IOSR Journal of Electrical and Electronics Engineering (IOSR-JEEE)
e-ISSN: 2278-1676, p-ISSN: 2320-3331, Volume 17, Issue 5 Ser. I (Sep. – Oct. 2022), PP 28-31
www.iosrjournals.org

The electron and heavy-hole effective masses in crystalline Diamond and the properties of the Metal-Oxide-Semiconductor hole device

Dr. Ravi Kumar Chanana
Retired Professor, Self-employed Independent Researcher, Greater Noida, India.
Corresponding author email: ravikumarchanana@yahoo.co.in

***Abstract*:** *This research study finds the electron and heavy-hole effective masses in crystalline (100) oriented type Ib and IIb Diamond semiconductor and the properties of the metal-oxide-semiconductor (MOS) hole device on Diamond theoretically. The universal mass-energy equivalence relation expressed as a first-order differential equation is given as dE/E equals dm/m. It is used to determine the effective masses in semiconductors and insulators and the MOS device properties. The properties are found without fabricating the device purely based on the above electron or hole particle physics universal concept that relates to the properties of the MOS device. The longitudinal electron effective mass of Diamond is found to be 0.43m for one conduction valley in the [100] direction and the heavy-hole mass is 0.57m. The transverse electron effective mass is also found to be 0.32m. The properties of the MOS hole device are further determined.*

Keywords: *Diamond,Effective Mass, Intrinsic Defects,MOS, FN-Tunnelling*

Date of Submission: 26-08-2022 Date of Acceptance: 10-09-2022

I. Introduction

Crystalline diamond is a wide bandgap semiconductor with high electron and hole mobilities making it suitable for high voltage applications such as a power MOSFET. Its bandgap is 5.5 eV giving a very low intrinsic carrier concentration and thus a high voltage can be applied without breakdown. The electron mobility is of the order of 3000 cm^2/V-s and the hole mobility is of the order of 2000 cm^2/V-s making it suitable for an n-channel or p-channel MOSFET device. However, the donor levels of Phosphorus and Nitrogen are deep at 0.6 eV and 1.7 eV resulting in ionization only with the help of ultraviolet illumination. The Boron acceptor level is at 0.37 eV above the Valence band and can result in partial ionization at room temperature also making a hole device more feasible than an electron device. In this article, a hole device is considered. Two hole-devices are already under study by Kawarada and co-researchers. One is an enhancement mode p-channel MOSFET giving a channel hole mobility of 106 cm^2/V-s and the other is a heterojunction high electron mobility transistor giving the 2D hole gas mobility of about 700 cm^2/V-s [1-2]. The MOSFET can also be used in designing a floating gate high temperature FLASH memory device which can further be considered for a solid-state drive to work at high temperatures of up to 200^{o}C at least. In the present article, the author finds the fundamental electron and hole effective masses of the diamond semiconductor along with the MOS properties of an enhancement mode p-channel MOSFET utilizing the concept of electron and hole effective masses being related to the intrinsic energy in the semiconductor band gap from the universal mass-energy equivalence relation dE/E equals dm/m expressed as a first order differential equation. Here, dE is the differential potential energy of the electron or hole, E is the semiconductor bandgap as the total potential energy, dm is the differential mass as the effective mass of electron or hole in the material and m is the free electron mass [3-5].

II. Theory

The research paper is divided into two parts. In the first part, the MIS characterization determines the intrinsic Fermi level E_i in the diamond semiconductor bandgap. The E_i determines the differential energy for the electron to the semiconductor conduction band (CB) and for the hole to the semiconductor valence band (VB). The total potential energy of the electron is the semiconductor bandgap. Thus, utilizing the universal mass-energy equivalence principle dE/E equals dm/m, the electron and hole effective masses in the semiconductor are determined [3-5]. The second part of the study determines theoretically the properties of the MOS hole device given the electron and hole effective masses of the diamond semiconductor based on say cyclotron resonance study or from the density functional theory of band structure determination. The known masses can be used to find E_i using the same equation dE/E equals dm/m. In the first part E_i was determined

first and now in the second part the masses are known first.Thus, the intrinsic Fermi energy level in the thermal oxide from the oxide CB, of 3.75 eV = 0.42 x 8.93 eV, aligns to the intrinsic Fermi level in the semiconductor as the relative electron or hole effective mass in the oxide is known accurately in advance as 0.42 and 0.58 respectively, with the oxide bandgap as 8.93 eV. The conduction band offset (CBO) from the oxide CB to the semiconductor CB can therefore be determined by subtracting the differential potential energy of electron from E_i to the semiconductor CB,from the oxide intrinsic Fermi energy level of 3.75 eV from the oxide CB. The valence band offset (VBO) from the oxide VB to the semiconductor VB can be determined by subtracting the differential potential energy of hole from E_i to semiconductor VB, from the oxide intrinsic Fermi energy of 5.18 eV from the oxide VB. After the determination of the CBO or the VBO of the electron or hole, the FN onset field is found by multiplying the CBO or VBO by 2 MV/cm-eV. This value is obtained by DiMaria et al. and confirmed by the author as the minimum electric field threshold for electron heating in the SiO_2 with 1 eV as the energy to create hot electrons in vacuum [6-7]. The intrinsic defects density in diamond N_{id} and the oxide breakdown field is further determined as described in the next section. Two earlier studies by the author, one on Si (100) and one on the 4H-SiC can also assist in elaborating and clarifying the above theory [8-9].

III. Results and Discussion

The intrinsic Fermi level E_i in the Diamond (100) semiconductor having small intrinsic defects density is found first by MIS characterization [3-4]. From the ratio of the intrinsic Fermi Level-Conduction band (CB) or Valence band energy difference to the bandgap energy, the electron effective mass in the longitudinal direction [100] having two conduction valleys or the heavy-hole effective mass can be obtained given that the (100) surface is used to fabricate the MOS device. The relation dE/E equals dm/m is utilized, where m is the free electron mass. Here, dE is the differential potential energy of electron from E_i to semiconductor CB, or differential kinetic energy of a moving electron when excited from E_i to the semiconductor CB, and dm is the differential mass as the effective mass [5]. E is the semiconductor bandgap as the total potential energy of the electron. The effective masses of the electron and hole in the crystalline Diamond semiconductor are calculated and presented in Table I below, and are compared to the values in references [10-11].

Table I. Effective masses of electron and hole in crystalline semiconductor Diamond

Semiconductor, (100) oriented	Indirect-Bandgap, E_g, in eV	Intrinsic Fermi Level from CB in eV	Heavy-hole effective mass	Longitudinal electron effective mass in [100] direction.
Diamond, Ref. [3-5]	5.5	2.35	0.57m	0.43m x 2 = 0.86m
Diamond, Ref. [10]	5.75		0.32m-0.40m	1.1m-1.5m
Diamond, Ref. [11]	5.45		0.614m	

It can be observed that the heavy-hole effective mass of reference [11] at 0.614m matches closely to the mass obtained by the MIS characterization method devised by the author, at 0.57m [3-5] and is lower than the hole mass in SiC polytypes at about 0.7m and wurtzite and zincblende GaN at about 0.8m, resulting in higher hole mobility in Diamond. The enhancement-mode p-channel MOSFET having a field-effect (FE) surface mobility of 106 cm^2/V-s, and 2-D Hole Gas hetero-devices in Diamond having a surface FE mobility of about 700 cm^2/V-s are therefore under study [1-2, 12]. Si (100) has an electron effective mass for one conduction valley as 0.49m and the heavy-hole mass as 0.51m. It makes an ideal candidate for both n-channel and p-channel MOSFETs with these values of electron and hole masses due to their high mobilities. The next semiconductor material could be Diamond for room temperature and high temperature Complementary-Metal-Oxide-Semiconductor (CMOS) technology development under ultraviolet (UV) illumination, apart from a power MOSFET development as the electron effective mass in Diamond is 0.43m for one conduction valley and the heavy-hole mass is 0.57m as calculated and presented above in the Table I, resulting in high electron and hole mobilities. The n-type donor dopants are deep, 0.6eV for Phosphorus and 1.7 eV for Nitrogen and the p-type acceptor dopant as Boron has the energy level at 0.37 eV. Doped Diamond therefore requires an UV illumination to ionize the dopants [13]. The enhancement type p-channel MOSFET is shown to exist in Diamond even without UV illumination and having partial hole ionization at 300 K in the p^+-I-p^+ channel region of the MOSFET with a hole mobility of 106 cm^2/V-s [1]. Integrated electronics with PMOS technology can flourish with the p-channel MOSFET. The matching hole mass in Diamond of 0.57m with that of 0.614m in reference [11] puts credibility into the longitudinal electron effective mass in [100] direction also of 0.86m for two conduction valleys, because the electron effective mass of one valley and the heavy-hole effective mass adds to be equal to the free electron mass. The longitudinal electron effective mass in [111] direction will be 0.86m multiplied by the long diagonal factor of $\sqrt{3}$, giving the mass to be 1.48m. The conduction valley at Γ=0

has a minimum at 7.3 eV from the valence band. Therefore, the transverse electron effective mass dm equals (2.35/7.3) m, where dE/E is (2.35/7.3). The transverse mass dm is thus 0.32m.

The properties of the Al/SiO_2/Diamond MOS hole device [1] with hole as a current carrier can be determined theoretically with the given heavy-hole mass of 0.57m and the bandgap of 5.5 eV in the type Ib or IIb crystalline diamond semiconductor, similar to the determination of properties of a MOS device with electron as a carrier in Si (100) or 4H-SiC semiconductors [8-9]. It needs to be noted that the Al-SiO_2 barrier height is 3.13 eV and the Diamond (100)-SiO_2 VBO is lower at about 2.0 eV resulting in Fowler-Nordheim (FN) hole tunnelling current with the MOS device in accumulation having Al gate as the cathode [1, 13]. The electric field in the thermal SiO_2 having negligible bulk defects is oriented in the [100] direction for the MOS device fabricated on the Diamond (100) surface. The intrinsic Fermi level E_i, is located at 0.57 x 5.5 eV = 3.135 eV above the Valence band (VB) of Diamond, given that the relative energy equals relative mass of a moving electron or hole from the equationdE/E equals dm/m [3-5]. This value is 2.35 eV from the CB in the earlier MIS characterization study with electron as a current carrier [3-5]. The VBO of the oxide/semiconductor interface is 5.18-3.135 = 2.045 eV and the FN onset field in the oxide is 2 x 2.045 = 4.09 MV/cm with hole as a current carrier. This is because the FN onset field divided by the CBO in a MOS device equals 2 MV/cm-eV as the electron heating threshold in the thermal SiO_2, where 1 eV is the energy to create hot electrons in vacuum. This has been found by direct observation of electron heating threshold in the oxide as 2 MV/cm, with confirmation by the author's study. The FN onset field in the MOS device is thus 2 MV/cm-eV x CBO [6-7]. The same is valid for the hole as a current carrier. Therefore, the FN onset field for the hole carrier is 4.09 MV/cm as presented above. Here, 5.18 eV is the position of the E_i in SiO_2 from its VB and identifies the position of E_i in Diamond for the oxide/semiconductor interface. The 5.18 eV equals 0.58 x 8.93 eV, where 0.58 is the relative hole effective mass in the oxide and 8.93 eV is the oxide bandgap [3-4]. The theoretical value of the slope constant B for the FN tunnelling hole current can now be decided using the formula [14-15]:

$$B = 68.3\, x \left(\frac{m_{ox}}{m}\right)^{1/2} x(\emptyset_0)^{3/2} \dots\dots MV/cm \qquad (1).$$

Here, hole effective mass m_{ox} for SiO_2 is 0.58m and the oxide/semiconductor interface barrier height $\emptyset_0$ for hole is found above theoretically as 2.045 eV. These values give the theoretical slope constant B as 152.12 MV/cm. The FN hole current density for this B and an FN onset field of 4.09 MV/cm found above will be about 1.5 x 10^{-9} A/cm^2 theoretically. The oxide will exhibit a breakdown field of about 5.8 MV/cm for a 10^{-4} A/cm^2 current density for thick oxide of say 40 to 150 nm, given that two points on the Fowler-Nordheim (FN) current-voltage (I-V) characteristics at high fields are (1.5 x 10^{-9} A/cm^2, 4.09 MV/cm) and (10^{-4} A/cm^2, E_{bkdn} in MV/cm). From the first point, FN slope constant B can be calculated as 152.12 MV/cm, and from the second point, the E_{bkdn} can be calculated to be 5.8 MV/cm [14-15].A recent experimental study of MOS capacitors on p-type diamond having 50 nm atomic layer deposited oxide shows a FN onset voltage of -8V giving a FN onset field of only 1.6 MV/cm at 296 K temperature and even lower at 373 K temperature. It is low and indicates presence of border traps at the Si-rich oxide/diamond interface [16, 17]. E_i, located at 2.35 eV from the Diamond (100) CB or 3.135 eV from the Diamond VB close to the mid-bandgap of 2.75 eV translates to a very small intrinsic defect density, N_{id} of about 2.3 x 10^{-13}/cm^3 in natural diamond having a very small intrinsic carrier concentration because of its large bandgap of 5.5 eV [3-4].

IV. Conclusions

It is concluded from the study that the MIS characterization where the intrinsic Fermi level is determined first can lead to finding the electron and hole effective masses in the semiconductor Diamond. The electron effective mass comes out to be 0.43m and the hole effective mass is found as 0.57m. Conversely, if the effective masses of electron and hole in Diamond are known by a different theoretical or experimental method, then the intrinsic Fermi energy position in the diamond semiconductor can be found at 2.35 eV from the CB or 3.135 eV from the VB,leading to the theoretical determination of the properties the MOS hole device. For the hole device, the VBO is at 2.045 eV, the FN onset field for hole tunnelling is 4.09 MV/cm, the oxide hole leakage current density is about 1.5 x 10^{-9} A/cm^2 at FN onset field, and electrical breakdown strength is 5.8 MV/cm due to the hole tunnelling current. Intrinsic defects density N_{id} in type IIb Diamond (100) is about 2.3 x 10^{-13}/cm^3.

References

[1]. W. Fei, Te Bi, M. Iwataki, S. Imanishi, H. Kawarada, "Oxidized Si terminated diamond and its MOSFET operation with SiO_2 gate insulator", Appl. Phys. Letts., 116, 212103 (2020).

[2]. Y. Sasama, T. Kageura, M. Imura, K. Watanabe, T. Taniguchi, T. Uchihashi, Y. Takahide, "High-mobility p-channel wide bandgap transistors based on h-BN/diamond heterostructures, arXiv Preprint, 2102, 05982 (2021).

[3]. R.K. Chanana, "A new method for calculating charged deep level defects density in doped semiconductors from the band offsets of MIS device interfaces", IOSR-J. Appl. Phys., 8(4), 53-56 (2016).
[4]. R.K. Chanana, "Intrinsic Fermi level and charged intrinsic defects density in doped semiconductors from the band offsets of MIS device interfaces", IOSR-J. Appl. Phys., 9(6), 1-7 (2017).
[5]. R.K. Chanana, "Linear model for the variation of semiconductor bandgap with high temperature for high temperature electronics", IOSR-J. Electrical and Electronics Engg., 16(6), 5-8 (2021).
[6]. D.J. DiMaria, M.V. Fischetti, E. Tierney, "Direct observation of the threshold for electron heating in silicon dioxide", Physical Review Letters, 56(12), 1284-1286 (1986).
[7]. R.K. Chanana, "On the ionization in silicon dioxide of a MOS device and its relation to the density of the oxide", IOSR-J. Appl. Phys., 12(6), 1-5 (2020).
[8]. R.K. Chanana, "Theoretical finding of the properties of a Si (100) MOS device", IOSR-J. Applied Physics, 14(3), 5-6 (2022).
[9]. R.K. Chanana, "N-channel 4H-SiC MOSFET device on $(11\bar{2}0)$ oriented epitaxial surface", IOSR-J. Electrical and Electronics Engineering, 17(3), 20-22 (2022).
[10]. H. Lofas, A. Grigoriev, Jan Isberg, Rajeev Ahuja, "Effective masses and electronic structure of diamond including electron correlation effects in first principles calculations using the GW-approximation", AIP Advances, 1, 032139 (2011).
[11]. A.T. Collins and E.C. Lightowlers, "Electrical Properties" in The Properties of Diamond, edited by J.E. Field, Academic Press, NewYork, 79. (1979).
[12]. T. Muta, T. Saito, M. Inaba, D. Matsumura, T. Kudo, Y. Kitabayashi, A. Hiraiwa, H. Kawarada, "Vertical MOSFET using C-H Diamond with trench channel", Extended Abstracts of the 2016 International Conference of Solid-State Devices and Materials, Tsukuba, pp-597-598 (2016).
[13]. M.W. Geis, J.A. Gregory, B.B. Pate, "Capacitance-Voltage measurements on Metal-SiO_2-Diamond structures fabricated with (100)- and (111)-oriented substrates", IEEE Trans. On ED, 38(3), 619-626 (1991).
[14]. R.K. Chanana, "Determination of electron and hole effective masses in thermal oxide utilizing an n-channel silicon MOSFET", IOSR-J. of Appl. Phys., 6(3), 1-7 (2014).
[15]. R.K. Chanana, "BOEMDET-Band offset and effective mass determination technique utilizing Fowler-Nordheim tunnelling slope constants in MIS devices in silicon", IOSR J. Appl. Phys., 6(4), 55-61 (2014).
[16]. J. Canas, C. Dussarrat, T. Teramoto, C. Masante, M. Gutierrez, E. Gheeraert, "High quality SiO_2/Diamond interface in O-terminated p-type diamond MOS capacitors", Appl. Phys. Letts, 121, 072101 (2022).
[17]. R.K. Chanana, "Border trap densities in metal-insulator-semiconductor devices and their correlation in Si and 4H-SiC devices", IOSR-JEEE, 16(2), 7-11 (2021).

Dr. Ravi Kumar Chanana. "The electron and heavy-hole effective masses in crystalline Diamond and the properties of the Metal-Oxide-Semiconductor hole device." *IOSR Journal of Electrical and Electronics Engineering (IOSR-JEEE)*, 17(5), 2022, pp. 28-31.