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Theoretical finding of the properties of a Si MOS device

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Abstract: *This article gives a method to find the properties of a Si (100) MOS device, given the transverse and longitudinal electron effective masses in the semiconductor and its bandgap, without fabricating the MOS device. The study also highlights 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 below the conduction band of the semiconductor through the relation dE/E equals dm/m, where dE is the differential kinetic or potential energy of the electron, E is the semiconductor bandgap as the total potential energy of the electrons, dm is the effective mass of the electron in the material, and m is the free electron mass.*

Keywords: *Metal-Oxide-Semiconductor, Silicon, Intrinsic defects, Fowler-Nordheim tunnelling*

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I. Introduction

This article is a repeat of the previous article with some improvements. The improvements are the inclusion of the theoretical and observed low-field leakage current at the Fowler-Nordheim onset field in n-Si (100) and n-4H-SiC (0001)-Si-faced MOS devices in accumulation. The improvements are included in the section III of this article in the form of a Table. The conclusions of the research remains the same as before.

The MIS characterization can lead to the determination of the intrinsic Fermi level E_i, in the semiconductor bandgap. The differential energy dE from E_i to the semiconductor conduction band (CB) determines the longitudinal effective mass in the semiconductor by using the relation dE/E equals dm/m. Here, E is the semiconductor bandgap, dm is the effective mass of the electron in the semiconductor and m is the free electron mass [1-3]. If the MOS device is fabricated on the transverse surface, then the MIS characterization will lead to the transverse effective mass in the semiconductor. This becomes a new method of determining the electron effective masses in a parabolic semiconductor. Alternatively, if the transverse and longitudinal effective masses in a parabolic semiconductor are determined correctly, by for example, the cyclotron resonance method [4], then the E_i in the semiconductor bandgap can be easily determined using the relation dE/E equals dm/m. The intrinsic defects density in the semiconductor N_{id}, can then be found using the equation of charge neutrality in the semiconductor [1-2]. Einstein first discovered the mass-energy equivalence relation $E=mc^2$ for a relativistic energy E and moving mass m. After differentiating this relation once on both sides, the relation dE/E equals dm/m as a first order differential equation is obtained. The kinetic energy of an electron or hole moving in a silicon crystal has also been shown to possess the same property under a changing thermal energy [3]. Thus, this equation becomes a universal mass-energy equivalence relation for all moving particles in materials and moving particles and objects in space. A recent article by the author discusses the relation in moving big or small relativistic masses and other energy transformations [5]. In parabolic semiconductors, dE is the differential potential energy of an electron from the semiconductor's intrinsic Fermi energy level E_i to the semiconductor conduction band (CB), E is the semiconductor bandgap as the total negative potential energy of electrons with reference to the valence band (VB) at zero energy, dm is the differential mass as the longitudinal electron effective mass, and m is the free electron mass. E-dE would be the differential potential energy for holes. In this article, the properties of a Si (100) MOS device such as, conduction band offset (CBO), the Fowler-Nordheim (FN) onset electric field, and the oxide electrical breakdown field, along with the intrinsic defect density N_{id} in Si (100) are all determined starting with the known transverse and longitudinal electron effective masses in Si (100) semiconductor as 0.19m and 0.98m and its experimental bandgap of 1.12 eV, without even fabricating the MOS device. Since there are two conduction valleys in Si (100) semiconductor in the [100] direction, therefore the longitudinal mass for one valley is 0.49m. The heavy-hole mass becomes 0.51m as the electron and hole effective masses add up to be free electron mass.

II. Theory

Four main properties of a MOS device are: the conduction and valence band offsets at the oxide/semiconductor interface, the FN onset field in the amorphous oxide (thermal SiO_2 in the present case) that is a measure of the leakage current in the oxide, oxide electrical breakdown strength, and the intrinsic defects density in the semiconductor that indirectly determines the surface field-effect (FE) mobility in the MOSFET. The band offsets can be determined from the known position of E_i from the conduction band (CB) of Silicon by comparing it to the E_i in the SiO_2. E_i can also aid in determining the intrinsic defects density in the semiconductor [1-2]. 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 [6-7]. The FN onset field can therefore be found once the CBO is known. Two points on the high field region of the Fowler-Nordheim electron tunneling current versus voltage characteristics can be used to find the tunneling slope constant B for the current and the dielectric breakdown field strength in MV/cm. One point can be the (10^{-9} or 10^{-10} A/cm^2, FN onset field in MV/cm) and the second point can be the (10^{-4} A/cm^2, E_{bkdn} in MV/cm). The 10^{-4} A/cm^2 current density is assigned as the breakdown current density in thick oxide of say 40 to 100 nm. This is described in the author's earlier studies [8-11]. Thus, all four main properties of a MOS device can be found without fabricating the MOS device.

III. Results and Discussion

Given the transverse and longitudinal electron effective masses in Si (100) semiconductor as 0.19m and 0.49m (for one conduction valley), where m is the free electron mass, substantial knowledge about a MOS device fabricated on the (100) surface can be gained. The electric field in the thermal SiO_2 having negligible bulk defects is oriented in the [100] direction. The intrinsic Fermi level E_i, is located at 0.49 x 1.12 eV = 0.55 eV from the CB of Silicon, given that the relative energy equals relative mass of a moving electron from the expression dE/E equals dm/m [1-3]. The conduction band offset (CBO) of the oxide/semiconductor interface is 3.75-0.55 eV = 3.20 eV and the FN onset field in the oxide is 2 x 3.2 = 6.4 MV/cm. This is because the minimum field for electron heating in the oxide is 2 MV/cm, which is FN onset field divided by the CBO with 1 eV as the minimum energy needed to see vacuum emission of hot electrons. The FN onset field in the MOS device is thus 2 MV/cm-eV x CBO, as presented above to be 6.4 MV/cm [6-7]. Here, 3.75 eV (= 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) is the position of the E_i in SiO_2 from its CB and identifies the position of E_i in Si (100) of the oxide/semiconductor interface [1-2]. The theoretical value of the slope constant B for the FN tunnelling electron current can now be decided using the formula [8-11]:

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

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 3.20 eV. These values give the theoretical slope constant B as 253.37 MV/cm. A value of 254 MV/cm is reported in reference [8] from experiments. The FN electron current density for this B and an FN onset field of 6.4 MV/cm found above will be 2.71 x 10^{-10} A/cm^2 theoretically [8-11]. The oxide will exhibit a breakdown field of about 9.5 MV/cm for a 10^{-4} A/cm^2 current density for thick oxide of say 100nm, given that two points on the Fowler-Nordheim (FN) current-voltage (I-V) characteristics at high fields are (2.71 x 10^{-10} A/cm^2, 6.4 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 254 MV/cm, and from the second point, the E_{bkdn} can be calculated to be 9.5 MV/cm. The observed current is 1.5 x 10^{-10} A/cm^2 at the FN-onset field for the Si-MOS device [12]. The lower observed current density is due to the presence of 4 x 10^{11}/cm^{2}eV density of border traps [13]. Similar is the case with n-4H-SiC MOS device where the observed current density is lower than the theoretically calculated value [14-15]. The theoretical and observed current densities for both the Si and SiC devices are presented in Table I below.

Table I. Theoretical and observed current density at FN onset field and border trap density in MOS devices

Device	FN onset field (MV/cm)	Slope Constant B (MV/cm)	Theoretical Current density (A/cm^2)	Observed Current density (A/cm^2)	Border Traps density (cm^{-2}eV^{-1})
n-Si-(100)	6.4	254	2.71 x 10^{-10}	1.5 x 10^{-10}	4 x 10^{11}
n-4H-SiC (0001)-Si-face	5.6	206	4.34 x 10^{-9}	1.0 x 10^{-9}	24 x 10^{11}

E_i, located at 0.55 eV from the Si (100) CB and close to the mid-bandgap of 0.56 eV translates to a small intrinsic defect density, N_{id} of about 2.1 x 10^{10}/cm^3 [1-2]. The surface field-effect (FE) electron mobility for the MOSFET can be known only from the I-V/C-V based characterization of a pair of n-MOS and p-MOS device, by finding the border trap density (D_{bt}) and the interface trap density (D_{it}), followed by a comparison to a Si-MOSFET with known surface mobility and total interface defect density. This is possible because the surface mobility is inversely proportional to the total interface traps density in the device [16]. The oxide electric field should thus be directed in the higher effective mass direction of the semiconductor giving lower N_{id}. This direction also gives lower FN onset field in the MOS device, but the minimum oxide field required with the MOSFET in the ON state is only 2 MV/cm as the electron heating threshold in the oxide. The lower effective mass transverse direction having a transverse mass of 0.19m can thus give larger mobility, as the oxide electric field and electron flow are directed perpendicular to each other.

IV. Conclusions

The above theoretical analysis corroborated with experimental evidence bring informed readers to the conclusion that, the properties of a Si (100) MOS device can be found without fabricating the device, simply with the knowledge of the transverse and longitudinal electron effective masses and its bandgap. The electron effective masses in the semiconductors and insulators are thus not only related to the mobility through drift velocity, but they are also related to the intrinsic Fermi energy level from the conduction band through the relation dE/E equals dm/m. This relation is universal to the moving particles and objects in materials and space alike, as the mass-energy equivalence relation first found by Albert Einstein as $E=mc^2$.

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