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Properties of a MOS device on (100) oriented cubic SiC

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Abstract: *This research study theoretically finds the properties of a MOS device on 3C-SiC semiconductor having a cubic crystal structure, and showing an anomaly of having a very high intrinsic defects density of about 1.8 x $10^{33}/cm^3$ in the [100] direction in the form of stacking faults. The properties are found without fabricating the device purely based on an electron particle physics concept that relates to the properties of the MOS device. The experimental longitudinal electron effective mass found by the cyclotron resonance is 5 times larger at 0.34m for one out of two conduction valleys in the [100] direction than the effective mass due to the band structure at 0.06m. The study also gives two ways of finding the intrinsic Fermi level E_i below the conduction band in 3C-SiC (100) oriented semiconductor.*

***Keywords*:** *Metal-Oxide-Semiconductor, Silicon Carbide, Intrinsic Defects, FN-Tunnelling*

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I. Introduction

Two research studies by the author, one on the Si (100) and the other on the a-face of 4H-SiC semiconductor, give a theoretical method to find the properties of a MOS device on any parabolic semiconductor, given the transverse and longitudinal electron effective masses in the semiconductor and its bandgap, without fabricating the MOS device [1-2]. The studies also highlight a significant scientific concept of physics that, the electron effective masses in semiconductors and insulators are not only related to the mobility through drift velocity, but are also related to the intrinsic Fermi energy E_i below the conduction band (CB) of the semiconductor through the relation dE/E equals dm/m which relates to the properties of the MOS device. This relation can be written as a first order differential equation. In this equation, dE is the differential kinetic energy of the moving electron when excited from E_i to the semiconductor CB, or it is the differential electron potential energy from E_i to the semiconductor CB, E is the semiconductor bandgap as the total potential energy of the electron, dm is the differential mass as the effective mass of the electron in the semiconductor or insulator material, and m is the free electron mass [1-3]. As mentioned in the earlier study [1], this relation of dE/E equals dm/m is a universal relation applicable to all moving particles in materials, and objects in space, as the mass-energy equivalence relation first discovered by Albert Einstein as $E = mc^2$ in 1905 as a conclusion of his special theory of relativity. The present study on 3C-SiC (100) MOS device is similar to the previous studies [1-2], but having an anomaly that the 3C-SiC semiconductor has a very high density of intrinsic defects that increases the experimental longitudinal effective mass of the electron in 3C-SiC(100)determined by the cyclotron resonance technique, by about 5 times the value based on the band structure of 3C-SiC (100). It thus causes the square of saturated electron drift velocity to decrease to (1/5) times the value based on the band structure of 3C-SiC (100) for the same thermal energy of 0.0388 eV given by (3/2)kT at 300 K temperature. In this article, the properties of a 3C-SiC-MOS device such as, conduction band offset (CBO), the Fowler-Nordheim (FN) onset electric field related to leakage current in the oxide, the oxide electric breakdown field strength, the intrinsic defect density in 3C-SiC (100), and the electron affinity in 3C-SiC semiconductor, are all determined starting with the known longitudinal electron effective mass in 3C-SiC (100) semiconductor as about 0.06m and its experimental indirect bandgap of 2.38 eV, without fabricating the MOS device. Graphene mono and bilayers, with the present state of process technology may be also exhibiting a larger longitudinal electron effective mass experimentally, due to high intrinsic defects density such as that of carbon vacancy defects.

II. Theory

The formula based on the theorem of equipartition of energy for a conducting electron or hole in a semiconductor at thermal equilibrium equates the kinetic energy of an electron in a semiconductor to the thermal energy of the electron at a given temperature T in Kelvin as [4]:

$$\frac{1}{2}m_{eff}{v_{th}}^2 = \frac{3}{2}kT \qquad (1).$$

Here, m_{eff} is the effective mass of the particle, v_{th} is the thermal velocity of the particle in the semiconductor material, k is the Boltzmann constant equal to 1.38 x 10^{-23} Joules/Kelvin. Thus, kT is the energy in Joules. Also, the saturated electron drift velocity of an electron in semiconductor is nearly equal to the thermal velocity of an electron at 300 K temperature. Therefore, the v_{th} in the above formula can be substituted for the saturated drift velocity v_d of an electron in the semiconductor. In relation to the above, a Monte Carlo simulation study for electron transport in n-type 3C-SiC by Zhang and Zhang [5], reveal that the saturated drift velocity of electrons at 300 K based on the band structure of 3C-SiC is about 4.8 x 10^7 cm/s. Plugging this value of v_d in the equation (1) above with the thermal energy at 300 K as 0.0388 eV, the m_{eff} is determined as 0.06m, where m is the free electron mass. Zhang and Zhang have also shown that the experimental value of the saturated electron drift velocity is about 2 x 10^7 cm/s [5]. This is about 0.45 times the v_d based on the band structure, of 4.8 x 10^7 cm/s. Square of the 0.45 v_d is 0.2 v_d^2. This means that if the square of the v_d is reduced by 0.2 times experimentally, then the m_{eff} should increase 5 times for the same thermal energy of 0.0388 eV at 300 K temperature. This makes m_{eff} as 0.06m times 5 which equals 0.30m. This is the experimentally observed m_{eff} of electron in 3C-SiC in the [100] direction. It is almost the same as 0.34m as the longitudinal effective mass of one conduction valley in 3C-SiC in the [100] direction observed experimentally by the cyclotron resonance technique [5-6]. Summarizing the above, the longitudinal electron effective mass m_{eff} of 3C-SiC in the [100] direction based on the band structure is about 0.06m, and that based experimentally is 5 times more at 0.30m. The electron essentially slows down due to the high density of intrinsic defects in 3C-SiC in the [100] direction at about 1.8 x 10^{33}/cm^3 [7-8]. The properties of a MOS device and the method for their determination theoretically without fabricating the device has been described in the author's earlier two research studies and is implemented in the present study for the 3C-SiC-MOS device on the (100) oriented surface [1-2].

There is a second interesting way of finding the intrinsic Fermi level $E_i$in cubic 3C-SiC. The E_i in elemental Si is 0.01 eV from the mid-bandgap, and E_i in the elemental Carbon as Diamond is 0.4 eV from the mid-bandgap [7-8]. The total shift in E_i for one part Si and one part C material as cubic SiC becomes 0.41 eV. Dividing this by the total electron potential energy in Si and C as Diamond as 1.12 eV + 5.5 eV = 6.62 eV, gives the shift in E_i per electron volt of potential energy of electron in SiC. This is 0.062. The dE/E equals dm/m relation gives dm as the electron effective mass in 3C-SiC(100) as 0.062m. For the 3C-SiC bandgap of 2.38 eV, the E_i as dE becomes 2.38 eV x 0.062 = 0.148 eV, using the same relation dE/E equals dm/m. This is the position of the E_i below the 3C-SiC(100) conduction band. Diamond form of Carbon is considered here instead of graphite or other forms because the Carbon atom in Diamond has sp^3 hybridization similar to that of Si atom and thus will form tetrahedral Si-C bonds in cubic 3C-SiC.

One can similarly find the electron effective mass of cubic Germanium Carbide as 0.043m based on the band structure starting with Ge and Diamond having cubic lattice structure. The intrinsic Fermi energy E_i in elemental Ge is -0.135 eV from the mid-bandgap, and E_i in the elemental Carbon as Diamond is 0.40 eV from the mid-bandgap [7-8]. The total shift in intrinsic E_i for one part Ge and one part C material as cubic GeC becomes (-0.135+0.40 = 0.265) eV. Dividing this by the total electron potential energy in Ge and C as Diamond as 0.67 eV + 5.5 eV = 6.17 eV, gives the shift in E_i per electron volt of potential energy of electron in cubic GeC. This is 0.043. The dE/E equals dm/m relation gives dm as the electron effective mass in cubic GeC as 0.043m. At present there is no study on cubic Germanium Carbide. The above is purely an educated speculation based on cubic 3C-SiC study above. Devices will be possible on cubic GeC that can operate at 300 K, but the high temperature stability and formation of stacking fault defects is unknown as the material does not exist as yet though Ge is known not to work beyond 90^{o}C temperature and the compound GeO_2 is water-soluble and degrades at high temperatures [9]. Cubic GeC is expected to be similar to cubic 3C-SiC. The polytypes of GeC could also be similar to polytypes of SiC with a large heavy-hole mass that would not allow efficient p-type devices to form, similar to SiC.

III. Results and Discussion

Given the longitudinal electron effective mass in 3C-SiC for one conduction valley in the [100] direction as about 0.06m and the semiconductor bandgap of 2.38 eV, the properties of the MOS device are determined theoretically as follows. 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 3C-SiC(100) surface. The intrinsic Fermi level E_i, is located at 0.06 x 2.38 eV = 0.14 eV below the CB of 3C-SiC, given that the relative energy equals relative mass of a moving electron from the expression dE/E equals dm/m [1-3]. This value is 0.15 eV from the earlier MIS characterization study [7-8]. The CBO of the oxide/semiconductor interface is 3.75-0.14 eV = 3.61 eV and the Fowler-Nordheim (FN) onset field in the oxide is 2 x 3.61=7.22 MV/cm. 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, as presented above to be 7.22 MV/cm [10-11]. Here, 3.75 eV is the position of the $E_i$in $SiO_2$from its CB and identifies the position of E_i in 3C-SiC for the oxide/semiconductor interface. The 3.75 eV equals 0.42 x 8.93 eV, where 0.42 is the relative electron effective mass in the oxide and 8.93 eV is the oxide bandgap [7-8]. The theoretical value of the slope constant B for the FN tunnelling electron current can now be decided using the formula:

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

Here, electron effective mass m_{ox} for SiO_2 is 0.42m and the oxide/semiconductor interface barrier height $\emptyset_0$is found above theoretically as 3.61 eV. These values give the theoretical slope constant B as 303.6 MV/cm or 304 MV/cm. The FN electron current density for this B and an FN onset field of 7.22 MV/cm found above will be about 2.7 x 10^{-11} A/cm^2 theoretically. The oxide will exhibit a breakdown field of about 11 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 FN current-voltage (I-V) characteristics at high fields are (2 x 10^{-11} A/cm^2, 7.22 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 304 MV/cm, and from the second point, the E_{bkdn} can be calculated to be 11 MV/cm [12-14]. The experimentally obtained slope constant B was also 308 MV/cm [15].It can be observed from the reference [15] that the current near the FN onset field of 7.22 MV/cm is about 3 x 10^{-11} A/cm^2. At lower fields the current is about 10^{-9} A/cm^2. This is unusual for the FN tunnelling current and is caused due to the presence of border traps in the oxide near the SiC CB. There is a high density of intrinsic defects in the semiconductor, some of which will be at the surface forming part of the oxide grown on it and developing border traps in the oxide near the oxide/semiconductor interface [16-17]. The border traps can be identified by comparing the low-field current density to the oxide displacement current density. Here, the low-field current density at 10^{-9} A/cm^2 is lower than the oxide displacement current density of 5.3 x 10^{-9} A/cm^2, giving a border trap density D_{bt} of about 3 x 10^{12}/cm^2-eV. The calculation is described in the references [16-17]. Also, there is electron trapping in the border traps during the current-voltage measurements causing some reduction in the current at high fields beyond the FN onset field leading to a higher than 10 MV/cm oxide breakdown field. Destructive breakdowns may also occur below 11 MV/cm oxide field. E_i, located at 0.14 or 0.15 eV from the 3C-SiC(100) CB and away from the mid-bandgap of 1.19 eV translates to a significant intrinsic defect density, N_{id} of about 1.8 x 10^{33}/cm^{3}that slows down the electron when performing cyclotron resonance experiment [7-8]. The defects are in the form of stacking faults [18]. The FN onset field of 7.22 MV/cm is demonstrated experimentally, and acts as corroboration of the theoretical determination above [15]. The electron affinity for 3C-SiC semiconductor oriented in [100] direction is 4.51 eV. It is found by adding the electron affinity of SiO_2 of 0.9 eV to the CBO of 3.61 eV of the oxide/semiconductor interface [2, 19].

IV. Conclusions

The properties of the MOS device on 3C-SiC (100) surface are theoretically determined and experimentally supported, once the longitudinal electron effective mass in the [100] direction based on the band structure is decided to be about 0.06m for one conduction valley. The finds of the properties reinforce the physical concept introduced at the beginning of this article. The CBO at the oxide/semiconductor interface is 3.61 eV, the FN onset field is 7.22 MV/cm giving a low leakage current through the oxide in the MOS device, and the oxide has a high breakdown strength of about 11MV/cm. However, the 3C-SiC semiconductor exhibits a high intrinsic defects density of about 1.8 x 10^{33}/cm^{3}in the form of stacking faults, and a border trap density of about 3 x 10^{12}/cm^2-eV near the SiC CB in the oxide, that will degrade the obtained surface mobility in the MOS transistor. The electron affinity in 3C-SiC is 4.51 eV. GeC could be a new semiconductor material like SiC with the longitudinal electron effective mass in cubic GeC (100) as 0.043m.

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