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# Properties of a MOS Device on Single Layer Molybdenum Disulfide

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**Abstract:** The properties of a metal-oxide-semiconductor device on a single layer $MoS_2$ (molybdenum disulfide) semiconductor are determined theoretically utilizing the concept of physics that the carrier effective masses in materials are related to the intrinsic Fermi energy levels in materials by the universal mass-energy equivalence equation given as $dE/E = dm/m$, where $E$ is the energy and $m$ is the mass of the free electron. The known parameters of electron effective mass of 0.48 m and the direct bandgap of 1.8 eV for monolayer $MoS_2$ semiconductor are utilized to determine the properties of the MOS (metal-oxide-semiconductor) device, with the given previous research consequence that the threshold for electron heating in $SiO_2$ is 2 MV/cm-eV.

**Key words:** Molybdenum disulfide, mass-energy equivalence, MOS device, Fowler-Nordheim tunnelling.

## 1. Introduction

A good review of the two-dimensional materials such as $MoS_2$ and their prospects in transistor electronics is published recently [1]. C. N. R. Rao has described the attributes of the 2D-nanosheets of $MoS_2$ and researchers in his group have attempted to fabricate a transistor on it [2, 3]. It has also found use in water-splitting reaction with hydrogen evolution [4]. Furthermore, it has been shown by the author in his earlier studies that the electron and hole effective masses in parabolic semiconductors and insulators are related to the intrinsic Fermi energy level in the bandgap of the materials by the universal mass-energy equivalence relation $dE/E$ equals $dm/m$, where $dE$ is the differential potential energy from the intrinsic Fermi energy level $E_i$ to the conduction band of the material, $dm$ is the differential mass as the longitudinal electron effective mass in the materials, $E$ is the bandgap of the semiconductor or insulator as the total potential energy of the electrons, and $m$ is the free electron mass [5-7]. The intrinsic Fermi energy level $E_i$ is the CNL (charge neutrality level) in the materials. This universal mass-energy equivalence equation is obtained by differentiating Einstein's equation $E=mc^2$ in its relativistic form once on both sides, with $E$ as the total relativistic energy and $m$ as the relativistic moving mass giving the equation $dE/E$ equals $dm/m$. The parameters applicable to semiconductors and insulators are defined above. It is valid for all energy transformations and moving big or small masses [8]. In this research paper the above concept is utilized to determine the properties of a MOS device on 1L-$MoS_2$ chalcogenide semiconductor theoretically. It is known that the MOS device is the heart of a MOSFET (metal-oxide-semiconductor field-effect transistor), the properties of which can determine the viability and reliability of a high or low voltage and high frequency power FET. 1L-$MoS_2$ having a bandgap of 1.8 eV at 300 K is found to be a viable semiconductor for a low voltage MOSFET.

## 2. Theory

The current-voltage characterization of a MOS device in accumulation or inversion gives the properties of low-field leakage current through the oxide insulator, the onset electric field for FN (Fowler-Nordheim)

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electron tunnelling current, and the electron tunnelling current at high electric fields across the oxide insulator that leads to the breakdown of the oxide. The oxide/semiconductor interface properties from the capacitance-voltage measurements give the oxide charge densities and the interface trap densities in the MOS device. These are the two groups of properties, interrelated and well-studied, and are discussed at length in a 900 pages book on MOS Physics and Technology [9, 10]. In this research paper, the properties based on current conduction are determined theoretically, that identifies a reliable $MoS_2$ MOS device for a low voltage and high frequency MOSFET. The oxide/semiconductor interface properties obtained by other research groups are utilized to determine the surface field effect mobility in the FET channel. The electron effective mass for 1L-$MoS_2$ has been determined theoretically and experimentally to be 0.483 m at the K-symmetry point of the Brillouin zone [11]. The electron mobility in bulk $MoS_2$ is estimated in the 200 to 500 $cm^2/V\text{-}s$ [12]. It is low as compared to silicon due to the presence of a high density of intrinsic point defects such as Molybdenum and Sulphur vacancies and antisites in the range of $5 \times 10^{12}/cm^2$ to $5 \times 10^{13}/cm^2$ [13]. The interlayer spacing in $MoS_2$ is 0.615 nm, giving the volume defect density of about $10^{20}/cm^3$ to $10^{21}/cm^3$.

## 3. Results and Discussion

The properties of the metal/$SiO_2$/1L-$MoS_2$ MOS device with electron as a current carrier can be determined theoretically with the given electron effective mass of 0.48 m and the direct bandgap of 1L-$MoS_2$ as 1.8 eV. The MOS device fabricated on the $MoS_2$ surface and in accumulation with metal gate as the anode has the electric field in the thermal $SiO_2$ having negligible bulk defects. This results into FN electron tunnelling current through the oxide at high electric fields. The intrinsic Fermi level $E_i$, is located at 0.48 × 1.8 eV = 0.864 eV below the CB (Conduction Band) of $MoS_2$, given that the relative energy equals relative mass of a moving electron or hole from the equation $dE/E$ equals $dm/m$. The CBO (conduction band offset) of the oxide/semiconductor interface is 3.75-0.864 = 2.886 eV and the FN onset field in the oxide is 2 × 2.886 = 5.77 MV/cm with electron as a current carrier. 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 thermal $SiO_2$ 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 × CBO [14, 15]. Therefore, the FN onset field for the electron carrier is 5.77 MV/cm as presented above. Here, 3.75 eV is the position of the intrinsic Fermi energy level $E_i$ in $SiO_2$ from its CB and identifies the position of $E_i$ in $MoS_2$ for the oxide/semiconductor interface due to charge neutrality. The 3.75 eV equals 0.42 × 8.93 eV, where 0.42 is the relative electron effective mass in the oxide and 8.93 eV is the oxide bandgap [16, 17]. The theoretical value of the slope constant $B$ for the FN tunnelling electron current can now be decided using the formula [18, 19]:

$$B = 68.3 \times (m_{ox}/m)^{1/2} \times (\Phi_0)^{3/2}\text{---(MV/cm)} \qquad (1)$$

Here, electron effective mass $m_{ox}$ for $SiO_2$ is 0.42 m and the oxide/semiconductor interface barrier height $\Phi_0$ for electrons is found above theoretically as 2.886 eV. These values give the theoretical slope constant $B$ as 217.0 MV/cm. The FN electron current density for this $B$ and an FN onset field of 5.77 MV/cm found above will be about $1.96 \times 10^{-9}$ $A/cm^2$ theoretically. The oxide will exhibit a breakdown field of about 7.95 MV/cm for a $10^{-4}$ $A/cm^2$ current density for thick oxide of, say 25 to 100 nm, given that two points on the FN current-voltage ($I$-$V$) characteristics at high fields are ($1.96 \times 10^{-9}$ $A/cm^2$, 5.77 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 217 MV/cm, and from the second point, the $E_{bkdn}$ can be calculated to be 7.95 MV/cm [18, 19]. $E_{bkdn}$ is the breakdown electric field in the amorphous

silicon dioxide. $E_i$, located at 0.864 eV from the $MoS_2$ CB translates to an intrinsic defect density, $N_{id}$ of about $1.61 \times 10^{21}/cm^3$ as 1L-$MoS_2$ has a large intrinsic carrier concentration of about $10^{20}/cm^3$ because of the monolayer and a bandgap of 1.8 eV [16, 17]. This defect density is nearly the same as determined experimentally and presented in the theory section above [13]. Thus, the electronic properties of intrinsic Fermi energy level $E_i$ in the semiconductor, the CBO at the oxide/semiconductor interface, FN onset field in the $SiO_2$, leakage current density at the FN onset field in the $SiO_2$, and the electric breakdown strength of the oxide are all determined for the MOS device theoretically, given the electron effective mass in the semiconductor 1L-$MoS_2$ of 0.48 m and its direct bandgap of 1.8 eV, without even fabricating and characterizing the MOS device experimentally. However, the MOS device has to be fabricated and characterized for the interface properties that will lead to the determination of surface FE (field-effect) electron mobility in the MOSFET device channel.

The property of surface FE mobility of the *n*-channel $MoS_2$ MOSFET transistor is considered next which are obtained from the fabricated n-MOS device in conjunction with the concept that the mobility is inversely proportional to the total interface trap density for a Coulomb-scattering limited mobility. This concept is applied on the 1L-$MoS_2$ MIS device with the $SiO_2$ layer as insulator. Atomic layer deposited $Al_2O_3$ has also been tried as an insulator. Utilizing Eq. (4) in the author's earlier study [20] gives the mobility of about 14 to 56 $cm^2$/V-s for the $SiO_2$ and $Al_2O_3$ based MIS device having total interface state density varying from $25 \times 10^{11}/cm^2$-eV to $100 \times 10^{11}/cm^2$-eV for the two hetero-interfaces with $MoS_2$ monolayer [21-25]. Obtaining a better interface for higher mobility is an on-going research endeavour with $MoS_2$. The combined densities of border traps or near-interface traps in the oxide near the semiconductor CB and the oxide/semiconductor interface traps constitute the total interface trap density. They can be said to form two parallel capacitances, one due to the near-interface traps in the oxide and the other due to the traps at the oxide/semiconductor interface. The oxide/semiconductor interface trap density is much larger than the border trap densities in the case of $MoS_2$/insulator interfaces. This, when compared to the Si MOS device as a control sample having a mobility of 140 $cm^2$/V-s for a $10 \times 10^{11}/cm^2$ eV total interface state density gives the calculated mobility presented above. The above calculation shows that the Coulomb-scattering limited mobility can be obtained with the concept of mobility being inversely proportional to the total interface state density with the total interface state density characterization of only the fabricated MOS device [20].

## 4. Conclusion

The *n*-channel MOSFET device on 1L-$MoS_2$ semiconductor is a reality as a low voltage and high frequency device as shown above with theoretical calculations. The insulator/semiconductor interface trap density is high as compared to that of $SiO_2$/Si interface of the Si-MOSFET because of the heterogeneous nature of the interface. This may limit the achievable mobility in the channel and the device characteristics may not surpass those of the silicon MOSFET of comparable dimensions unless the interface trap densities are reduced further. However, other applications of the semiconductor could prove advantageous.

## Conflict of Interest

The single corresponding author declares that there is no conflict of interest.

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