

Investigation of electron effective mass in C.B. of dilute nitride semiconductors.

Ahad Khan Pyawarai^{1,2,*}

- 1- Polytechnics University, Karte-Mamorin, Kabul, Afghanistan
 2- Physics Department, Electromechanics Faculty, Kabul, Afghanistan

ABSTRACT

Dilute Nitride Semiconductor (low nitrogen-containing ternary and quaternary alloys) have recently attracted much attention due to their fundamental properties promising for device applications in optoelectronics and photonics such as highly efficient near infrared lasers, multi-junction solar cells, as well as heterojunction bipolar transistors (HBTs). The effect of N on the electronic band structure in dilute III-N-V nitrides has been explained in terms of a band anticrossing interaction between highly localized N states and the extended conduction band states of the semiconductor matrix. The interaction leads to a splitting of the conduction band into two non-parabolic subbands. The downward shift of the lower subband edge relative to the valence band is responsible for the reduction of the fundamental band gap. The profound effects on the optical and electrical properties of the dilute nitrides such as the significant increase in the electron effective mass can be quantitatively account for using this model.

Keyword: Semiconductor, HBT, effective mass

1 Introduction

Band gap of semiconductors are the most important parameters that scientist reporting in their consideration. Finding a relation between bandgap and effective mass that is one of important factor playing important role in transport, is also demanding. According to the band structure of a semiconductor, based on the relationship between energy and the k-wave vector, the effective mass can be expressed as [1-8].

$$\frac{1}{m^*} = \frac{1}{\hbar^2 K} \frac{dE}{dK}$$

It shows that the effective mass is inversely proportional to the changes of E in terms of the wave vector inside the crystal. As shown in Figure 1, in most semiconductors, the effective mass decreases with decreasing band gap [9].

But in the case of dilute nitrogen semiconductors, the opposite is true, and they exhibit unusual behavior. By adding nitrogen to the host semiconductor and bending the band gap as well as reducing it, the effective mass increases. The main reason for the increase in effective mass by reducing the band gap is due to the addition of nitrogen and according to the band repulsion model, the non-parabolic conduction band is due to its presence [10].

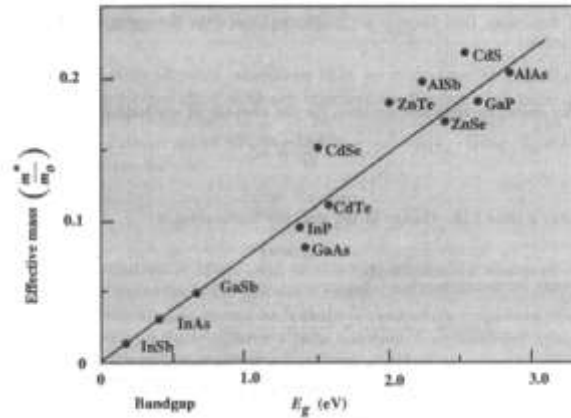


Figure 1 - Reduction of the effective mass of the electron along with the reduction of the semiconductor band gap [9]

2 Experimental details

The samples studied in this paper are low-nitrogen group III-V semiconductors including a series of GaN_xAs_{1-x} volumetric samples and two series of $In_yGa_{1-y}N_xAs_{1-x}$ multiple quantum well samples with 0.13 and 0.32 indium levels with percentages. There are different nitrogens grown by MOVPE method. Stimulation and measurement of emitted light of samples was done by photoluminescence method [11].

3. Results and discussion

According to the band repulsion model, nitrogen causes the conduction band to separate into two sub-levels E_+ and E_- and therefore the effective mass relationship of the states can be determined as follows in these alloys:

$$\frac{1}{m_{\pm}^*} = \frac{1}{\hbar^2 k} \left| \frac{dE_{\pm}(k)}{dk} \right|$$

And according to the relations obtained using the disorder theory for E_{\pm} :

$$\frac{1}{m_{\pm}^*(k)} = \frac{1}{\hbar^2 k} \left\{ \frac{1}{2} \frac{dE_M(k)}{dk} \pm \frac{(E_M(k) - E_N)}{2\sqrt{[E_M(k) - E_N]^2 + 4V_{MN}^2}} \frac{dE_M(k)}{dk} \right\} =$$

$$\frac{1}{2\hbar^2 k} \frac{dE_M(k)}{dk} \left\{ 1 \pm \frac{[E_M(k) - E_N]}{\sqrt{[E_M(k) - E_N]^2 + 4V_{MN}^2}} \right\} = \frac{1}{2m_M(k)} \left\{ 1 \pm \frac{[E_M(k) - E_N]}{\sqrt{[E_M(k) - E_N]^2 + 4V_{MN}^2}} \right\}$$

Where $m_M(k)$ is the mass of the electron in the conduction band of the nitrogen-free structure. Therefore, according to the relationship between effective mass and energy obtained in Equation (2), the effective mass changes can be investigated by performing the necessary calculations related to the changes of E_M , E_N and V_{MN} in terms of nitrogen increase in different samples. This condition can be proved based on various experimental data. As an example, the results obtained by Penn [11] can be seen in Figure (2), which shows the effective mass changes of electrons as well as the band gap in the structure of $In_{0.3}Ga_{0.7}NAs / GaAs$ with nitrogen percentage. Therefore, despite the same amount of In, the value of m^* in $InGaNAs$ is much higher than $InGaAs$.

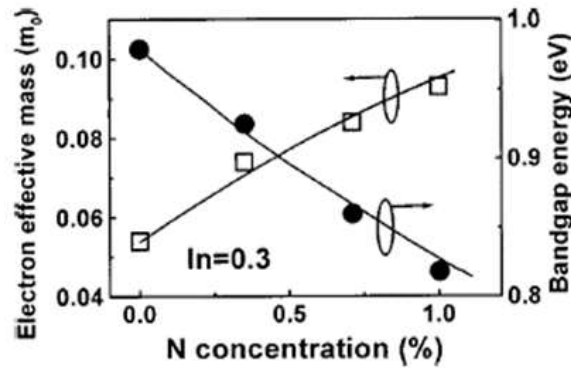


Figure 2 - Dependence of band gap and effective electron mass on nitrogen concentration in In_{0.3}Ga_{0.7}NAs / GaAs structure[11].

Knowledge of masses affecting atmospheric pressure provides valuable information about the nature of the band structure of semiconductors and alloys, which is very useful in optimizing III-V-N alloys due to their many applications in the manufacture of various parts [12]. We now examine the effective mass change with increasing nitrogen for both GaNAs and InGaNAs.

Figure (3) shows the effective mass changes of electrons in the conduction band in terms of the percentage of nitrogen in the sample. As can be seen, the effective mass increases with increasing percentage of nitrogen. Calculate the effective mass of the electron according to Equation (2) and use the values of E_N^0 , E_M^0 and C_{MN} , which for this alloy are equal to 1.65, 1.407 and 2.7 electron volts. By placing these values in relation (4-5) we reach the following relation:

$$\frac{1}{m_*} = \frac{1}{2m_M} \left\{ 1 - \frac{1.05x - 0.42}{\sqrt{(1.05x - 0.42)^2 + 19.589x}} \right\}$$

The same is true for InGaNAs with an indium content of 0.32, and with increasing nitrogen, the effective mass of the electron in the conduction band increases. The values E_N^0 , E_M^0 and C_{MN} for this sample are equal to 1.2755, 1.03 and 1.9, respectively, so we have:

$$\frac{1}{m_*} = \frac{1}{2m_M} \left\{ 1 - \frac{1.05x - 0.245}{\sqrt{(1.05x - 0.245)^2 + 14.44x}} \right\}$$

In the above cases, m_M is the effective mass of the electron in the conduction band of the nitrogen-free structure, which is calculated from the following equations:

$$\frac{1}{m_*} = \frac{1}{\hbar^2 K} \frac{dE}{dK}$$

$$E^{In_xGa_{1-x}As} = (x)E^{InAs} + (1-x)E^{GaAs} - bx(1-x)$$

$$\frac{1}{m_{InGaAs}^*} = \frac{1}{m_M} = \frac{1}{\hbar^2 K} \left| (x) \frac{dE^{InAs}}{dK} + (1-x) \frac{dE^{GaAs}}{dK} \right|$$

$$\frac{1}{m_M} = x \left(\frac{1}{m_{InAs}^*} \right) + (1-x) \left(\frac{1}{m_{GaAs}^*} \right)$$

By placing the effective mass values of InAs and GaAs, which are 0.0310 and 0.0812, respectively [1], m_M is obtained for InGaAs with an indium value of 0.13 equal to 0.067 and for indium 0.32 equal to 0.03535.

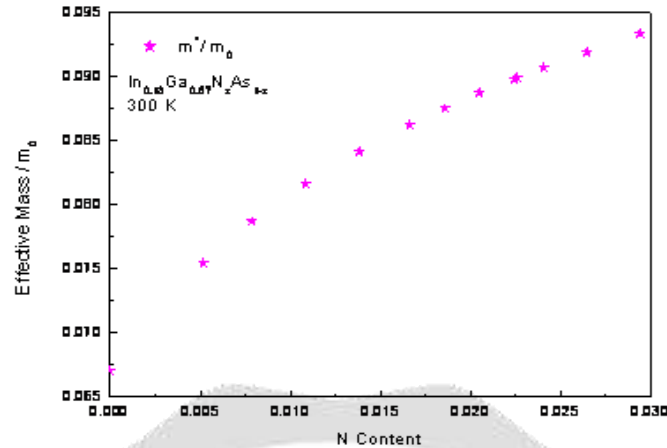


Figure 4 - Increase in the effective mass of the electron by increasing the percentage of nitrogen in $\text{In}_{0.13}\text{Ga}_{0.87}\text{N}_x\text{As}_{1-x}$

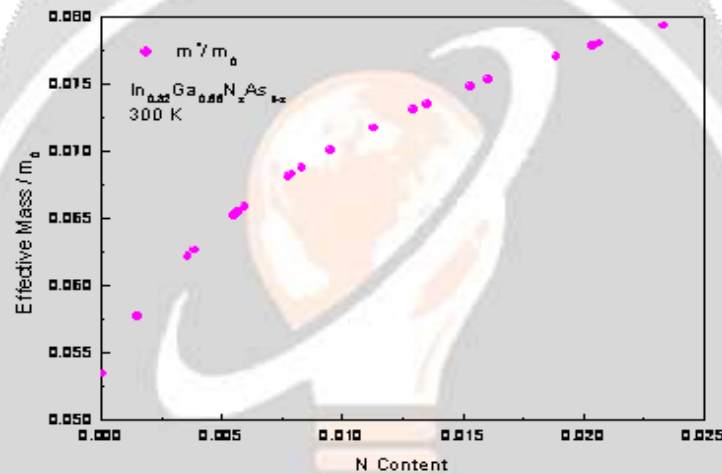


Figure 5 - Increasing the effective mass of the electron by increasing the percentage of nitrogen at $\text{In}_{0.32}\text{Ga}_{0.68}\text{N}_x\text{As}_{1-x}$

4. Conclusion

In III-V alloys, adding a very small percentage of nitrogen causes a change in the band structure and unusual behaviors such as a sharp decrease in the band gap, an increase in the effective mass of the electron, which can be changed by previous models (VCA and dielectric ...) They were not justified, but the BAC model justifies them well. x), compared to the same sample without indium but with the same amount of nitrogen ($\text{GaN}_x\text{As}_{1-x}$), decreases and in addition the graph of effective mass increase with increasing amount of nitrogen also reaches saturation later.

5. References

- [1]. Mohsen Jamshidia, Mostafa Razmarab, Banafsheh Nikfarc, Masoud Amiri, First principles study of a heavily nitrogen-doped (10,0) carbon nanotube, *Physica E: Low-dimensional Systems and Nanostructures* 103 (2018) 201–207.
- [2] Ali Baharia, Amir jalalinejadb, Mosahhar Bagheria, Masoud Amiri, First principles study of electronic and structural properties of single walled zigzag boron nitride nanotubes doped with the elements of group IV, *Solid State Communications* 267 (2017) 1–5.
- [3] A. Bahari and M. Amiri, Simulation Study of the Electron and Hole Transport in a CNTFET, *Commun. Theor. Phys.* 59 (2013) 121–124.
- [4] M. Amiri and A. Bahari, Renormalization of Fermi Level of Carbon Nano Tube Field Effect Transistors, *Archives of Physics Research*, 2010, 1 (2):84-88

- [5] Masoud Amiri and Ali Bahari, A New Consideration of Carrier Transport Through Carbon Nanotubes Which Has Been Placed as a Channel of Field Effect Transistor, World Applied Sciences Journal 12 (1): 68-71, 2011
- [6] Mosahhar Bagheri, Ali Bahari, Masoud Amiri, Behnam Dehbandi, Electronic and structural properties of Au-doped zigzag boron nitride nanotubes: A DFT study.
- [7] Ahad Khan Pyawarai, Simulating of Boron Atoms Interacting with a (10,0) Carbon Nano Tube: A DFT Study, International Journal of Physics, 2020, Vol. 8, No. 1, 29-34.
- [8] Ahad Khan Pyawarai, Interaction of Au and Boron Nitride Nanotube: A DFT Study, International Journal of Physics. **2020**, 8(2), 42-47.
- [9] J. Singh, Semiconductor Optoelectronics, Mc Grow-Hill. Inc (1995), p. 66-68
- [10] I. A. Buyanova, W. M. Chen and B. Monemar, MRS Internet Journal. Nitride Semiconductor Research. 6, 2(2001)
- [11] Doping, Electrical Properties and Solar Cell Application of GaInNAsK. Volz, W. Stolz, J. Teubert, P. J. Klar, W. Heimbrod, F. Dimroth, C. Baur, A. W. Bett Dilute III-V Nitride Semiconductors and Material Systems Physics and Technology(2008), p.369-404
- [12] Z. Pan, L. H. Li, Y. W. Lin, B. Q. Sun, D. S. Jiang, W. K. Ge, Appl. Rhys. Lett. 78, 2217 (2001)

