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The Electron and Hole Effective Masses in Thermal Silicon Dioxide Determined from the Perspective of a Semiconductor

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ABSTRACT

Three experimentally determined parameters of valence band to oxide conduction band offset, the bandgap of 4H-SiC, and the longitudinal electron effective mass in 4H-SiC, coupled with the universal mass-energy equivalence relation, facilitate the determination of the electron and hole effective masses in thermal silicon dioxide of a metal-oxide-semiconductor (MOS) device without prior knowledge of any of the oxide masses.

Keywords: Bandgaps, 4H-SiC, MOS device, Composite materials.

INTRODUCTION

4H-SiC semiconductor is technologically important semiconductor for high voltage power electronics applications. Wolfspeed in the USA, and Infineon in Germany have already manufactured low voltage SiC power MOSFETs of 650V and 1.2KV where thermally grown reliable and native silicon dioxide is used as an insulator. SiC is also important for making blue light emitting diode (LED), for ultraviolet detection and H_2 gas sensor applications. This research paper finds the electron and hole effective masses in thermal silicon dioxide as 0.42m and 0.58m with m as the free electron mass from the perspective of a semiconductor, without prior knowledge of one of the effective masses in thermal silicon dioxide. The internal photoemission of electrons on 4H-SiC MOS device gives the valence band to oxide conduction band offset of 6.0 ± 0.1 eV, and the photoacoustic spectroscopy helps determine the bandgap of doped 4H-SiC semiconductor [1-3]. These parameters coupled the longitudinal electron effective mass in 4H-SiC and the universal mass-energy equivalence relation of $dE/E = dm/m$ facilitate the determination of the oxide effective masses.

THEORY

The theory consists of utilizing the universal mass-energy equivalence relation $dE/E = dm/m$. It has been discussed in the author's earlier studies [4-6]. It suffices to say that it is derived from differentiating the energy-mass equation for both big and small relativistic masses in the universe [5]. When applied to the semiconducting and insulating materials, dE is the differential potential energy of the electron from the intrinsic Fermi energy level E_i to the conduction band of the material, E is the bandgap of the semiconductor or insulator, dm is the differential mass as the longitudinal electron effective mass in the material, and m is the free electron mass.

RESULTS AND DISCUSSIONS

The semiconductor perspective starts with the experimental determination of the top of the SiC valence band to be located at 6.0 ± 0.1 eV from the thermal SiO_2 conduction band by Afanasev et al. in 1996 [1]. The bandgap of doped 4H-SiC has also been experimentally found to be 3.23 eV for a doping of 7 x $10^{18}/cm^3$ [2]. This bandgap becomes 3.234 for a lower doping of 9 x $10^{16}/cm^3$, given that the intrinsic bandgap of 4H-SiC from the density functional theory calculations is 3.26 eV. Doping causes bandgap narrowing that reduces the bandgap by 20 to 40 meV [3]. The above two determinations give the conduction band offset of the SiO_2/semiconductor interface of 2.766 eV. Now, the universal mass-energy equivalence relation dE/E = dm/m is applied on the (0001) oriented Si-terminated 4H-SiC. It has a longitudinal electron effective mass of 0.297m giving dm/m as 0.297. The bandgap is determined above as 3.234 eV. These two give the dE in 4H-SiC as 3.234 x 0.297 = 0.96 eV below the conduction band. This is the position of the intrinsic Fermi energy level E_i below the conduction band of 4H-SiC. This will align to the SiO_2 intrinsic Fermi energy level due to charge neutrality. Therefore, the dE for the SiO_2 at the oxide/4H-SiC interface will be the sum of the conduction band offset of 2.766 eV and the E_i in 4H-SiC of 0.96 eV. These total to 3.726 eV. The relative electron effective mass in the SiO_2 is now 3.726/8.93 as the dE/E = dm/m = 0.417 or 0.42, rounded to two decimal places. Furthermore, the universal mass-energy equation of dE/E = dm/m gives the hole effective mass to be 0.58m as the differential energy for holes dE in the SiO_2 is E-dE of electrons with the SiO_2 bandgap E as 8.93 eV [4-6]. The dE for the electrons in SiO_2 is 8.93 eV x 0.42 = 3.75 eV in place of 3.726 eV obtained above when using 0.42m for the electron mass. If the electron effective mass is 0.42m, then the hole effective mass has to be 0.58m, where m is the free electron mass. The hole effective mass in thermal SiO_2 has been determined experimentally also as 0.58m [7-9]. The masses are correct to two decimal places. The electron and hole effective masses in thermal SiO_2 can also be determined using Silicon as a semiconductor in a similar way [6]. The same values of 0.42m and 0.58m are obtained. It is worth noting that the universal mass-energy equivalence relation applicable to the semiconductors and insulators was discovered by the author after the experimental measurements of electron and hole effective masses through Metal-Insulator-Semiconductor (MIS) characterization [7-8]. The author in a collaborative study has determined experimentally a conduction band offset of 2.7876 eV at the SiO_2/4H-SiC with the 4H-SiC being Si-terminated and (0001) oriented, and with the electron effective mass in SiO_2 of 0.42m [7]. The experimentally determined conduction band offset of 2.7876 eV when added to the bandgap of 4H-SiC of 3.234 eV gives the position of valence band below the SiO_2 conduction band as 6.0216 eV. This value is nearly equal to 6.0 eV and well within the resolution limit of internal photoemission measurements reported by Afanasev et al. of ± 0.1 eV [1]. The results presented above makes 0.42m as the electron effective mass in the SiO_2 to be correct. The hole effective mass in SiO_2 has to be 0.58m as explained in the previous paragraph.

CONCLUSION

The electron and hole effective masses in the thermal silicon dioxide are determined from the perspective of 4H-SiC semiconductor without prior knowledge of any of the oxide masses. The obtained values of the electron and hole effective masses in thermal SiO_2 are 0.42m and 0.58m respectively, where m is the free electron mass. These values are correct to two decimal places. They can also be determined similarly utilizing Silicon as the semiconductor.

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