

On the ionization in silicon dioxide of a MOS device and its relation to the density of the oxide

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Abstract: Ionization in the amorphous thermal silicon dioxide in a metal-oxide-semiconductor device begins at the onset field for Fowler-Nordheim carrier tunnelling current. The calculated mean free path of electrons in the oxide is higher by 0.22 nm for the denser oxide on 4H-SiC than on Si. It is generally observed that a lower conduction band offset of a native oxide/semiconductor interface is indicative of a denser native oxide of a denser semiconductor material, particularly after removing the intrinsic defects in the semiconductor materials. Si is found to be the least dense semiconductor material giving the least dense native oxide on it with the highest conduction band offset at the SiO₂/Si interface of 3.2 eV.

Keywords: Density, Metal-Oxide-Semiconductor, Ionization, Mean Free Path

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I. Introduction

When a metal-oxide-semiconductor (MOS) device is biased in accumulation or inversion with a voltage applied across the device, then electrons having potential energy tunnel from the triangular barrier into the conduction band of the oxide and get accelerated as the field is increased. At high electric fields, ionization begins in the oxide and carriers increase exponentially causing the current through the device to increase exponentially also. This current is called the Fowler-Nordheim (FN) carrier tunnelling current. This research paper relates the concept of ionization in the semiconductors to the onset field for FN carrier tunnelling current in a MOS device and shows that the ionization in the oxide begins at this field. This relation enables the determination of the mean free path of electrons in the thermal silicon dioxide before collision. The mean free path of electrons in the oxide reflects on the density of the native oxide grown on the semiconductor surfaces. It is found that a lower conduction band offset (CBO) of the native oxide/semiconductor interface is indicative of a higher density oxide.

II. Theory

Ionization takes place in a semiconductor or insulator materials, when free electrons in the material accelerate due to the applied electric field, collide with the lattice atoms and break the covalent bonds, freeing carriers and then scatter. Every accelerated free carrier creates two additional carriers. Next, the three carriers free additional carriers causing the avalanching process [1]. If the density of excited electrons arriving at a particular point in the material is n^* that have sufficient energy to create electron-hole pairs, then n^* is given as:

$$n^* = n \exp\left(-\frac{d}{\lambda}\right) \quad (1).$$

Here, n is the total electron density and $\exp(-d/\lambda)$ is the probability that an electron has not collided in the distance d necessary to gain sufficient energy, and λ is the mean free path. The distance d is given as:

$$d = \frac{E_1}{qE} \quad (2).$$

Here, E_1 is the minimum energy necessary for an ionizing collision, and E is the average field that accelerates the electron [1]. The exponential term of ionization coefficient is equal to the exponential term in the FN carrier tunnelling equation as is shown next. It is observed that the FN onset field when the current starts to increase exponentially to the CB barrier height is a constant of value 2 MV/cm in Si and 4H-SiC MOS devices as shown in the Table I below. The data of FN onset field and conduction band offsets (CBO) in Si and 4H-SiC devices is obtained from the author's earlier study [2]. It is to be noted that the unit of barrier height is already included in

the FN slope constant B given in MV/cm, and so the constant is a field of 2 MV/cm which is the minimum average field required for electron heating or acceleration in the amorphous silicon dioxide and the Table I thus acts to confirm it [3].

Table I. Field constant, FN onset field to conduction band offset (CBO) in MOS devices as the minimum average field for electron heating in SiO₂.

Device	FN onset field (MV/cm)	CBO	Field Constant (MV/cm)
Si-MOS	6.5	3.2	2.03
4H-SiC MOS	5.5	2.8	1.96

The minimum energy E₁ required for electron-hole pair generation is theoretically given as 2.8 E_g [4] and experimentally measured as 24.2 eV for SiO₂ which involves plasmons in creating electron-hole pairs [4]. The theoretical value is 25.00 eV given the bandgap of SiO₂ as 8.93 eV. The author has used this value for calculations in this article. Fowler-Nordheim carrier tunnelling current equation through a MOS device in accumulation or inversion having a triangular barrier is given by [5, 6]:

$$J = AE_{ox}^2 \exp(-B/E_{ox}) \quad (3).$$

Here, A and B are constants given as follows:

$$A = \frac{e^3 m}{16\pi^2 \hbar m_{ox} \phi_0} \quad (4)$$

$$A = 1.54 \times 10^{-6} \frac{m}{m_{ox}} \frac{1}{\phi_0} \dots A/V^2$$

$$B = \frac{4}{3} \frac{(2m_{ox})^{1/2}}{e\hbar} \phi_0^{3/2}$$

$$B = 6.83 \times 10^7 \left(\frac{m_{ox}}{m} \right)^{1/2} \phi_0^{3/2} \dots V/cm \quad (5).$$

$$B = 68.3 \times (m_{ox}/m)^{1/2} \phi_0 \phi_0^{1/2} \dots MV/cm$$

In the above constants A and B, e is the electronic charge in Coulombs, m is the free electron mass in Kg, m_{ox} is electron mass in the oxide in Kg, ħ is the reduced Planck's constant in Joule-sec, φ₀ is the electron barrier height in eV, and B is called the FN tunnelling slope constant in V/cm at a particular temperature in Kelvin. E_{ox} is the oxide field in V/cm. Equation (1) models the current-voltage characteristics across the oxide at high electric fields E_{ox}. The Fowler-Nordheim tunnelling current equation for an elementary triangular barrier and a 'general barrier' is revisited by Forbes and Deane after the original work of Fowler and Nordheim in 1928 [7-10]. The studies by Forbes greatly help to understand the derivation of the current-voltage characteristics due to field emission of electrons from the barriers [9]. He has made small improvements in the correction factor v(y) due to which the FN slope constant is dependent on the field in a general barrier. In v(y), y is Δφ₀/φ₀, where Δφ₀ is the change in barrier height due to the Schottky barrier lowering at a high field, and φ₀ is the unreduced potential barrier [10, 11]. It is nearly equal to 1 at 0.9370 at 6 MV/cm field across a MOS device [11]. The calculated Field constant in Table I above which is the same as the direct measurement of the minimum field for electron heating of 2 MV/cm [3] is an indication that the above error in barrier heights due to v(y) is not very significant at a particular set of two high fields where the FN slope constant B is determined experimentally by finding $B = \Delta \ln(J/E_{ox}^2) / \Delta(1/E_{ox})$. The B includes v(y) as part of the experimentally determined slope constant. Equating the exponential terms of the ionization coefficient and the FN carrier tunnelling current gives the equation:

$$-\frac{E_1}{qE\lambda} = -\frac{B}{E_{ox}} \quad (6).$$

Here, E_{ox} is taken as the FN onset field where ionization begins given as 5.5 MV/cm for the n-4H-SiC MOS device in Table I above, and FN slope constant B for the n-4H-SiC MOS device is 206 MV/cm [6]. An example calculation of the two sides of equation (6) shows that the equation (6) is valid. The left hand side is (-25 V)

/(2MV/cm x 3.3 nm) giving -37.88. The right hand side is (-206 MV/cm)/(5.5 MV/cm) giving -37.45. It can be observed that the left side is equal to the right side indicating that the ionization in the oxide begins at the FN onset field when the average energy of carriers required to create electron-hole pairs reaches 25 eV. Substituting B from equation (5) in equation (6) on the right hand side and substituting the values of E₁ and E on the left hand side and eliminating the minus sign from both sides gives:

$$\frac{25.00}{E\lambda_1} = \frac{68.3x(m_{ox}/m)^{1/2}\phi_0^{1/2}}{5.5/\phi_0} \quad (7).$$

Here, E in the denominator on the left side is equal to 5.5/φ₀ in the denominator on the right hand side. These are the same field constant of 2 MV/cm as the minimum average field required for electron heating in SiO₂ given in Table I above, where φ₀ is 2.79 (≈2.8) in n-4H-SiC MOS device. These cancel and equation (7) reduces to:

$$\frac{0.366}{\lambda_1} = \left(\frac{m_{ox}}{m}\right)^{1/2} \phi_0^{1/2} \quad (8).$$

In equation (8), λ = λ₁ x 10⁻⁶. λ is the mean free path of electrons before collision in the oxide given in nanometres, and λ₁ is in centimetres.

III. Results and Discussion

The mean free path in amorphous thermal SiO₂ has been determined in 1971-72 by internal photoemission as 3.4 and 3.5 nm, and then in 1985 as 3.0 nm by observing the ratio of the substrate to channel currents in p-channel FETs on Si [12-14]. This mean free path forms the direct carrier tunnelling regime in MOS devices [14]. The mean free path in the oxides on 4H-SiC and Si are calculated by using equation (8) in the present study and presented in the Table II below. It can be observed that this new method is also giving the same mean free path in thermal oxide as about 3.2 to 3.4 nm.

Table II. Calculation of the mean free path in SiO₂ for the 4H-SiC and Si MOS devices using equation (8)

MOS Device	m _{ox}	Φ ₀	m _{ox} ^{1/2} φ ₀ ^{1/2}	λ ₁ , (cm)	mean free path, λ=λ ₁ x10 ⁶ , (nm)
n-4H-SiC	0.42m	2.8	1.08	0.338	3.38
n-Si	0.42m	3.2	1.16	0.316	3.16

In Fig.7 of the study by Ashley and Anderson [15], mean free path of electron in the crystalline form of SiO₂ known as quartz having a density of 2.65 g/cm³, and in silicon having a density of 2.33 g/cm³ has been presented. They observed that the mean free path of electron depends on the density of the material. Fig.7 clearly shows that the mean free path of electron in the less dense Si is smaller than that in quartz having a higher density [15]. The MOS devices on Si and 4H-SiC are both composed of amorphous SiO₂ having a density of 2.27 g/cm³ which is less dense than quartz and therefore the mean free path of electron at the average carrier energy of 25 eV is expected to be less than that in quartz where it is about 4 nm from Fig.7 of the reference [15]. It can be observed from Table II above that the mean free path of electrons in the amorphous oxide on 4H-SiC is more by 0.22 nm as compared to the mean free path in the amorphous oxide on Si indicating that the amorphous oxide on 4H-SiC is of a little higher density than the amorphous oxide on Si and it has a lower conduction band offset of 2.79 eV. Thus, the lower conduction band offset (CBO) of a native oxide/semiconductor interface is indicative of a higher density native oxide. This is demonstrated further in Table III below, where the oxides of materials like Si, Al, Zr and Hf show lower and lower band offsets with Si as the density of the their oxides increase, given the fact that denser metals and semiconductors have denser native oxides grown on them [6, 16-18]. The CBO of Si/SiO₂ interface is 3.2 eV and the CBO of 4H-SiC/SiO₂ CBO is 2.79 eV. Both have amorphous SiO₂ on them but the oxide on 4H-SiC is little more dense than on Si according to the above analysis as the CBO on 4H-SiC/SiO₂ is lower. The above is also demonstrated in all the SiC polytypes after removing the effect of intrinsic defects in them as can be seen in column 8 of Table IV.

Table III. Conduction Band Offsets (CBO) of different oxides with Silicon and 4H-Silicon Carbide.

Material	Density (g/cm ³)	Native oxide	Density of oxide (g/cm ³)	CBO with Si or 4H-SiC (eV)	Comments
Si	2.33	SiO ₂	2.27	3.2	Denser material has denser oxide
Al	2.7	Al ₂ O ₃ (α or γ phase)	2.1 to 3.6	α-2.1 γ-2.5	
4H-SiC (Si-face)	3.21	SiO ₂ (denser)	2.27	2.79	CBO with Si is lower for a denser oxide.
Zr	6.49	ZrO ₂	4.66	1.83	
Hf	13.07	HfO ₂	7.97	1.54	

Intrinsic defects density in doped semiconductors has been determined by finding the intrinsic Fermi level in the semiconductors. The method is described in the author's earlier work [19]. Here, in Table IV below, the position of the intrinsic Fermi level in Si and SiC polytypes is reproduced from the earlier study in column 5, and the densities of the semiconductors are added in column 2. The CBO in these semiconductors with their native oxides do not follow the trend described earlier that, as the density of the material increases, the CBO with their oxides reduces. In particular, the CBO on the 3C-SiC/oxide interface of 3.6 eV is the odd one out where the density of 3C-SiC is less but the CBO is more at 3.6 eV. This CBO is with the intrinsic defects in the semiconductor material. In column 8 of the Table IV, the CBOs are determined after removing the intrinsic defects by placing the intrinsic Fermi level at the middle of the band gap. Now, the CBOs in column 8 follow the trend, that as the density of the semiconductors increase the CBOs with their native oxides decrease given the fact that denser materials have denser native oxides. Therefore, in general it is concluded that a denser semiconductor material will give a denser oxide and its CBO with the native oxide will be less, and so observing the CBO itself can indicate that the density of the oxide is less or more, comparatively. The 4H-SiC with the highest density among the polytypes will have a denser oxide and the CBO after removing the intrinsic defects is the least as indicated in column 8 of Table IV. The semiconductor Si is the least dense with the least dense oxide and its CBO with its native oxide is the largest at 3.2 eV.

Table IV. Relation between the density of Si and SiC polytypes and the conduction band offsets (CBO) of the native oxide/semiconductor interfaces with and without the intrinsic defects in the semiconductors.

1	2	3	4	5	6	7	8
Semiconductor	Density (g/cm ³)	Bandgap E _g (300K) (eV)	ΔE_c (CBO) with intrinsic defects (eV)	Intrinsic Fermi level E _i from CB E _c - E _i (eV)	Middle of bandgap E _c -E _v /2 (eV)	E _i -E _g /2 (eV)	ΔE_c (CBO) without intrinsic defects (eV) (4+7)
4H-SiC	3.21	3.23	2.79	0.97	1.63	-0.66	2.13
6H-SiC	3.21	3.02	2.95	0.80	1.51	-0.71	2.24
15R-SiC	-	2.96	3.0	0.75	1.48	-0.73	2.27
3C-SiC	3.16	2.38	3.6	0.15	1.19	-1.04	2.56
Si	2.33	1.12	3.2	0.55	0.56	-0.01	3.19

IV. Conclusions

Ionization in the amorphous thermal silicon oxide of a MOS device begins at the onset field for FN carrier tunneling current. The mean free path in the native oxide on 4H-SiC is larger by 0.22 nm than that on the native oxide on silicon indicating a denser oxide on 4H-SiC. The more dense oxide on denser semiconductor materials relates to the lower CBO of the oxide/semiconductor interface, particularly when the intrinsic defects in the semiconductors are removed. A field constant of 2MV/cm exists for the silicon dioxide in a MOS device on Si and 4H-SiC which is the minimum average field for electron heating in the oxide.

References

- [1]. R.S. Muller, T.I. Kamins, with M. Chan, "pn junctions" in Device Electronics for Integrated Circuits, 3rd edition, John Wiley and Sons, Singapore, 2003:174-225.
- [2]. R.K. Chanana, "Interrelated current-voltage/capacitance-voltage traces based characterization study on 4H-SiC metal-oxide-semiconductor devices in accumulation and Si device in inversion along with derivation of the average oxide fields for carrier tunneling from the cathode and the anode", IOSR-J. Electrical and Electronics Engg., 2019;14(3):49-63.
- [3]. D.J. DiMaria, M.V. Fischetti, E. Tierney, "Direct observation of the threshold for electron heating in silicon dioxide", Physical Review Letters, 1986;56(12):1284-1286.
- [4]. R.C. Alig, S. Bloom, C.W. Struck, "Scattering by ionization and phonon emission in semiconductors", Physical Review B, 1980;22(12):5565-5582.
- [5]. Z.A. Weinberg, "On tunneling in metal-oxide-silicon structures", J. Appl. Phys., 1982;53(7):5052-5056.
- [6]. R.K. Chanana, K. McDonald, M. Di Ventra, S.T. Pantelides, L.C. Feldman, G.Y. Chung, C.C. Tin, J.R. Williams, R.A. Weller, "Fowler-Nordheim hole tunneling in p-SiC/SiO₂ structures", Appl. Phys. Letts., 2000;77(16):2560-2562.
- [7]. R.G. Forbes, J.H.B. Deane, "Reformulation of the standard theory of Fowler-Nordheim tunneling and cold field electron emission", Proc. R. Soc. A, 2007;463:2907-2927.
- [8]. R.G. Forbes, J.H.B. Deane, "Transmission coefficients for the exact triangular barrier: an exact general analytical theory that can replace Fowler & Nordheim's 1928 theory", Proc. R. Soc. A, 2011;467:2927-2947.
- [9]. R.G. Forbes, "Use of energy-space diagrams in free-electron models of field electron emission", Surface and Interface Analysis, 2004;36:395-401.
- [10]. R.G. Forbes, "Simple good approximations for the special elliptic functions in standard Fowler-Nordheim tunneling theory for a Schottky-Nordheim barrier", Appl. Phys. Letts., 2006;89:113122.
- [11]. Z.A. Weinberg, W.C. Johnson, M.A. Lampert, "High-field transport in SiO₂ on silicon induced by corona charging of the unmetallized surface", J. Appl. Phys., 1976; 47(1):248-255. Appendix A.
- [12]. C.N. Berglund and R.J. Powell, "Photoinjection into SiO₂: Electron scattering in the image force potential well", J. Appl. Phys., 1971;42(2):573-579.
- [13]. R. Poirier and J. Olivier, "Energy losses of hot electrons in a thin layer of SiO₂ on Si", Appl. Phys. Letts, 1972;21(7):334-335.

- [14]. D.J. DiMaria, T.N. Theis, J.R. Kirtley, F.L. Pesavento, D.W. Dong, S.D. Brorson, "Electron heating in silicon dioxide and off-stoichiometric silicon dioxide films", *J. Appl. Phys.*, 1985;57(4):1214-1238.
- [15]. J.C. Ashley, V.E. Anderson, "Interaction of low-energy electrons with silicon dioxide", *J. Electron spectroscopy and related phenomenon*, 1981;24:127-148.
- [16]. R.K. Chanana, "Determination of electron and hole electron masses in thermal oxide utilizing an n-channel silicon MOSFET", *IOSR-J Appl. Phys.*, 2014;6(3):1-7.
- [17]. V.V. Afanasev, M. Houssa, A. Stesmans, C. Merckling, T. Schram, J.A. Kittl, "Influence of Al₂O₃ crystallization on band offsets at interfaces with Si and TiN_x", *Appl. Phys. Letts.*, 2011;99:072103.
- [18]. H.C. Shin, Lee Seul Son, K.R. Kim, S.K. Oh, H.J. Kang, Dahlang Tahir, Sung Heo, Jae Gwan Chung, J.C. Lee, Sven Tougaard, "Band alignment and optical properties of (ZrO₂)_{0.66}(HfO₂)_{0.34} gate dielectrics thin films on p-Si(100)", *J. Surface Analysis*, 2011;17(3):203-207.
- [19]. 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.*, 2017;9(6):1-7.

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