, \quad (1)$$

where  $u_{nk}$  is the Bloch wavefunction and has the periodicity of the lattice. At  $\Gamma$ -point, where  $k_0=(0,0,0)$ , the function reduce to:

$$\left(\frac{p^2}{2m} + V\right)u_{n0} = E_{n0}u_{n0}. \quad (2)$$

Similar equations could be obtained for other high symmetric  $k$ -point. Solving Equation 2 we can get  $E_{n0}$  and  $u_{n0}$ . Then we can treat  $\hbar\mathbf{k}\cdot\mathbf{p}/m$  as the perturbations using either degenerate or nondegenerate perturbation theory. This k-p method works best for small  $k$ . Beresford has presented full-zone k-p band structure calculation of wurtzite semiconductors [29], but the author still used the old parameters for InN and got bandgap of InN to be 1.9 eV. Recently, some key parameters of InN have been extracted using density-function theory [30], which would be helpful to calculate the band structure of InN using k-p method.

In this work we present the theoretical approaching of calculation of electronic band structure of wurtzite InN. The first step was calculate the nearly free electron band (also called empty lattice model) in wurtzite structure. In this model, the crystal potential is assumed to be vanishingly small. The electron energy band is simply a parabolical dispersion plotted in the reduce zone. The  $E - k$  relation thus becomes:

$$E = \frac{\hbar^2}{2m}(k + G)^2, \quad (3)$$

where  $G$  is the reciprocal lattice point and  $k$  is the wavevector in reduce zone. Eventhough this nearly free electron approach doesn't consider any crystal structure, it still looks very similar to other large-scale numerical calculation such as tight-binding and pseudopotential methods. Figure 1 shows the calculation of Ge band structure. We could see near free electron model could be a very good point to start. Based on that, we will derived the full-zone k-p calculation of wurtzite InN using new parameters.

to be continued...

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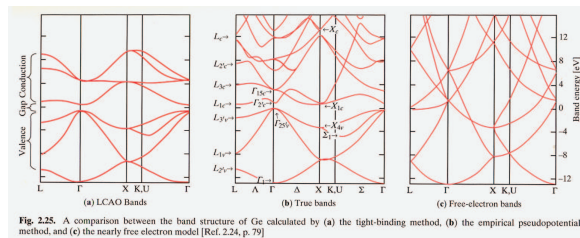


Fig. 2.25. A comparison between the band structure of Ge calculated by (a) the tight-binding method, (b) the empirical pseudopotential method, and (c) the nearly free electron model [Ref. 2.24, p. 79]

FIG. 1: Ge band structure calculated by (a) tight-binding method, (b) empirical pseudopotential method, (c) nearly free electron model. Reprint from [31].

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