IOSR Journal of Electrical and Electronics Engineering (IOSR-JEEE)
e-ISSN: 2278-1676, p-ISSN: 2320-3331, Volume 18, Issue 3 Ser. II (May. – June. 2023), PP 05-07
www.iosrjournals.org

On the Electron and Hole Effective Masses in SiO_2

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Abstract: *This review and research study provides convincing arguments and evidences based on experiments that the electron and hole effective masses in thermal silicon dioxide are 0.42m and 0.58m, where m is the free electron mass. Only one of the masses needs to be determined as the electron and hole masses in materials add up to be equal to free electron mass with the hole effective mass being larger than the electron effective mass. The review also convinces the reader that the conduction band offset or the Si-SiO_2 barrier height at the oxide/silicon interface of a Si MOS device is 3.20 eV.*

Keywords: *Band Offsets, Effective Masses, MOS Device, Materials, Tunnelling*

Date of Submission: 15-06-2023 Date of Acceptance: 25-06-2023

I. Introduction

The characterization of a Metal-Insulator-Semiconductor (MIS) device is important as it uncovers the Physics of the device and materials for the application of a reliable Metal-Insulator-Semiconductor-Field-Effect-Transistor (MISFET). An n-channel Si MOSFET was demonstrated in early 1960, where grown thermal SiO_2 was utilized as the insulator. A Si Metal-Oxide-Semiconductor (MOS) device has band offsets at the oxide/semiconductor interface along with the electron and hole effective mass values in the thermal SiO_2. The band offset values inform us about the amount of electron or hole current tunnelling through the oxide in the MOS device at low and high electric fields. This characterization has been in doubt ever since the invention of the transistor. One of the main reasons for this doubt has been that the hole effective mass in the Si-MOS device could not be found because the direct measurement and observation of FN hole tunnelling was not possible due to a large hole barrier at the anode of the Si-pMOS device of 4.6 eV which was higher than the electron barrier at the cathode causing electron current to be dominant in the two-terminal MOS device. Carrier separation method using a MOSFET device resulted in the observation of hole current but the polysilicon depletion in the MOSFET prevented from accurate measurement of the hole tunnelling current in the oxide. Also, it was not known then that the flatband voltage has to be added to the applied voltage to give the oxide voltage for hole tunnelling, meaning that the science was also unknown for hole tunnelling calculations. The advent of 4H-SiC eliminated this problem and direct measurement and observation of FN hole tunnelling current was possible because of a low hole barrier in the pMOS device on 4H-SiC in accumulation [1-2]. This paper puts to rest any doubts about the electron and hole effective masses in the thermal SiO_2 and the band offsets at the oxide/semiconductor interface of a Si or 4H-SiC MOS device by reviewing past research and providing corroborative evidence and science of a MOS device.

II. Theory

MIS characterization of a MOS device can be done easily in an Electronics laboratory of a University or College or at an Industry setting. The study of this device reveals the properties of the device that can make the transistor efficient and reliable. Some of the main properties are: Interface states at the oxide/semiconductor interface and in the oxide near the interface, charge densities in the oxide, Electrical breakdown strength of the oxide, leakage current in the oxide, the onset field for electron and hole tunnelling current, the carrier effective masses in the oxide and many others. An excellent 900 pages book on the MOS Physics and Technology is available from Wiley and Sons publishers, written by E.H. Nicollian and J.R. Brews that can provide detailed knowledge on the MOS device. This book can be supplemented with books on Solid-State Physics and Solid-State Device Electronics [3]. Now, the science of the MOS device through author's recent studies have revealed that the character of a MOS device can be obtained theoretically on all parabolic semiconductors given the longitudinal electron and hole effective masses in the semiconductors and insulators and the bandgap of the materials without even fabricating the device [4-6]. Theoretical results are a sure shot based on the universal mass-energy equivalence relation, dE/E=dm/m. The problems would lie in experiments if a mismatch is found.

III. Results and Discussions

Since the advent of 4H-SiC semiconductor material for the design and development of high voltage power electronics devices such as MOSFETs, direct measurement and observation of Fowler-Nordheim (FN) hole tunnelling current though the Metal-Oxide-Semiconductor (MOS) device is possible. The Au-SiO_2-p-4H-SiC-Si faced MOS device with Au as the cathode causes accumulation of holes at the semiconductor surface. The smaller hole barrier of 2.92 eV at the oxide/semiconductor interface as compared to the larger electron barrier at the Au cathode of 4.2 to 4.4 eV brings about the observation of FN hole tunnelling as the dominant current in the two-terminal MOS device. The hole effective mass in thermal SiO_2 is calculated to be 0.58m and is confirmed by a Japanese research group, Nemoto et al. [7]. It has also been shown by the author that the longitudinal electron and hole effective masses in parabolic semiconductors such as Si and 4H-SiC are related to the intrinsic Fermi energy level E_i in the semiconductors by the universal mass-energy equivalence relation dE/E = dm/m, where dE is the differential potential energy of electrons from E_i to the conduction band (CB) of the semiconductor, E is the semiconductor bandgap as the total potential energy of electrons relative to the valence band, dm is the differential mass as the longitudinal electron effective mass in the material, and m is the free electron mass. This universal relation is obtained by differentiating the mass-energy equivalence relation of Einstein, who first found that intrinsic energy E is equivalent to rest mass m_0 by the relation $E = m_0c^2$. The same relation holds for E as the total relativistic energy of a moving mass m, and c is the speed of light, given as $E=mc^2$, where $m = m_0/(\text{sqrt}(1-v^2/c^2))$ with v as the velocity of the moving mass m. This relation is differentiable in the velocity interval [0, c], giving dE/E=dm/m. Applying this universal mass-energy equivalence principle to the thermal oxide as an insulator which is modelled as a wide bandgap semiconductor, gives the electron effective mass in the oxide as 0.42m, given that the hole effective mass in the oxide is confirmed to be 0.58m, and the differential energy of holes from the intrinsic Fermi energy level E_i in SiO_2 to the oxide valence band (VB) is E-dE [4-6]. The universal mass-energy equivalence relation is also applicable to other energy transformations such as nuclear and chemical energies.

The above paragraph assures that the electron effective mass in thermal SiO_2 is 0.42m, where m is the free electron mass. The original establishment of this value is from the research study of Lenzlinger and Snow in 1969 [8]. The FN characteristics in Fig.6 of the research paper for Si gives the slope constant of the plot as 258 MV/cm and the reported Si-SiO_2 barrier height by photoemission is 3.25 eV. The equation for the slope constant of the FN characteristics of a MOS device is given as [9-10]:

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

Here, B is the slope constant at 258 MV/cm, m_{ox} is the electron effective mass in SiO_2, and $\emptyset_0$ is the Si-SiO_2 barrier height at 3.25 eV. The calculation by substituting the above values in the equation for the slope constant gives m_{ox} as 0.4156m which is reported as 0.42m in the graph for Si. Shifting the line of the slope a bit to the right from the bottom only, so as to properly fit the bottom most point on the graph reduces the slope to 254 MV/cm, which is also obtained for an 8.5 nm thermal oxide in another study [9-10]. Now, using the assured value of 0.42m as the electron effective mass from the above paragraph and 254 MV/cm as the slope constant for the FN characteristics for Si, gives the Si-SiO_2 barrier height as 3.205 eV instead of 3.25 eV reported by Lenzlinger and Snow. Three different internal photoemission (IPE) experiments to obtain the Si-SiO_2 barrier height has been reviewed by the author. The Si VB to SiO_2 CB reported by Yan et al. is 4.3 eV using a graphene/SiO_2/Si device [11]. Subtracting the Si bandgap of 1.12 eV gives the Si-SiO_2 barrier height as 3.18 eV. This is close to the obtained barrier height of 3.205 eV above. The photoemission experiment by Richard Williams with the Au/SiO_2/n-Si device gave a Si VB to SiO_2 CB barrier height of 4.25 ± 0.06 eV. This data supports the Si-SiO_2 barrier height of 3.19 eV if +0.06 eV variation is taken, and after subtracting the Si bandgap of 1.12 eV [12]. Gobeli and Allen showed electron emission into vacuum from p-Si giving energy from Si VB to vacuum of 5.2 eV [13]. After subtracting 0.9 eV as the electron affinity of the SiO_2, the Si VB to SiO_2 CB barrier height becomes 4.3 eV same as what Yan et al. had obtained. This again gives the Si-SiO_2 barrier height as 3.18 eV after subtracting the Si bandgap of 1.12 eV. This is close to 3.205 eV. The Polish experimenters, Piskorski and Przewlocki, have found the Si VB-SiO_2 CB barrier height to be 4.4 eV [14]. After subtracting the Si bandgap of 1.12 eV, the Si-SiO_2 barrier height is higher at 3.28 eV. It is to be noted that Al is hydrophilic whereas graphene and Au are hydrophobic. This may cause the Al-based MOS device to give a higher Si-SiO_2 barrier height due to water adsorption which is known to reduce the work function by as much as 1 eV [15]. Reduction in Al work function results in increase in metal-semiconductor work function difference $\emptyset_{ms}$ which being negative reduces the gate voltage and consequently the photoelectron current. This means that a higher photon energy is required to compensate the reduction in the photocurrent. Higher photon energy implies a higher Si-SiO_2 barrier height of 3.28 eV. It needs to be noted that the difference in barrier height is only of 0.1 eV from 3.18 to 3.28 eV. The results of Yan et al., Richard Williams, and Gobeli and Allen is consistent to a Si-SiO_2 CB barrier height of 3.20 eV. Thus, the author vouches for a Si-SiO_2 barrier height at the oxide/Si interface of a Si MOS device of 3.20 eV instead of 3.25 eV as reported by Lenzlinger and Snow. Moreover, a variation of $\pm$ 0.05 eV in the photoemission experiments is known to be present as shown by Richard Williams. IPE of holes is not efficient. Both, Yan et al.

and Goodman reported a SiO_2 bandgap of about 8 eV instead of 8.93 eV based on the incorrect IPE of holes [11, 16].

Observing the FN onset electric field across a MOS device can also lead to determine the Si-SiO_2 barrier height. The minimum field for electron heating in the thermal SiO_2 is 2 MV/cm-eV, where 1 eV is the minimum energy needed for vacuum emission of hot electrons. This has been shown by DiMaria et al. and confirmed by the author in his earlier study on ionization in the thermal SiO_2 [17-18]. The FN onset field in a MOS device divided by this minimum field for electron heating of 2 MV/cm-eV gives the Conduction Band Offset (CBO) in the MOS device. Lenzlinger and Snow reported an FN onset electric field of 6.41 MV/cm as shown in the graph for electron emission from Si cathode in Fig. 5 of their study [8]. This divided by the electron heating threshold in SiO_2 of 2 MV/cm-eV gives the CBO of 3.205 eV in the Si MOS device. This method further assures the Si-SiO_2 barrier height of 3.205 eV. It is to be noted that the thermal oxide is a grown oxide on semiconductors such as Si and 4H-SiC, whereas plasma or atomic layer deposited oxides of Si and Al are utilized on hetero-surfaces of GaN, GaAs or Ga_2O_3 semiconductors. They show lower bandgaps and electrical breakdown strengths and higher density of interface traps, compared to the thermally grown oxide.

The Si-SiO_2 barrier height of 3.20 eV is substantiated by the photoemission experiments as described above. The intrinsic Fermi energy level E_i in Si is 0.55 eV below the CB, giving 3.75 eV as the Si-SiO_2 CBO from E_i [19]. Applying the theoretical universal mass-energy equivalence relation of dE/E = dm/m, where dE is 3.75 eV divided by the SiO_2 bandgap E of 8.93 eV gives the electron effective mass in thermal SiO_2 as 0.42m [19]. From the universal mass-energy relation the hole effective mass has to be 0.58m.

IV. Conclusions

The electron and hole effective masses in thermal silicon dioxide is convincingly 0.42m and 0.58m. The CBO at the oxide/semiconductor interface of a Si-MOS device is 3.20 eV. The universal mass-energy equivalence relation applied to SiO_2 shows that only one of the masses needs to be determined correctly. The hole mass in materials is always larger than the electron effective mass. The character of a MOS device on any parabolic semiconductor can be known theoretically given the electron and hole effective masses in materials and their bandgaps including the total intrinsic defects density in semiconducting materials.

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