Design and Investigation of Double Gate Field Effect Transistor Based H2 Gas Sensor Using Ultra-Thin Molybdenum Disulfide

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Design and Investigation of Double Gate Field Effect Transistor Based H_2 Gas Sensor Using Ultra-Thin Molybdenum Disulfide

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Abstract: In this article, a low-power hydrogen (H_2) gas sensor has been proposed using a two-dimensional (2D) material based Double Gate Field Effect Transistor (2D-FET). It is imperative to highlight that the conventional three-dimensional (3D) materials cannot be scaled down to an ultra-low dimension due to the presence of dangling bonds, surface roughness scattering etc. This creates a major challenge in developing low-dimensional sensors for next generation sensing and computing. In this context, we have developed an extensive simulation model, which articulates the physical phenomena behind a catalytic metal gate-based hydrogen gas sensor using a 2D-FET. A 5 nm thin Molybdenum disulfide (MoS_2) film has been used as the channel material for the proposed 2D-FET based gas sensor. The sensor has been modelled by emphasizing on the catalytic metal (Palladium) gate approach, where the work function of the gate metal deposited on top of the channel region varies after the absorption of the hydrogen gas. Moreover, the Technology Computer Aided Design (TCAD) based gas sensor model has been developed by considering a change in the pressure of H_2 gas as well. We have also highlighted the effect of Metal/MoS_2 contact on sensor performance. In terms of results, a maximum threshold voltage (V_{th}) shift of 100 mV has been obtained against a gas pressure of 10^{-10} torr, whereas the maximum percentage of change in I_{ON}/I_{OFF} is 100.

Index Terms—2D Materials, Field Effect Transistor, Hydrogen Gas Sensor, Sensitivity, Schottky Barrier Effect

Introduction:

Field effect transistors (FETs) are extensively used and closely packed to develop logic gates or any other integrated circuit for the last two decades. These devices are also developed to sense different gas molecules [1] at room temperature and have gained a lot of popularity in the research community. Low power consumption, CMOS compatibility, reconfigurability etc. make a FET based gas sensor efficient and attractive. It must be mentioned that the change in the metal (gate) work function against the adsorption of the gas molecules is the backbone of the FET based gas sensors, where the dipole generation changes the work function of the metal [2]. In addition, the change in the metal work function gets reflected on the threshold voltage of the FET, which shifts significantly.

For the past few years, there have been multiple gas sensor models reported in the literature with an emphasis on different FET architectures. A gate-all-around nanowire junctionless transistor was proposed to work as a hydrogen gas sensor based on the catalytic metal gate approach [2]. Similarly, the scientists have also proposed an alternative to the MOSFET based gas sensors, where they have considered Tunnel FETs (TFETs) to minimize the short channel effects and to reduce the sub-threshold slope of the device [3]. It is imperative to say that planar MOSFET, gate all-around MOSFET [4], TFET [5] based gas sensors have shown a lot of promise, but all these devices are prone to scaling challenges as most of them are made of 3D materials [6]. On the other hand, to design and develop low-dimensional nanoelectronic devices for next generation sensing primitives, we need semiconducting materials that can be thinned down even to the atomic scale. It is to be noted that the 2D materials [7] have gained a lot of attention in the vast area of semiconductor devices owing to the atomically thin body, which also opens an opportunity for aggressive scaling of the device dimension. Moreover, the 2D materials such as the transition metal dichalcogenides (TMDs) are immune to surface roughness scattering as there are no dangling bonds present in the material [8], which makes them an ideal choice in terms of developing low-dimensional FETs for ultra-low power sensing/circuit applications and non-von-Neumann computing [9].

In this paper, we have tried to articulate the gas sensing behavior of a MoS_2 based double gate FET by considering the catalytic metal gate approach. It is imperative that pressure plays a crucial role in changing the electrical characteristics of the device as it changes the work function of the gate metal. After the metal (Pd) gate is exposed to the H_2 gas, a decomposition of the gas molecules take place at the metal surface and then the disassociated molecules diffuse into the metal gate. Moreover, an electrical dipole layer gets generated at Pd/HfO_2 interface due to the adsorption of the gas molecules into the gate metal and thus the metal work function changes accordingly. In this context, we have evaluated the performance of the proposed device in terms of shift in threshold voltage and I_{ON}/I_{OFF} ratio. Furthermore, we have also depicted the potential distribution along the channel and the density of states. In addition, we have also included the effects of a Schottky contact between MoS_2 and source/drain metal (Ag) contacts

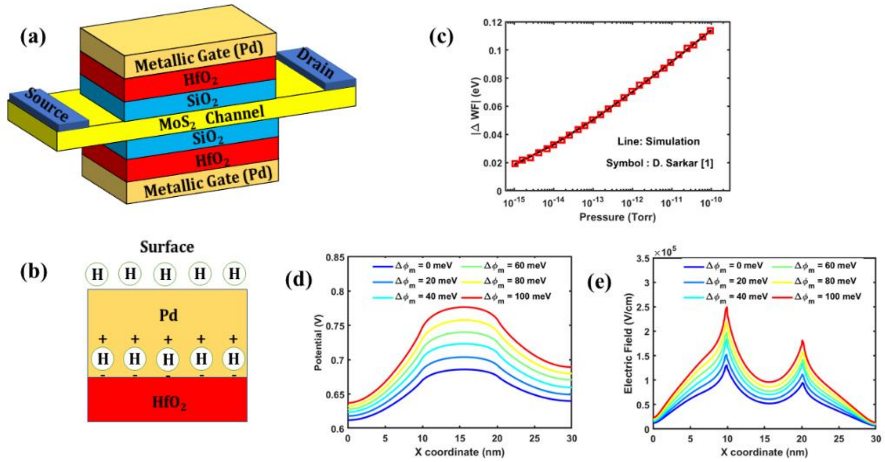

Fig. 1. (a) 3D schematic of the 2D-FET with **(b)** 2D schematic of electrical dipole formation at the Pd/HfO_2 interface, **(c)** Change in gate metal work function ($\Delta\phi_m$) with respect to the hydrogen gas pressure, **(d)** Surface potential distribution of 2D-FET for different $\Delta\phi_m$ and **(e)** Electric field distribution of 2D-FET for different $\Delta\phi_m$.

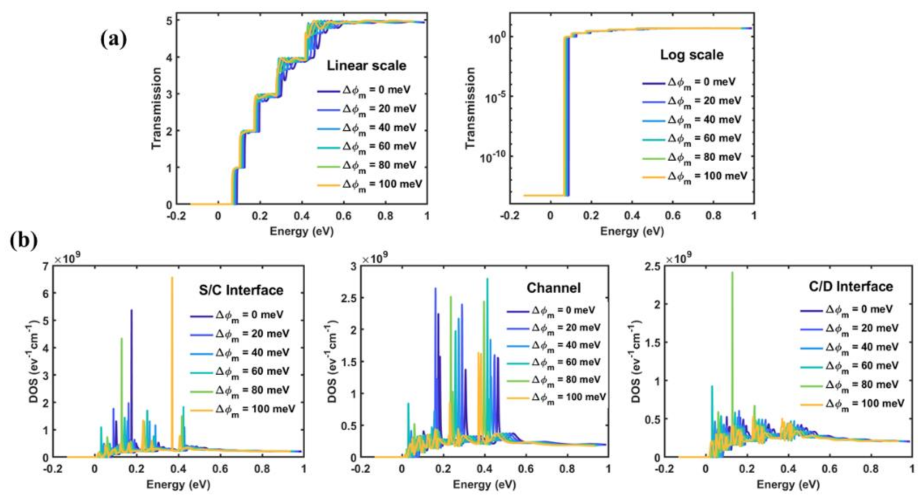

Fig. 2. (a) Transmission probability across the energy levels in linear and log scale for different $\Delta\phi_m$ and **(b)** Density of States (DOS) at source, channel and drain for different $\Delta\phi_m$.

on the sensor performance for different gas pressures in our simulation framework.

Device Description and Simulation Methodology:

In this article, we have tried to evaluate the electrical performance of a 2D-FET as a hydrogen gas sensor, and the transistor schematic is depicted in Fig. 1(a). A palladium (Pd) gate metal is used to sense the hydrogen gas molecules with a work function (ϕ_m) of 5.22 eV. The gate metal is deposited on top of a high-k oxide stack, where a 1 nm SiO_2 is the low-k dielectric layer, and the high-k dielectric layer is a 2 nm HfO_2. Moreover, a 5 nm thin MoS_2 film has been considered as the channel material and the length of the channel is 10 nm. It must be mentioned that the MoS_2 film is intrinsic here with a carrier concentration of 10^{14} atoms/cm^3. Fig. 1(a) shows the dipole formation mechanism at and near the Pd/ HfO_2 interface after the adsorption of the gas molecules. It must be noted that the hydrogen gas molecules undergo a significant amount of dissociation and adsorption at the gate metal surface and therefore some of the hydrogen atoms diffuse through the gate metal, which ultimately forms the dipole at and near the interface followed by a change in the metal work function. In this context, the change in the metal work function has been shown in Fig. 1(b) as a function of the hydrogen gas pressure. Moreover, the metal work function reduces as we increase the pressure due to the increased surface coverage of the hydrogen gas on the metal surface. Thus, it is observed that the $|\Delta\phi_m|$ or $|\Delta WF|$ increases with increasing gas pressure [1]. In this work, the 2D-FET has been simulated using the SILVACO ATLAS TCAD tool [10] at room temperature. The carrier transport mechanism in the 5 nm thin MoS_2 channel has been captured through NEGF simulations. Furthermore, the Schrodinger-Poisson equation is generally coupled with the NEGF formalism for extracting the electron density and eventually current [10]. In addition, the material parameters have been defined in ATLAS to develop the simulation framework, where the electron affinity of 5 nm thin MoS_2 is 4.0 eV, electron and hole effective mass is $0.52m_o$ and $0.64m_o$. Also, the permittivity of MoS_2 is 11 and the bandgap is 1.6 eV [10].

Results and Discussions:

In this article, we have assessed the electrical characteristics of the proposed 2D-FET based H_2 gas sensor based on the catalytic metal gate approach, where the absorbed gas molecules on the palladium gate metal, cause a modulation in the work function of the metal. Here, the potential distribution has been shown in Fig. 1d along the channel for different $\Delta\phi_m$ values. It has been depicted in Fig. 1c that the maximum change in ϕ_m is close to 120 meV, when the gas pressure (P) is 10^{-10} torr. The potential distribution shows that with an increase in the $\Delta\phi_m$, the surface potential also increases at and near the channel region. Moreover, the relative change is almost 15 % when P is 10^{-10} torr with respect to no gas molecules absorbed. The electric field distribution has been depicted in Fig. 1e for different $\Delta\phi_m$ values. In this case, the maximum electric field near the source/channel and drain/channel interface has increased with an increase in the $\Delta\phi_m$, where the work function (ϕ_m) of the Pd metal has reduced with an increase in the gas pressure.

It is a known fact that, the electric field is nothing but a differential quantity of the surface potential and thus the electric field profile follows the slope of the surface potential.

Fig. 2a shows the transmission probability in linear and log scale across the filled energy levels and it illustrates that for different $\Delta\phi_m$, there is a clear transition in the transmission probability, and it attains a lower energy level as ϕ_m reduces after the gas molecules are absorbed at the metal surface. Moreover, the relative change in the occupied energy levels with a specific transmission probability is not very significant for different $\Delta\phi_m$. Furthermore, the variation in the density of states (DOS) has been shown with respect to the energy levels at source, channel and drain regions of the 2D-FET. It must be noted that the change in the DOS as a function of occupied energy levels depicts the modulation in the band gap (E_G) and carrier density across the 2D-FET. Fig. 2b shows the change in density of states for different $\Delta\phi_m$, where a reduction in the metal work function reduces the filled energy level of the first sub-band that reduces the E_G of MoS_2.

Here, the transfer characteristics has been shown in Fig. 3(a) for different gas pressures ($P = 10^{-14}$, 10^{-12} and 10^{-10} torr etc.) at a drain-to-source voltage or V_{DS} of 0.2 V. It has been already shown in Fig. 1(c) that the metal work function, ϕ_m, changes with the change in the gas pressure. We have assessed that ϕ_m reduces gradually as the gas pressure increases from 10^{-15} torr to 10^{-10} torr due to catalytic reactions between the gas and the metal. The threshold voltage of the 2D-FET reduces with an increase in the gas pressure as shown in Fig. 3(b). Moreover, the I_{ON}/I_{OFF} ratio reduces significantly with an increase in the gas pressure as the off-state current (I_{OFF}) increases as ϕ_m goes down as shown in Fig. 3(b). It must be noted that the on-state current of the 2D-FET does not get affected largely by the catalytic reaction between metal and the gas as the change in ϕ_m is less as a function of the gas pressure. Furthermore, the transfer characteristics of a 2D-FET is expected to get affected by the interface trap charges (N_{it}) localized at and near the SiO_2/MoS_2 interface due to defect states. Fig. 3(c) shows that the transfer characteristics has shifted significantly due to the trapped charges (positive) and the threshold has reduced by 400 mV, when N_{it} is 5×10^{12} /cm^2 before the absorption of any gas molecules at the metal surface. Furthermore, the I_{ON}/I_{OFF} ratio has also shifted significantly by 7 orders of magnitude as shown in Fig. 3(d) against the variation of N_{it} from 1×10^{11} to 5×10^{12} /cm^2. Additionally, the variation in the transfer characteristics, threshold voltage and I_{ON}/I_{OFF} ratio has also been illustrated in Fig. 4(a-c) for different gas pressures to validate the gas sensing behavior against the variation of N_{it}.

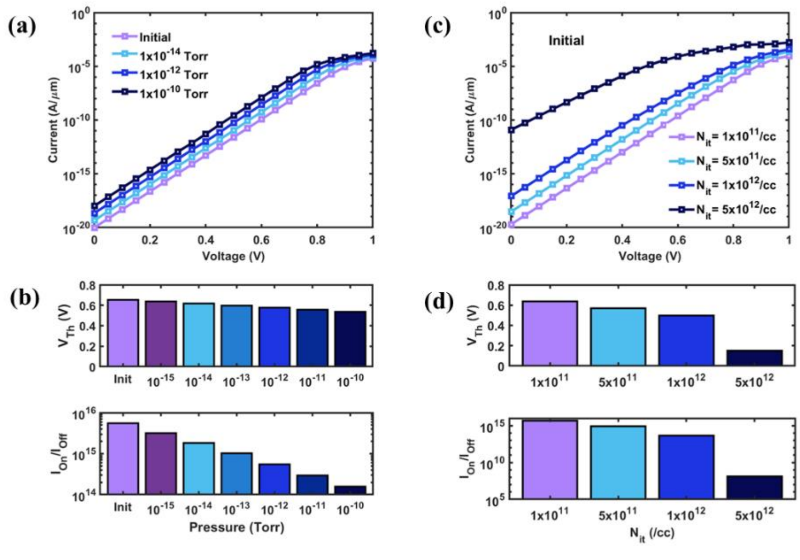

Fig. 3. (a) Transfer characteristics of 2D-FET for different gas pressures at $V_{DS} = 0.2$ V without considering interface trap charges, **(b)** Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different gas pressures, **(c)** Transfer characteristics of 2D-FET for different interface trap charges before absorption of gas molecules at metal surface and **(d)** Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different interface trap charges before absorption of gas molecules at metal surface

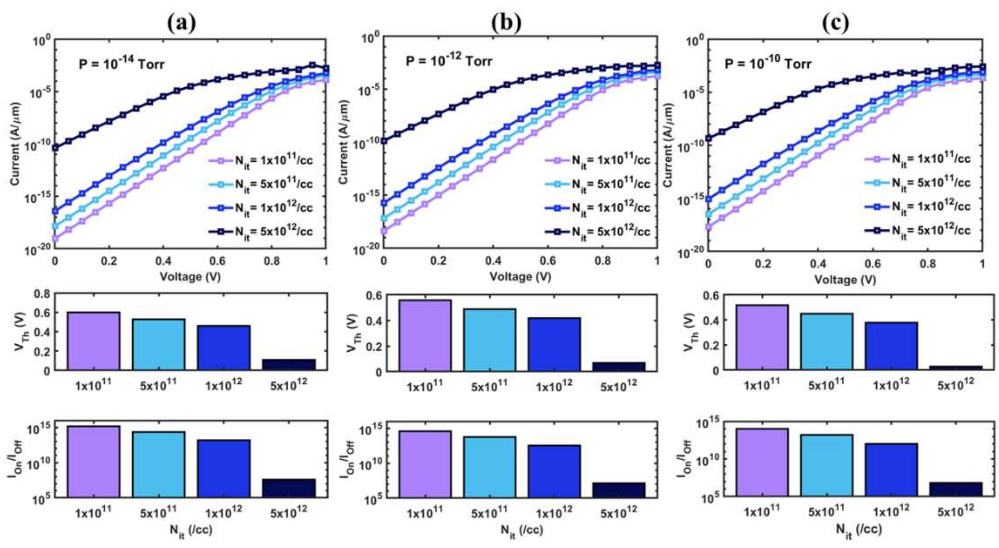

Fig. 4. (a) Transfer characteristics, Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different interface trap charges at $P = 10^{-14}$ torr and $V_{DS} = 0.2$ V, **(b)** Transfer characteristics, Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different interface trap charges at $P = 10^{-12}$ torr and $V_{DS} = 0.2$ V and **(c)** Transfer characteristics, Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different interface trap charges at $P = 10^{-10}$ torr and $V_{DS} = 0.2$ V

Fig. 5(a) shows the threshold voltage sensitivity (S_{Vth}) as a function of both gas pressure (P) and interface trap charges (N_{it}). The maximum percentage of S_{Vth} is nearly 100. In addition to this. the change in the I_{ON}/I_{OFF} ratio has also been considered as a sensing metric and the maximum percentage of $S_{ION/IOFF}$ is 100 for P = 10^{-10} torr as shown Fig. 5(b). Although most of the previously reported FET (MOSFET or TUNNEL FET) based gas sensors have shown high sensitivity values while sensing H_2, NH_3 or NO_2, but the channel materials used in those devices do suffer from either quantum confinement [11] or surface roughness scattering [12] or both. In an ultra-thin Si based FET, the quantum confinement phenomena play an important role as it increases the effective band gap of silicon and thus, we observe a decrement in the current. Most of the previously published papers on FET based gas sensors have not really considered the effect of metal/semiconductor contact while evaluating the sensing behavior. In a 2D-FET based gas sensor, the interface between the MoS_2 and the source/drain metal contacts plays a crucial role in the carrier injection mechanism [13] and thus can govern the sensing behavior as well. It must be noted that the MoS_2/metal interface is immensely affected by the Fermi level pinning [14] phenomena near the CB (conduction band) of MoS_2 as shown in Fig. 6(a). As we know that, the formation of a Schottky barrier (SB) takes place due to the difference between the metal (source/drain) ϕ_{mc} and the electron affinity (χ) of the semiconductor and in our case the Schottky barrier height (Φ_{SBH}) is roughly 0.3 eV as ϕ_{mc} is 4.3 eV. Moreover, the selection of the source/drain metal contacts plays a pivotal role in determining the amount of carrier injection and metals with low work functions would be a better. Fig. 6(b) shows the surface potential distribution across the channel for different $\Delta\phi_m$. We can say that the maximum change in the potential value is around 0.1 V by considering the SB effect. Fig. 6(c) shows the transfer characteristics of the 2D-FET, and the on-state current has reduced a bit due to the Φ_{SBH} of 0.3 eV compared to Fig. 3(a). Furthermore, the change in the threshold voltage is 85 mV for a $\Delta\phi_m$ of 100 meV, whereas it was 100 mV in Fig. 5(a) without the SB effect. Therefore, we can say that it is imperative to carefully consider the SB effect in 2D-FET and assess the sensor performance. However, if the ϕ_{mc} is low, then we can minimize the Φ_{SBH} further and carrier injection will be more. Thus, it

is very much crucial to consider this non-ideal effect while designing a 2D-FET based gas sensor [15].

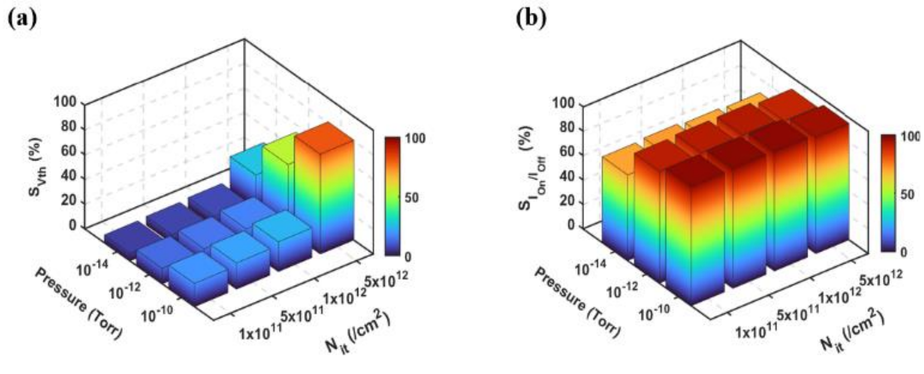

Fig. 5. (a) Threshold voltage sensitivity (S_{Vth}) and **(b)** I_{ON}/I_{OFF} Sensitivity ($S_{ION/IOFF}$) of 2D-FET for different interface trap charges and gas pressures at $V_{DS} = 0.2$ V.

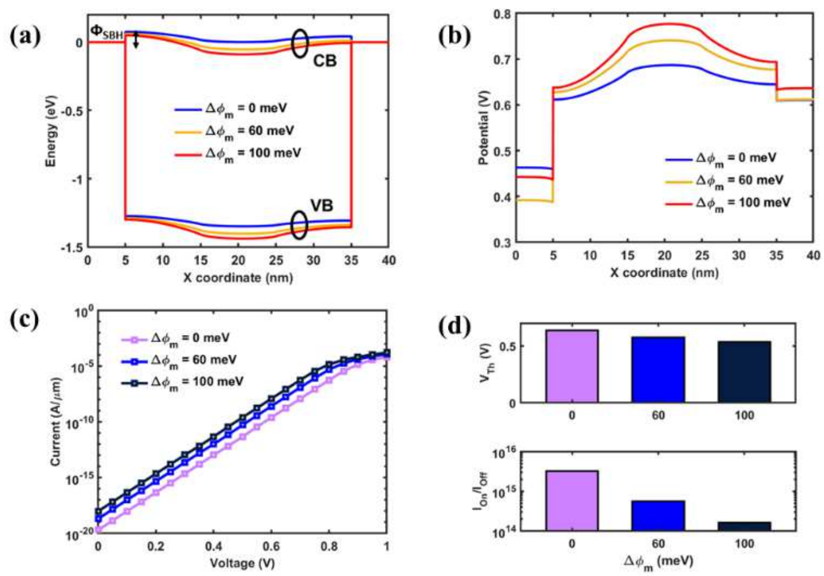

Fig. 6. (a) Energy band diagram of 2D-FET for different $\Delta\phi_m$ at $V_{DS} = 0.2$ V, **(b)** Surface potential distribution of 2D-FET for different $\Delta\phi_m$ at $V_{DS} = 0.2$ V, **(c)** Transfer characteristics of 2D-FET for different $\Delta\phi_m$ at $V_{DS} = 0.2$ V and **(d)** Threshold voltage and I_{ON}/I_{OFF} ratio of 2D-FET for different $\Delta\phi_m$ considering Schottky barrier effect.

CONCLUSION:

In this article, we have tried to evaluate the electrical performance of a 2D-FET as a hydrogen gas sensor. One of the reasons behind selecting a 5 nm thin MoS_2 film as the channel material is the area efficiency as we can thin down a MoS_2 film up to the atomic scale and it does not suffer from surface roughness scattering or any quantum mechanical effect. The proposed 2D-FET has been modelled using SILVACO TCAD and the catalytic metal gate approach helped us to realize the gas sensing phenomenon. The maximum threshold voltage shift is 100 mV after the variation of the gas pressure. Moreover, we have tried to include the effect of interface trap charges and investigated the change in the electrical characteristics of the device. Furthermore, the study of the Metal/MoS_2 contact (source/drain) was included in the paper to highlight the effect of the Schottky barrier height and how we can minimize the barrier height to have more amount of carrier injection.

Conflict of Interest:

The authors declare that they have no conflict of interest.

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