

Article

Combined Influence of Gate Oxide and Back Oxide Materials on Self-Heating and DIBL Effect in 2D MoS₂-Based MOSFETs

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Abstract: In this paper, degradation effects, such as self-heating effect (SHE) and drain-induced barrier lowering (DIBL) effect in 2D MoS₂-based MOSFETs are investigated through simulations. The SHE is simulated based on the thermodynamic transport model. The dependence of the DIBL effect and the lattice temperature in the middle of the channel on the gate length is considered for transistors with different gate oxide and back oxide (BOX) materials. The effects of Al₂O₃ and HfO₂ as gate oxide and SiO₂ and HfO₂ as BOX materials are compared. Transistors, in which the channel is fully and partially (i.e., just below the gate) covered by a gate oxide, are considered. It is shown that the transistors with Al₂O₃ as gate oxide and SiO₂ as BOX materials have higher immunity to DIBL effect and transistors with HfO₂ as gate oxide and HfO₂ as BOX materials have higher immunity to SHE.

Keywords: self-heating effect; DIBL effect; lattice temperature; thermal conductivity; 2D MoS₂



Citation: Atamuratov, A.E.; Saparov, K.S.; Yusupov, A.; Chedjou, J.C. Combined Influence of Gate Oxide and Back Oxide Materials on Self-Heating and DIBL Effect in 2D MoS₂-Based MOSFETs. *Appl. Sci.* **2023**, *13*, 6131. <https://doi.org/10.3390/app13106131>

Academic Editor: Pablo Guardia

Received: 10 April 2023

Revised: 8 May 2023

Accepted: 15 May 2023

Published: 17 May 2023



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1. Introduction

In accordance with some viewpoints, the scaling of silicon-based planar MOSFETs has approached its physical limit. However, according to some other outlooks, there is still an opportunity to continue size scaling of MOSFETs by modifying the structure or choosing the appropriate functional materials. In this context, intensive research was carried out to find alternative transistor structures and channel materials for future devices. A promising material that can be used as a channel material is the transition metal dichalcogenide (TMD), especially two-dimensional TMD. Among other materials, transition metal dichalcogenides have shown great potential in device applications due to their satisfactory bandgaps, thermal stability, carrier mobility, and compatibility with silicon CMOS processes [1]. MOSFETs with channels based on two-dimensional materials, namely TMDs, offer superior electrostatics and excellent immunity to short-channel effects [2]. One of the most popular TMD materials considered as channel material in MOSFETs and also considered to be the most thoroughly and widely studied material is the two-dimensional molybdenum disulfide (MoS₂) [3–5].

In addition to short channel effects, self-heating is also a noticeable effect that can influence the characteristics of MOSFETs based on two-dimensional (2D) materials [6–8]. This means that the top of the transistor's two-dimensional channel is covered with gate oxide and the bottom has a border with back oxide. The low thermal conductivity of oxide materials can cause low heat flow in the channel, resulting in a self-heating effect. The effect of temperature on the drain current of single-layer MoS₂-based MOSFETs has been investigated in [9,10]. It has been observed in [10] that temperature has various impacts on different regions of drain current-gate voltage (Id-Vg) dependence. The drain current decreases slowly in the saturation region and increases quite sharply (or abruptly) in the leakage current region as the lattice temperature in the channel increases. Therefore,

in order to realize high-performance MOSFETs based on MoS₂ or other transition metal dichalcogenides, important problems, such as SHE, must be solved.

As mentioned above, a 2D MoS₂-based MOSFET has sufficient immunity against short channel effects, especially against the DIBL effect [2]. The DIBL effect is one of the noticeable effects in short channel transistors. It appears as an additional (however undesirable) control of the threshold voltage due to the lowering of the barrier by the drain voltage [11]. This effect depends on the electrical parameters of the channel material and the materials surrounding the channel, in particular on the dielectric constant of these materials [12]. However, thermal parameters of the same materials, namely thermal conductivity and heat capacitance, are responsible for thermal properties or thermal effects in the transistor. Thermal conductivity is mainly responsible for the rate of heat dissipation, while heat capacitance is the main parameter that determines the resulting temperature in the channel at a given heat generation or dissipation rate. Therefore, in order to study the transistor immunity to degradation effects, such as the DIBL effect and the self-heating effect, the combined influence of materials surrounding the channel on the above effects must be considered. In this context, this work considers the SHE and DIBL effects for 2D MoS₂-based MOSFETs with the most commonly used oxide materials, such as SiO₂, Al₂O₃, and HfO₂ as gate oxide and back oxide (BOX) in different combinations to compare them. Due to the small dielectric constant, SiO₂ is not considered as a gate oxide in this work.

The rest of the paper is organized as follows. Section 2 describes both the simulation conditions and the parameterization of the transistor. The simulation results are presented in Section 3 and discussed thereafter. Finally, concluding remarks are formulated in Section 4.

2. Simulation Conditions and Parameterization of the Transistor

The advanced TCAD tool Sentaurus is used to numerically simulate the device. Since 2D MoS₂ is not included in the standard version of Sentaurus, the parameters and simulation methods proposed in [2,13] are implemented. The main idea of the method for simulating 2D material-based MOSFETs proposed in [2,13] consists of the following steps: (1) the compilation of data for the material and transport parameters needed for the simulation of 2D material-based MOSFET; (2) the elaboration of a suitable approach to correctly describe the density of states (DOS) and the quantum capacitance in 2D material-based MOS structures; and (3) the implementation of these features in TCAD. It has been shown that carrier transport in 2D MoS₂ MOSFETs with channels of dimensions 10 nm and even sub 10 nm are still far from ballistic but dissipative and scattering dominated channels [14–16]. The drift–diffusion approach is also considered a reasonable guide in the presence of transient and quasi-ballistic transport in short-channel MOSFETs as it correctly accounts for both device geometry and electrostatics [17]. In order to account for thermal effects, the thermodynamic transport model is used in conjunction with the drift–diffusion transport model in our simulation. To calibrate the model used, simulation results of the Id–Vg characteristics are compared with the results in [2]. The comparison for different gate lengths of the transistor (see Figure 1) has led to a good agreement.

The channel of the simulated transistor consists of a MoS₂ monolayer with a thickness of 0.65 nm, and the total length of the device varies between 60 nm and 300 nm depending on the gate length. For all considered transistors, the channel length is three times longer than the gate length. The aluminum gate has a thickness of 2 nm and lengths of 20 nm, 30 nm, 50 nm and 100 nm. The charge carrier mobility in the channel depends on the gate oxide material, so we used a mobility of 125 cm²/(V·s) for Al₂O₃ [2] and 320 cm²/(V·s) for HfO₂ gate oxide (see ref. [18]).

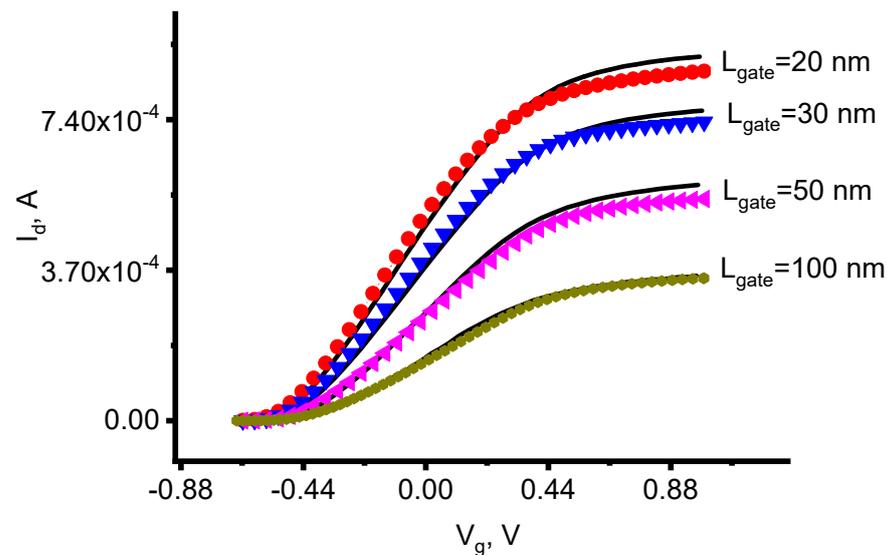


Figure 1. I_g - V_d characteristics of the considered 2D MoS₂-based MOSFETs with different gate lengths. The gate oxide material is Al₂O₃ and the BOX material is SiO₂ with a thickness of 1020 nm. The drain voltage is $V_d = 1$ V. Solid lines correspond to the results in [2], and colored markings are the results of our simulation.

In order to define the optimal structure of the transistor to increase the immunity against degradation effects, the SHE and DIBL effects for a MOSFET with 2D MoS₂ as transistor channel are simulated in two cases (see Figure 2). In the first case, the length of the gate oxide is equal to the length of the MoS₂ channel (Figure 2a), and in the second case, the length of the gate oxide is equal to the length of the gate (Figure 2b).

The simulation is performed considering the four combinations of gate oxide and back oxide materials (see Table 1). An equivalent gate oxide thickness of 1 nm is chosen for all combinations. Therefore, SiO₂-based gate oxide is not considered to likely rule out possible gate leakage current at such thicknesses. Since Al₂O₃ is practically not used as a back oxide material in MOSFETs, Al₂O₃ is not considered as a back oxide material in this work. The thickness of the BOX material has a high impact on the temperature of the transistor channel [19]. The temperature in the channel is increased with increasing thickness of the BOX. In our simulation, we have chosen a thickness of BOX 80 nm. This thickness is in the range of BOX thicknesses of the field effect transistors considered in many works, for example in [20] which was devoted to the investigation SHE in hybrid FinFET [20].

Table 1. Combination of the gate and back oxide materials considered in the work.

Number of Combination	Gate Oxide Material	Back Oxide Material
1	Al ₂ O ₃	SiO ₂
2	HfO ₂	SiO ₂
3	Al ₂ O ₃	HfO ₂
4	HfO ₂	HfO ₂

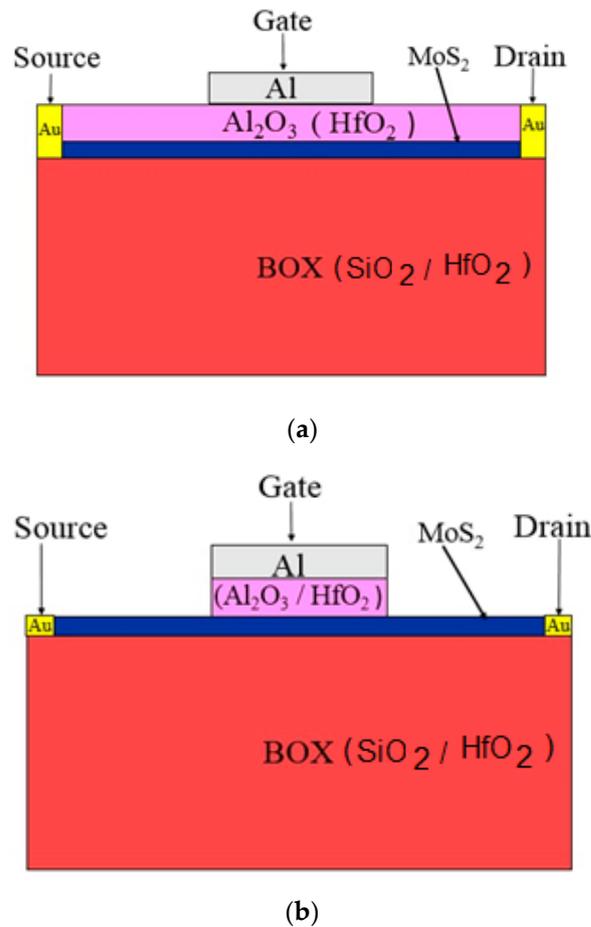


Figure 2. Structure of the simulated MoS₂ MOSFET. Two cases are considered: (a) the gate oxide length is equal to the MoS₂ channel length (first case); (b) the gate oxide length is equal to the gate length (second case).

3. Simulation Results and Discussion

3.1. SHE for Different Combinations of the Gate Oxide and Back Oxide Materials

One of the main parameters of the SHE effect is the temperature in the middle of the channel. The resulting temperature at the center of the channel is defined by the rate of heat generation as well as the rate of heat dissipation through the oxide surrounding the channel. In this study, only heat dissipation is considered, assuming that heat generation is similar in all cases considered. The similar heat generation rate in all the considered cases is provided by choosing the appropriately applied voltages on the gate and drain electrodes. The rate of heat dissipation in the channel is defined by the transistor structure as well as the properties of the oxide materials surrounding the channel. Various considered structures are shown in Figure 2, and various combinations of gate oxide and back oxide materials are shown in Table 1.

The simulation results of the lattice temperature dependence of the gate length at the center of the channel for case 1 (channel surface fully covered) and case 2 (channel surface partially covered) are shown in Figure 3. For all transistors, the temperature distribution along the channel was simulated at fixed (or constant) gate and drain voltages: $V_g = 0.1$ V and $V_d = 0.4$ V. As the resistance of long channel transistors is higher, their drain current is lower than the drain current of short channel transistors at the same applied voltages. Higher drain current in short channel transistors results in higher temperature in the middle of the channel compared to the temperature at the center of the channel in the case of long channel transistors. Our different numerical simulations have shown that the temperature at the center of the channel for short channel transistors is higher in both cases

(i.e., cases 1 and 2) and for two specific combinations (i.e., combinations 1 and 4). Moreover, although the temperature depends on the length of the channel, it is important to note that it also depends on the structure and the oxide materials. These dependencies are discussed later in this section. The temperature dependence on the applied voltages V_g and V_d was also addressed in our previous work (see ref. [9]).

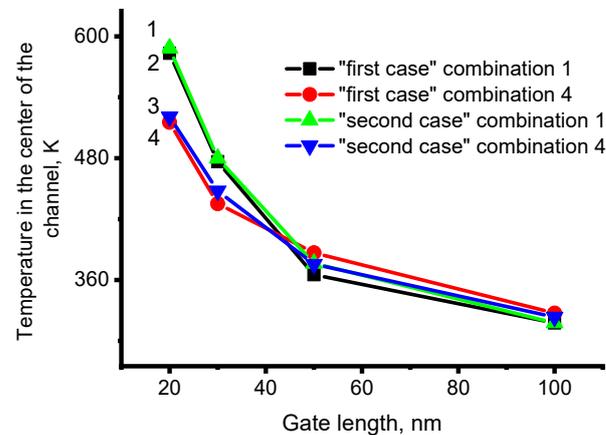


Figure 3. Dependence of lattice temperature at channel center on gate length for 2D MoS₂ MOSFETs with Al₂O₃ gate oxide (1, 2) and HfO₂ gate oxide (3, 4) with fully covered channel (2, 4) and with partially covered channel (only under the gate) (1, 3).

With a gate length less than 40 nm, for combinations 1 and 4, the lattice temperature in the middle of the channel is slightly higher for transistors where the channel is covered with gate oxide only under the gate (second case) than for the transistors of the first case. This is related to the quite different thermal conductivity of gate oxide materials and air. In the first case, the transistor channel is fully covered with oxide (Figure 2a), while in the second case it is partially covered with air (Figure 2b). In the wide temperature range (between 90 K and 1473 K), the thermal conductivity of air has values between 0.0084 and 0.0915 W/(m·K). These values of the thermal conductivity of air (even appropriate for 1473 K) are 2–3 orders of magnitude lower than the thermal conductivity of aluminum- and hafnium-oxides. Thermal conductivities of Al₂O₃ and HfO₂, depending on the size and temperature, are in the ranges of 6–30 W/(m·K) [21–24] and 0.27–4.3 W/(m·K) [25,26], respectively.

The effect of the thermal expansion of the channel is not taken into account in this simulation, because the coefficient of thermal expansion is too low (i.e., very small). According to [27], the coefficient of thermal expansion of the MoS₂ monolayer at 550 K is $6.5 \cdot 10^{-3}$ 1/K, which means a channel expansion of only 1.95% at a change in the temperature of 300 K.

For transistors with a channel length greater than 40 nm, the mid-channel temperature for the transistors of the first case became higher than for the transistors of the second case (Figure 3). This means that the impact of oxide materials on the establishment of the resulting temperature at the center of the channel becomes greater than the impact of the transistor structure (cases 1 and 2) for long channel transistors. In other words, for long-channel transistors, heat dissipation through oxides is much greater than in short-channel transistors, and heat dissipation through gas has no decisive role (i.e., is not so important) in establishing the resulting temperature in the channel.

For long-channel transistors, the temperature tends to be the same for all types of transistor structures considered. In this case, it is observed that the heat generation rate plays a more sufficient role than the heat dissipation rate, since the resulting temperature is the same for both structures (case 1 and case 2) and for both combinations 1 and 4. From the temperature distribution along the channel for case 1 (fully covered channel top) and case 2 (partially covered channel top), it can be seen that with the same applied gate and drain voltages, the temperature variation when lengthening the gate, for the transistor with combination 1 is higher than for the transistor with combination 4 (Table 1) (Figures 4 and 5).

The change in center channel temperature is 264 K and 192 K in case 1, 270 K and 194 K in case 2 for combinations 1 and 4, respectively. Apparently this is mainly related to the higher thermal conductivity of Al_2O_3 compared to the thermal conductivity of HfO_2 (Table 2), which is used as gate oxide materials in combinations 1 and 4, respectively. Although the thermal conductivity of SiO_2 used as BOX material in combination 1 is lower than the thermal conductivity of HfO_2 used as BOX material in combination 4, it differs only by 1.5 times, while the thermal conductivity of gate oxide materials is about 5 times different (Table 2).

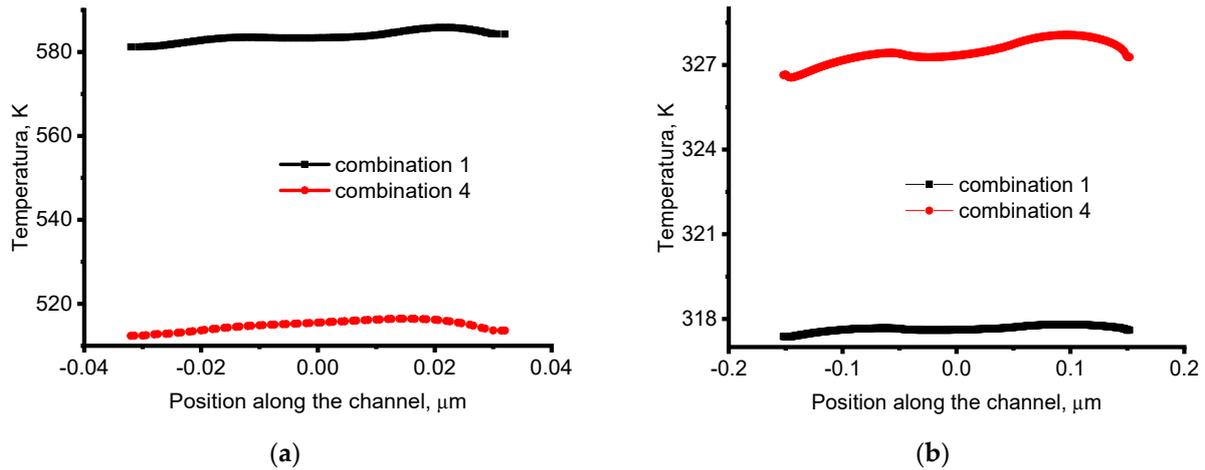


Figure 4. Temperature distribution along the channel for “case 1” transistors with gate oxide materials Al_2O_3 and HfO_2 , while BOX material is SiO_2 and HfO_2 , respectively. The gate lengths are 20 nm (a) and 100 nm (b). $V_g = 0.1$ V, and $V_d = 0.4$ V.

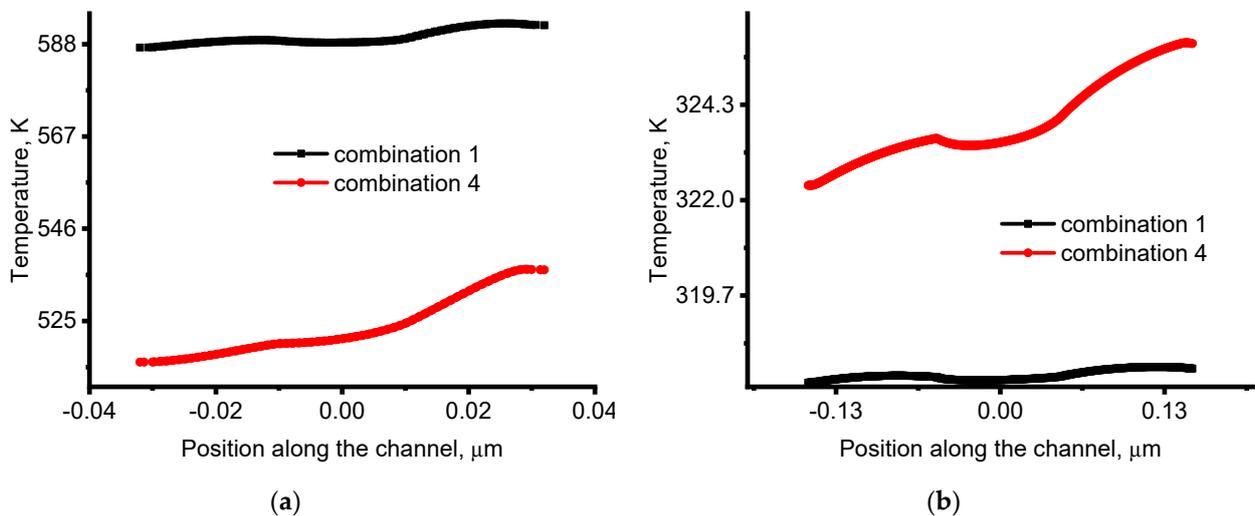


Figure 5. Temperature distribution along the channel for “case 2” transistors with gate oxide materials Al_2O_3 and HfO_2 , while BOX material is SiO_2 and HfO_2 , respectively. The gate lengths are 20 nm (a) and 100 nm (b). $V_g = 0.1$ V, and $V_d = 0.4$ V.

The simulation results for a wider range of oxide material combinations show that SHE is gate length-sensitive for all combinations of gate and back oxide materials in the transistor (Figure 6). The SHE dependence on gate length has only been shown for transistors of case 1, since this dependence is the same for transistors of case 2. The sensitivity of SHE to gate length can be explained by the dependence of drain current on channel length, which in our analysis is based on gate length. Therefore, since the drain current defines the heat

generation rate, a long channel (small drain current) reduces the heat generation rate. The reduction in temperature for long channel transistors and its convergence to the same value for all four oxide material combinations supports our assumption that for long channels the main mechanism responsible for the formation of the resulting temperature is the heat generation rate.

Table 2. Thermal conductivities used for simulation.

Material	Thickness (nm)	Thermal Conductivity $\frac{W}{K \cdot m}$
SiO ₂	80	1.4
Al ₂ O ₃	2.385	12
HfO ₂ (gate oxide)	5.641	2.3
HfO ₂ (Box)	80	2.3

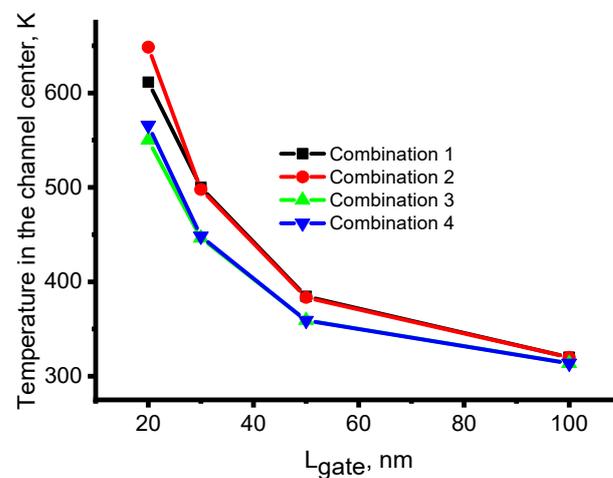


Figure 6. SHE dependence on the gate length for different combinations of gate oxide and back oxide materials.

The temperature dynamics (or behavior) shown in Figure 6 can be explained by the heat dissipation through the gate oxide and BOX. It is known that “low thermal conductivity of oxide materials” results in slower heat dissipation from the material and formation of a higher equilibrium channel temperature than in “higher thermal conductivity of oxide materials”. Therefore, the thermal conductivity of the gate oxide and BOX materials is a very important parameter in SHE. Depending on the thickness, the thermal conductivity of HfO₂ films has values in the range of 0.27–4.3 W/(m·K) at temperatures between 300 °C and 500 °C [26,28]. The values of the thermal conductivity of SiO₂ are in the range between 0.5 W/(m·K) and 2.5 W/(m·K) [29,30]. In our simulation, we used the thermal conductivity values shown in Table 2. We chose the thermal conductivities for HfO₂ and SiO₂ as average values from the indicated above ranges. Thermal conductivity for Al₂O₃ considerably depends on the thickness and the temperature. It is varied in the range between 6 and 30 W/(m·K) [21–24] as mentioned above, in Section 3.1. The value 12 W/(m·K) was chosen as the value corresponding to the nanoscale (less than 10 nm) oxide layer and for a temperature range of approximately between 100 and 300 °C.

With gate lengths up to 100 nm, the mid-channel temperature is higher for transistors with combinations 1 and 2 than for transistors with combinations 3 and 4. Apparently, this is mainly related to a lower thermal conductivity of the BOX material in combinations 1 and 2 (which is SiO₂) than the thermal conductivity of the BOX material in combinations 3 and 4 (which is HfO₂). With the smallest gate length (e.g., a length of less than 30 nm) for combinations with the same BOX material, the temperature is higher for combinations with HfO₂ as the gate oxide material. With gate lengths between 30 nm and 100 nm, the

temperature for combinations with the same BOX material is approximately the same and practically independent of the gate oxide material. With a gate length of 100 nm, the temperature is practically the same for all four combinations, which means that with long gate lengths, the resulting center channel temperature does not depend on the gate oxide and BOX materials.

3.2. DIBL Effect for Different Combinations of the Gate Oxide and Back Oxide Materials

The DIBL effect is one of the SHE-like degradation effects which also depends on the properties of the gate oxide and BOX materials. For comparison with the SHE effect, the DIBL effect was simulated in a MOSFET with 2D MoS₂ as transistor channel with the four combinations of gate oxide and BOX materials mentioned above. The simulation results show that the DIBL effect for transistors with combinations 3 and 4 is more sensitive to gate length (Figure 7). In all ranges of transistor length, the DIBL effect is higher for transistors with combinations 3 and 4 than for transistors with combinations 1 and 2. This observation can be understood in the context of a simple model describing the capacitive coupling between the channel and the device electrodes, proposed in [12]. Within the context of a simple model, the modified expression for DIBL is expressed as follows [12]:

$$DIBL = \frac{C_D}{C_G} \quad (1)$$

where, C_D and C_G are drain-channel and gate-channel capacitances, respectively (Figure 8). Three components contribute to the drain-channel capacitance (C_D): the capacitive coupling through the channel layer ($C_{D, ch}$), the coupling through the BOX ($C_{D, box}$), and the coupling through the gate oxide ($C_{D, ox}$). Therefore, the drain-channel capacitance (C_D) is expressed as follows:

$$C_D = C_{D, ch} + C_{D, box} + C_{D, ox} \quad (2)$$

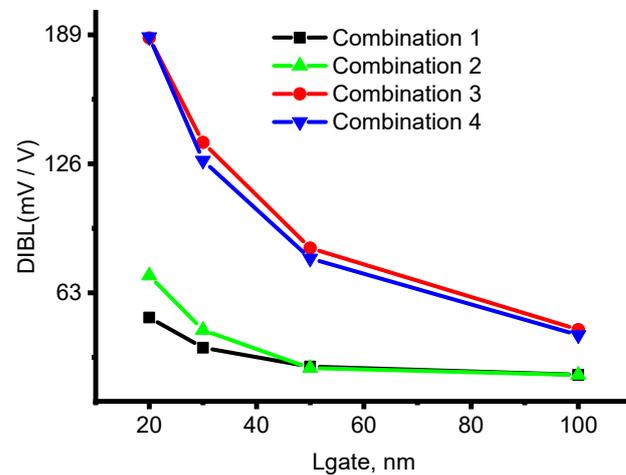


Figure 7. DIBL effect dependence on the gate length for different combinations of gate oxide and back oxide materials.

The capacitance components C_G , $C_{D, ch}$, and $C_{D, ox}$ depend on the dielectric constant of the channel ϵ_{MoS_2} , while $C_{D, box}$ is unaffected by ϵ_{MoS_2} and depends on the dielectric constant of the BOX material. In our case, $\epsilon_{Al_2O_3} = 9.3$, $\epsilon_{SiO_2} = 3.9$ and $\epsilon_{HfO_2} = 25$ and $\epsilon_{MoS_2} = 3$. Therefore, since the dielectric constant of the channel ϵ_{MoS_2} is smaller, the gate capacitance C_G and the components $C_{D, ch}$ and $C_{D, ox}$ are reduced, and the DIBL effect is mainly defined by $C_{D, box}$. Thus, for the considered transistors, the DIBL effect is defined by the dielectric constant of the BOX. In the range of combinations, the BOXs with the highest dielectric constant are in combinations 3 and 4, where oxide materials are HfO₂ with $\epsilon_{HfO_2} = 25$, hence these combinations should show the highest DIBL effects. Therefore,

while the BOX material for the transistors with combinations 1 and 2 is SiO_2 with a lower dielectric constant ($\epsilon_{\text{SiO}_2} = 3.9$), the DIBL effect for these transistors should be low. These suggestions are in perfect agreement with Figure 7. It can also be seen in Figure 7 that the gate oxide material does not have a considerable impact (or influence) on the DIBL effect in the considered range of variation of the gate length.

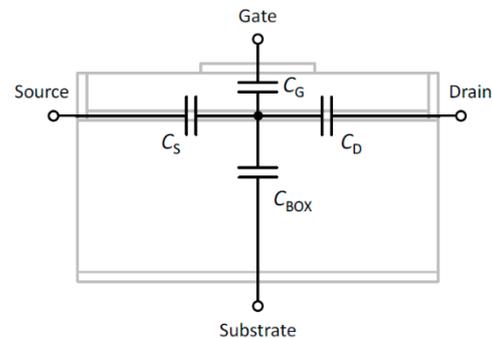


Figure 8. Equivalent circuit describing the capacitive coupling between the channel and the device electrodes in MOSFET.

3.3. Optimization of the Combination of the Gate Oxide and Back Oxide Materials

The dependence of lattice temperature and DIBL on the number of combinations that can be seen from Figures 6 and 7 for a gate length of 20 nm is shown in Figure 9. It is clear from Figure 9 that the SHE and DIBL effects compete for the combination of the oxide materials. As already discussed above, the electrical and thermal properties of the back oxide material, namely dielectric constant and thermal conductivity, are mainly responsible for the SHE and DIBL effect in the considered 2D MoS_2 MOSFETs.

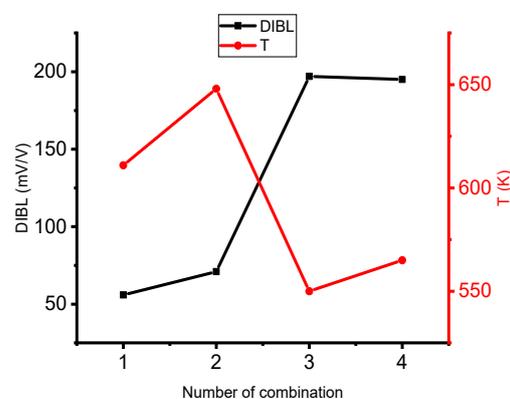


Figure 9. DIBL effect and SHE dependence of combinations of gate oxide and back oxide materials in MOSFET.

Achieving a small DIBL effect requires a low dielectric constant back oxide material, while reducing the gate temperature in the transistor channel requires a high thermal conductivity back oxide material. We have considered two popular and commonly used back oxide materials: SiO_2 and HfO_2 . When the back oxide material is SiO_2 , it has a small dielectric constant, resulting in a decrease in DIBL; at the same time, it also has low thermal conductivity, which leads to high lattice temperature in the transistor channel. Conversely, as a back oxide material, HfO_2 material has a high dielectric constant, resulting in a high DIBL effect, while also exhibiting a relatively high thermal conductivity, resulting in a reduction in the lattice temperature in the transistor channel.

From our results, it is possible to define the range of electrical and thermal parameters of oxide materials that allow to achieve optimal immunity to SHE as well as the DIBL effect. From Figure 7, it can be concluded that using the BOX material with a relative dielectric

constant in the range between 3.9 and 25 and a thermal conductivity between 1.4 and 2.3 W/Km is a perfect choice to achieve (or for achieving) optimal immunity to degradation effects, such as SHE and DIBL effects in 2D MoS₂-based MOSFETs. The gate oxide material has practically no significant influence on SHE as well as on the DIBL effect.

4. Conclusions

The results of the simulation of the SHE effect have revealed that with a gate length of less than 40 nm, a greater influence on the resulting temperature was exerted on the considered structures of the transistor (see case 1 and case 2) than the influence of the gate oxide and the BOX materials. Furthermore, it was observed that SHE is sensitive to gate length for all combinations of gate and back oxide materials in the transistor, while the DIBL effect is more sensitive to gate length for transistors with combinations 3 and 4.

Moreover, our simulation results revealed that the choice of gate and BOX oxide materials to ensure the highest possible immunity against degradation effects, such as SHE and DIBL effects, is an optimization task in 2D MoS₂-based MOSFETs. The electrical and thermal properties of the back oxide material have been shown to have a major influence on the SHE and DIBL effects in 2D MoS₂-based MOSFETs. Indeed, the use of the BOX material with a relative dielectric constant between 3.9 and 25 and a thermal conductivity between 1.4 and 2.3 W/(K·m) makes it possible to obtain optimum immunity against degradation effects, such as SHE and DIBL effects, in 2D MoS₂-based MOSFETs. Finally, it was observed that the gate oxide material has almost no considerable impact on the SHE effect as well as the DIBL effect.

Author Contributions: Conceptualization, A.E.A.; methodology, A.E.A. and A.Y.; software, K.S.S.; validation, A.E.A. and K.S.S.; formal analysis, J.C.C. and A.Y.; investigation, K.S.S.; resources, K.S.S.; data curation, K.S.S.; writing—original draft preparation, A.E.A.; writing—review and editing, A.E.A. and J.C.C.; visualization, J.C.C. and A.Y.; supervision, A.E.A.; project administration A.E.A.; funding acquisition, A.E.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Ministry of Innovation Development of the Republic of Uzbekistan, grant number Ind-Uzb-2021-80.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data is unavailable due to privacy.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

SHE	Self-Heating Effect
DIBL	Drain-Induced Barrier Lowering
MOSFET	Metal-Oxide-Semiconductor Field Effect Transistor
BOX	Back oxide
TMD	Transition Metal Dichalcogenide
CMOS	Complementary Metal-Oxide-Semiconductor
DOS	Density of States
2D	Two Dimensional
TCAD	Technology Computer Aided Design

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