JOURNAL LA MULTIAPP
VOL. 01, ISSUE 02 (007-013), 2020
DOI: 10.37899/journallamultiapp.v1i2.107

Simulation of Energy Bands for Metal and Semiconductor Junction

Wut Hmone Kyaw[1], May Nwe Myint Aye[1]

[1] *Technological University (Sagaing), Sagaing, Myanmar*

**Corresponding Author: Wut Hmone Kyaw*
Email: lillian.wuthmone@gmail.com

Article Info
Article history:
Received 09 June 2020
Received in revised form 12 June 2020
Accepted 18 June 2020

Keywords:
MOSFET
Band Structure
Gallium Nitride
Metal-semiconductor

Abstract

This paper presents the metal-semiconductor band structure analysis for metal-oxide semiconductor field effect transistor (MOSFET). The energy bands were observed at metal-semiconductor and semiconductor-metal junctions. The simulation results show energy variations by using gallium-nitride (GaN) material. Gallium nitride based MOSFETs have some special material properties and wide band-gap. From the energy band, the condition of contact potential, conduction and valence band-edges can be analyzed. The computerized simulation results for getting the band layers are investigated with MATLAB programming language.

Introduction

The metal-oxide semiconductor field effect transistor called MOSFET is very important electronic device in these modern days. If a voltage source is connected across drain and source terminal with positive terminal at drain and negative terminal at source, there will be no current flowing from drain to source because there is no conducting channel between drain and source (Soubra et al., 1994). Due to the apply positive voltage at drain, p-n junction between n-type drain and p-type substrate is reversed biased and due to negative voltage at the source, the p-n junction between n-type source and p-type substrate is forward biased. Since the reverse bias junction is in series with the forward bias junction between drain and source, there will be no current between drain and source of the device. But, when positive voltage is applied at gate terminal, minority carriers in p-type substrate are concentrated between drain and source and this makes a conducting channel. Therefore, current starts flowing from drain to source. The conductivity of the channel depends on the amount of positive voltage applied at gate terminal (Son et al., 2009). If the gate voltage is not applied, there will be no current from drain to source, except that there is a negligible amount of constant saturation current due to minority carriers. The gate voltage is gradually increased by keeping fixed the drain to source voltage. After certain minimum gate voltage is applied, drain to source current will start flowing. And this voltage is called threshold voltage. In other words, the voltage needed to create the channel is called the threshold voltage, V_T.

Figure 1 shows an example of n-channel enhancement mode metal-oxide semiconductor field effect transistor. For an n-channel enhancement-type MOSFET, V_T is positive and for a p-channel device it is negative. If the gate voltage is less than the threshold voltage, the device will behave as a non-conducting or an OFF-mode. On the other hand, if the gate voltage is larger than the threshold voltage, it behaves as a conducting or ON-mode. Therefore, this type of MOSFET is suitably used as a gate controlled switching device (Chaudhr & Roy, 2010; Gang, 2010; Wan et al., 2012).

ISSN: 2716-3865 (Print), 2721-1290 (Online)

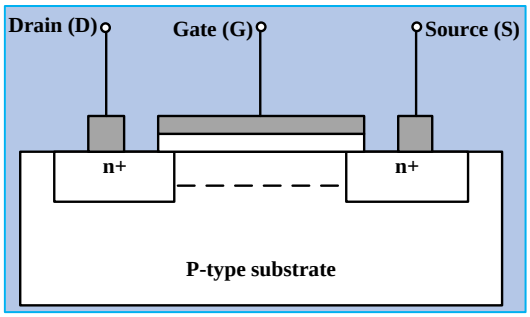

Figure 1. N-channel MOSFET

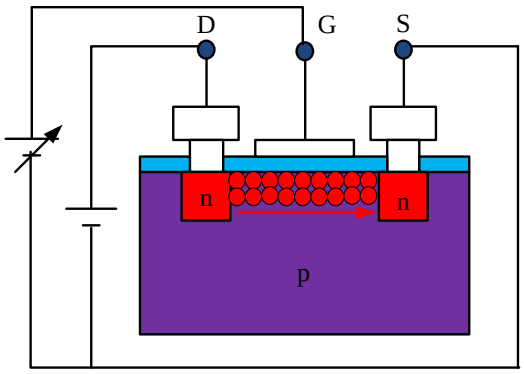

Figure 2. N-Channel Enhancement Mode MOSFET

Analysis of Energy Band Structure

The investigation of energy band structure is mainly focused on the band-gap energy for MOSFET (Ma et al., 2011). There are two types in analyzing the energy band diagrams for metal and semiconductor junction. The first type is for the work-function of metal greater than that of semiconductor. In such case, the semiconductor is going to lose its electrons. The Fermi level of semiconductor material is above that of metal. Therefore, metal will gain its electrons. For second type of work-function of metal which is less than that of semiconductor, the metal will lose its electrons. The semiconductor material will achieve the electrons. In such condition, the energy of conduction band is closer to the Fermi level and that of valence band is far away from the Fermi level near metal and semiconductor junction (Grigelionis et al., 2011; Zhang et al., 2011; Kordoš et al., 2012).

Implementation Procedure for Energy Band

The modelling of metal-oxide semiconductor field effect transistor is considered to use gold (Au) and n-type gallium nitride material system. Gallium nitride is used as a semiconductor material. The implementation plan includes step-by-step procedure to model the device. The doping concentrations are considered with three different values: $2x10^{17}$, $1x10^{18}$ and $2x10^{18}$ cm^{-3}. The work-function of Au is 5.0eV and that of GaN is 3.7eV are considered in the paper. Therefore, semiconductor loses the electrons. The values of electron and hole mass and fundamental parameters are known to be constants for each material. The band-gap energy of gallium nitride is 3.4eV.

Before calculating band edges for both conduction and valence band, carrier concentrations must be observed. Then, the contact potential, energy levels and depletion width of the junction are derived with mathematical calculations. Finally, the structures of energy band associated

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with Fermi level are drawn for the device. The detail calculation for device design can be investigated based on the following equations.

$$E_{cn} - F_n = -k_B T \ln \frac{N_d}{N_c} \quad (1)$$

$$x_n = \left[\frac{2\varepsilon_n V_0}{qN_d N_A \left(N_A + \frac{\varepsilon_p}{\varepsilon_N} N_d \right)} \right]^{1/2} N_A \quad (2)$$

$$V_{on} - V_n = \frac{qN_d}{2\varepsilon_n} x_n^2 \quad (3)$$

Table 1 shows the values of depletion width for the n-type material used to design band structure of the device.

Table 1. Values of Depletion Width for Various Concentrations

Concentrations (cm^{-3})	Depletion Widths (m)
$2x10^{17}$	0.329
$1x10^{18}$	0.115
$2x10^{18}$	0.0667

Results and Discussion

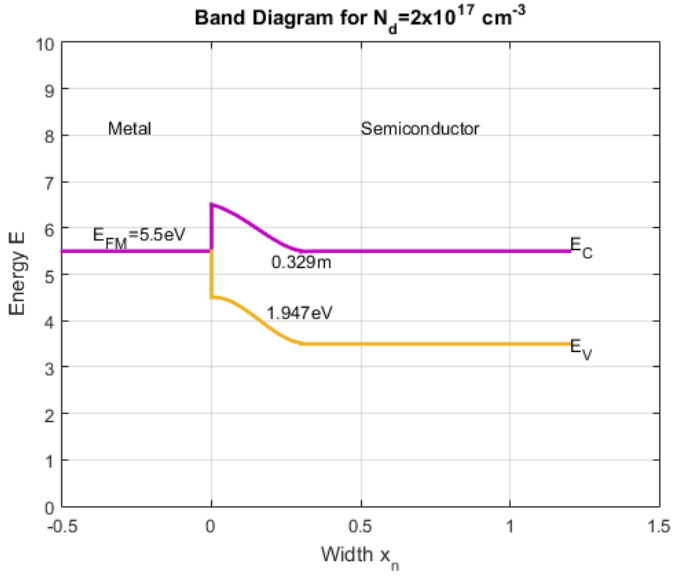

Figure 3. Band Diagram of Gold and Gallium Nitride Junction

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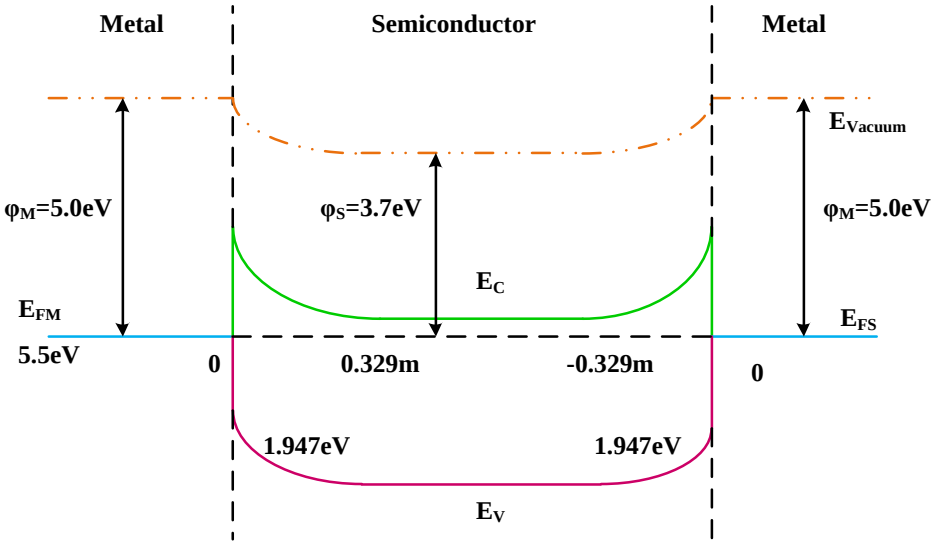

Figure 4. Energy Levels for Metal-Semiconductor-Metal Junctions

Figure 3 shows the simulation result for energy level investigation for metal-oxide semiconductor field effect transistor. From the figure, it can be seen that the conduction band and valence band of the semiconductor material are contacted with the metal portion. It also shows energy changes depending on the width of the region.

Figure 4 illustrates the energy levels for metal-semiconductor junction and semiconductor-metal junction occurring at both conduction band and valence band. The work-function is defined as Φ_M and it is the energy required to take electron between vacuum level and the Fermi level. The work-function must be considered for the band analysis. The work-function of metal is 5.0eV and that of semiconductor is 3.7eV in order to get the Schottky barrier junction design for the device.

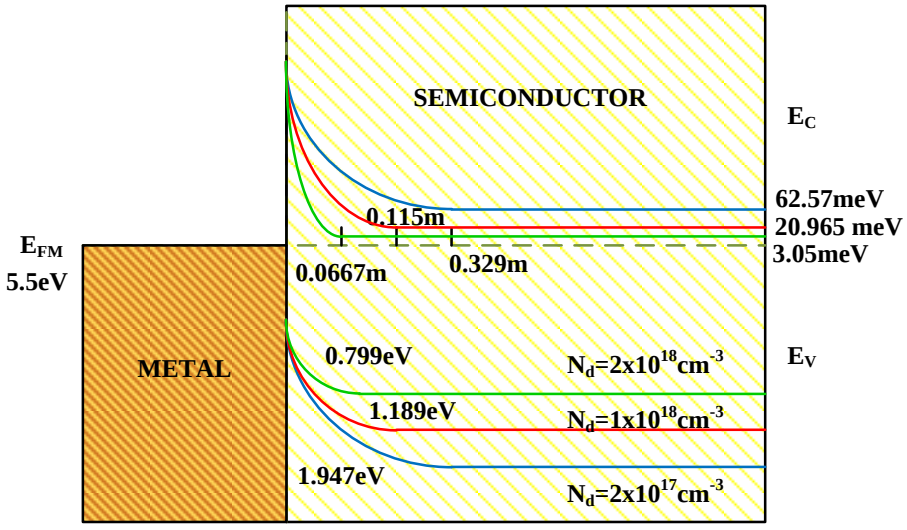

Figure 5. Metal-Semiconductor Junction Using Different Donor Concentrations

It can be seen from Figure 5 that the concentrations are used as three different values for the investigation of band structure. The band edges values are calculated from the respective equations. For the conduction band, the green line is the resultant curve for donor concentration of the highest value. This band closes to the Fermi level than the other bands for conduction

ISSN: 2716-3865 (Print), 2721-1290 (Online)

band. On the other hand, when the concentration is higher, the valence band closes to the Fermi level than the bands of lower concentrations.

Comparison of Band-Edges with Gallium-Arsenide Material

The resultant data of metal and gallium nitride material are compared with that of metal and gallium arsenide material for the device. Table 2 describes the data for comparing band edges of the two.

Table 2. Comparison of Band Edges

Donor Concentrations	Materials	Conduction Band Edges (meV)	Valence Band Edges (eV)
$N_d=2x10^{17}$ cm^{-3}	Au-nGaAs	19.79	1.067
	Au-nGaN	62.57	1.947
$N_d=1x10^{18}$ cm^{-3}	Au-nGaAs	21.82	0.6395
	Au-nGaN	20.965	1.189
$N_d=2x10^{18}$ cm^{-3}	Au-nGaAs	39.74	0.42
	Au-nGaN	3.05	0.799

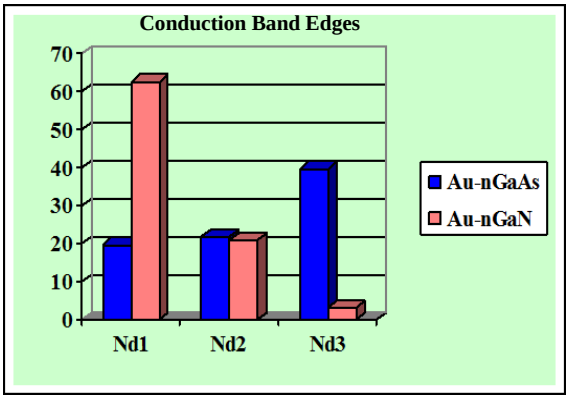

Figure 6. Comparison of Conduction Band Edges

Figure 6 is the comparison data for conduction band edge values of band analysis between gallium arsenide material and gallium nitride material. It can be seen that the highest band edge for gallium nitride and gold junction is achieved when donor concentration is $2x10^{17}$ cm^{-3}. Also, Figure 7 gives the difference between the two materials in relation with valence band edges.

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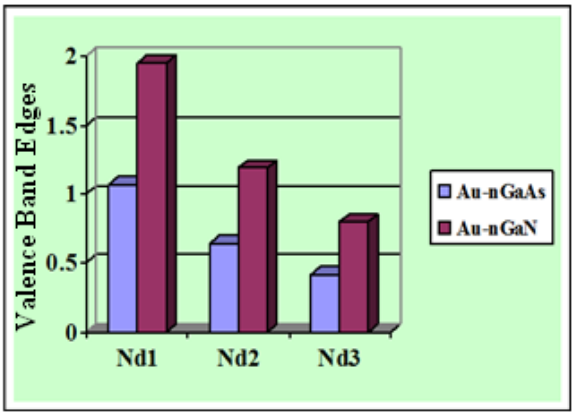

Figure 7. Comparison of Valence Band Edges

Conclusion

The paper mainly focuses on the analysis of energy band diagrams for metal and semiconductor junction for MOSFET modeling. The concentrations ranges used are 10^{17} and 10^{18} cm^{-3}. It also shows the differences between the band edges of gallium arsenide and gallium nitride. From the energy analysis, the condition of current can further be analyzed for the device performance.

Acknowledgment

The authors wish to thank semiconductor research group of our Technological University.

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ISSN: 2716-3865 (Print), 2721-1290 (Online)