Universal Mass-Energy Equivalence Relation in Materials

Ravi Kumar Chanana ✉ iD

Retired Professor, Self-Employed Independent Researcher, Gr. Noida-201310, India

Abstract:

A new discovery of the universal mass-energy equivalence relation applicable to materials having a bandgap, was initiated in the year 2014 and concretized in 2022-23. It is described in this short research paper. The relation is dE/E = dm/m, where E is the energy and m is the mass.

Keywords: *Mass-Energy Equivalence, Semiconductors, Insulators, MOS device, Fowler-Nordheim tunneling.*

Introduction

The relation dE/E = dm/m, has E as the energy and m as the mass. When applied to materials having bandgaps such as Silicon, Silicon Carbide, Silicon Dioxide and Hafnium Oxide, dE is the differential potential or kinetic energy of electrons or holes in the materials from the intrinsic Fermi energy level E_i to the conduction band (CB) or valence band (VB) of the materials, and dm is the differential mass in materials as the longitudinal electron or hole effective masses, E is the material bandgap as the total potential or kinetic energies of the electrons and holes and m is the free electron mass (Chanana, 2017; 2021; 2022a; 2022 b).

Materials and Methods

Consider a Metal-Oxide-Semiconductor (MOS) device on Silicon (100) surface with a dry thermal oxide as the oxide insulator. It has band offsets at the Si/oxide interface with the oxide bandgap larger than the silicon bandgap. In the year 2014, while characterizing 5-10 nm SiO_2 films by the Fowler-Nordheim (FN) carrier tunneling currents through the MOS device in accumulation or inversion by utilizing n-channel silicon MOSFET, the band offset and effective mass determination technique was introduced as BOEMDET. In this technique, the electron and hole effective masses in the oxide at high electric fields when the FN carrier tunneling occurs, were modified by the universal mass-energy equivalence relation of dE/E = dm/m. dE/E was taken as the differential kinetic energy of electrons in the oxide having a saturation velocity v at high fields in the oxide as:

$$\frac{dE}{E} = \frac{0.5\, m_{ox,e} v^2}{\left(0.5(m_{ox,e} + m_{ox,h})v^2\right)} \qquad (1)$$

Here $m_{ox,e}$ and $m_{ox,h}$ are the electron and hole effective masses in the oxide. This dE/E can also be written as the differential potential energy of electrons from E_i in Si to the oxide CB divided by the oxide bandgap E_g as the total potential energy of electrons with the VB at zero energy. E_i in the oxide is also the charge neutrality level (CNL) and is aligned with the E_i in Si semiconductor because of charge neutrality. The intrinsic E_i in Si is related to the longitudinal electron effective mass in [100] direction. There are two conduction valleys in the [100] direction in Si (100) and the longitudinal electron effective mass is 0.98m at 300 K temperature. The effective mass for one conduction valley is

0.49m. This gives dm/m as 0.49. dE can now be calculated by multiplying the bandgap of Si of 1.12 eV to the dm/m. This gives dE as 0.55 eV. This is the position of E_i in the Si (100) below its CB. The position of E_i from the VB will be 0.57 eV. The 0.55 eV for Si is added to the CB offset of the Si-SiO$_2$ interface of 3.20 eV to give the total dE for the oxide as 3.75 eV, because the E_i in Si is aligned to the E_i in the SiO$_2$ due to charge neutrality. The universal mass-energy equivalence relation of dE/E = dm/m can thus be also written in terms of potential energy of electrons as:

$$\frac{dE}{E} = \frac{(\phi_e + 0.55)}{E_g} \tag{2}$$

Here ϕ_e is the CB offset for electrons at the Si-SiO$_2$ interface from the Si CB to Oxide CB and E_g is the oxide bandgap. A similar equation for holes is also present (Chanana, 2014a; 2014b). The change in potential energy of electrons as in equation (2) is equal to the change in kinetic energy of electrons in the oxide as in equation (1). An analogy for this can be given that when a ball of mass m_b is dropped from a height h, it has the change in potential energy as $m_b gh$, and when it reaches the ground, it has a change in kinetic energy as 0.5 $m_b v_f^2$. Here v_f is the final velocity of the ball when it reaches the ground. Similarly, the electron overcomes the potential energy when photo-excited from E_i energy position in the bandgap and moves into the CB of the oxide where it travels at the saturation velocity v at high fields with an effective mass $m_{ox,e}$. The universal relation is concretized in 2022-23 with the MIS characterization utilizing MOS devices fabricated on 4H-SiC semiconductor oriented in the (0001) direction and Si-terminated (Chanana, 2023a; 2023b). Now, a generalized BOEMDET technique for MIS characterization utilizing FN carrier tunneling currents is available for future research on materials and devices (Chanana, 2023a).

Results

MIS characterization by the BOEMDET technique of the Si-SiO$_2$ interface of the MOS device in 2014 (Chanana, 2014a; 2014b), and of the 4H-SiC/SiO$_2$ interface in 2023 (Chanana, 2023a; 2023b) has given the following results. The CB and VB offsets at the Si-SiO$_2$ interface are 3.205 eV and 4.605 eV respectively. The electron and hole effective masses in the oxide are 0.42m and 0.58m, and the SiO$_2$ bandgap is 8.93 eV. For the 4H-SiC-SiO$_2$ interface, the CB and VB offsets are 2.785 eV and 2.915 eV respectively. The oxide effective masses are the same as in the Si device at 0.42m and 0.58m, and the oxide bandgap is also the same at 8.93 eV.

Discussion

Two important points are to be made. One, that because of the universal mass-energy equivalence relation, only one of the masses need to be determined as the other mass is complementary. The electron and the hole effective masses add up to be equal to the free electron mass and the hole effective mass is always larger than the electron effective mass. Second, it is through the universal relation that the E_i in the semiconductor is related to the longitudinal electron effective mass in the semiconductor. Thus the E_i is determined in Si and in 4H-SiC through this equation. This E_i has to be added to the CB offset or the VB offset at the oxide/semiconductor interface to be able to get equation (2), which then gives the electron and hole effective masses in the oxide after completing the MIS characterization (Chanana, 2023a). Up until now, the intrinsic Fermi energy levels in the semiconductors were not related to their electron and hole effective masses. Only the CB and VB offsets were known (Robertson, 2002). Another important point to consider is that the BOEMDET technique uses only electrons having a maximum of 5eV energy for characterization through FN carrier tunneling currents whereas, the internal photoemission (IPE) technique of band offset determination utilizes higher energy photons. IPE can give the band offsets but the electron and hole effective masses can be determined easily with the help of the universal mass-energy equivalence relation of dE/E = dm/m after finding the band offsets,

without having to perform current-voltage characterization after IPE. For example, a MOS device on Si having a magnetron grown HfO$_2$ gives the VB offset of -2.5 eV and the oxide bandgap of 5.82 eV after IPE in a research study (Tan et al., 2009). Since the position of E$_i$ in Si is 0.55 eV from the CB and 0.57 eV from the VB as shown by the universal mass-energy relation above, the 0.57 eV can be added to 2.5 eV to give 3.07 eV as the total VB offset in the oxide from the E$_i$ in Si. This can now give the hole effective mass in the HfO$_2$ as $3.07/5.82 = 0.527m$ from the relation $dE/E = dm/m$. Since the electron mass is complementary, therefore it equals $0.473m$. Here, m is the free electron mass. One last important advantage of the FN tunneling based technique called BOEMDET is that the instrumentation is simpler than that of IPE.

Conclusion

The universal mass-energy equivalence relation of $dE/E = dm/m$ is a significant discovery. It relates the intrinsic Fermi energy level E$_i$ below the CB of the material to the longitudinal electron and hole effective masses in all materials having a bandgap. It also makes it possible to characterize oxides of both high and low bandgaps utilizing MOS devices on 4H-SiC and Si semiconductors, respectively. The electron and hole effective masses can be easily determined in the oxides now utilizing this relation along with the BOEMDET technique.

Conflict of Interests

The single contributing author states that there is no conflict of interest.

References

Chanana, R.K. (2014a). BOEMDET-Band Offsets and Effective Mass Determination Technique utilizing Fowler-Nordheim tunnelling slope constants in MIS devices on Silicon. *IOSR Journal of Applied Physics, 6*(4), 55-61. https://doi.org/10.9790/4861-06634855

Chanana, R.K. (2014b). Determination of electron and hole effective masses in thermal oxide utilizing an n-channel silicon MOSFET. *IOSR Journal of Applied Physics, 6*(3), 1-7.

Chanana, R.K. (2017). Intrinsic Fermi level and charged intrinsic defects density in doped semiconductors from the band offsets of MIS device interfaces. *IOSR Journal of Applied Physics, 9*(6), 1-7. https://doi.org/10.9790/2834-1204025760

Chanana, R.K. (2021). Linear model for the variation of semiconductor bandgap with high temperature for high temperature electronics. *IOSR journal of electrical and electronics engineering, 16*(6), 5-8. https://doi.org/10.9790/1676-1606010508

Chanana, R.K. (2022a). N-channel 4H-SiC MOSFET device on (11$\bar{2}$0) oriented epitaxial surface. *IOSR-J. Electrical and Electronics Engineering, 17*(3), 20-22. https://doi.org/10.9790/1676-1703012022

Chanana, R.K. (2022b). Theoretical finding of the properties of a Si (100) MOS device, *IOSR-J. Applied Physics, 14*(3), 5-6. https://doi.org/10.9790/4861-1403010506

Chanana, R.K. (2023a). Metal-Insulator-Semiconductor characterization by Fowler-Nordheim carrier tunneling currents through MOS devices. *Transactions on Engineering and Computing Sciences, U.K., 11*(5), 45-50. https://doi.org/10.14738/tecs.115.15489

Chanana, R.K. (2023b). The electron and hole effective masses in thermal silicon dioxide determined from the perspective of a semiconductor. *Transactions on Engineering and Computing Sciences, U.K., 11*(4), 172-174. https://doi.org/10.14738/tecs.114.15367

Robertson, J. (2002). Band offsets of high dielectric constant gate oxides on silicon. *Journal of Non-Crystalline Solids, 303,* 94-100. https://doi.org/10.1016/S0022-3093(02)00972-9

Tan, T., Liu, Z., Lu, H.,Liu, W.,Yan, F., Zhang, W. (2009). Band structure and valence-band offset of HfO$_2$ thin film on Si substrate from photoemission spectroscopy. *Applied Physics, A, 97,* 475-479. https://doi.org/10.1007/s00339-009-5245-8.