HYDROGEN SENSOR BASED ON MOS CAPACITOR

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A MOS capacitor structure used as hydrogen sensor is defined and simulated. The maximum operating temperature, as well as the influence of structure defects and hydrogen environment on the C-V characteristic were determined. The analysis was performed on structures based on silicon (Si) and silicon carbide (SiC). Results showed that the Si-MOS structure is best suited for hydrogen detection at low temperatures up to 430K. The SiC-MOS sensor can be used at high temperatures up to 1150K.

Keywords: MOS capacitor, hydrogen sensor, silicon, silicon carbide

1. Introduction

Hydrogen has become one of the most utilized gases in the industry. It is used as raw material or clean energy source in industries such as chemical, food, semiconductor and transport. The processes that include hydrogen need sensors for leakage detection and gas distribution monitoring.

In the last years, a great research was conducted on hydrogen micro sensors. This type of sensors has many advantages over conventional gas detectors. Their characteristics are represented by low cost, compactness, easy maintenance, reliability and manipulation by less experienced personnel. Also, they are well suited for remote applications and multi sensor systems [1].

MOS capacitors are highly used as hydrogen sensors. Their structure is simple and easy to fabricate. Also, they can be integrated in sensor arrays. They can operate at room and high temperatures and provide a great sensibility and selectivity [2].

The current paper presents a study of the MOS capacitor used as hydrogen sensor. Both Si and SiC were employed for the semiconductor layer. The structure's maximum operating temperature and the influence of a hydrogen environment on the sensor's C-V characteristic were obtained by extensive simulations.

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2. Structure

The general structure used to simulate the hydrogen sensor is illustrated in Fig. 1. It consists of a 1.5μm n-type semiconductor layer with a doping of 1 x 10^{16} cm^{-3}. Two semiconductor materials were utilized: Si and 3C-SiC. On top of the semiconductor layer, a 50nm SiO_2 is deposited. Over the oxide layer a metallic anode is considered. The metal work function was configured to 5.12eV, which represents the work function value of palladium (Pd). Hydrogen has a high solubility in this material [3].

When the structure is introduced in a hydrogen environment, the gas molecules dissociate in contact with the metal electrode at temperatures as low as 150°C. Some of the atoms remain at the surface of the metal and others diffuse through the metal until they reach the metal-oxide interface. Here, they create a dipole layer which decreases the metal work function. This determines a parallel shift of the structure's C-V characteristic towards negative voltages [4].

At temperatures over 700K, the hydrogen atoms diffuse further into the structure until they reach the oxide-semiconductor interface. Here, they passivate the interface states charges. This passivation reduces the transition from accumulation to inversion of the structure's C-V characteristic [4].

The sensor's response to hydrogen ambient is determined by keeping the device at a constant capacitance in the depletion region of the C-V characteristic and by measuring the voltage needed to maintain that capacitance [4].

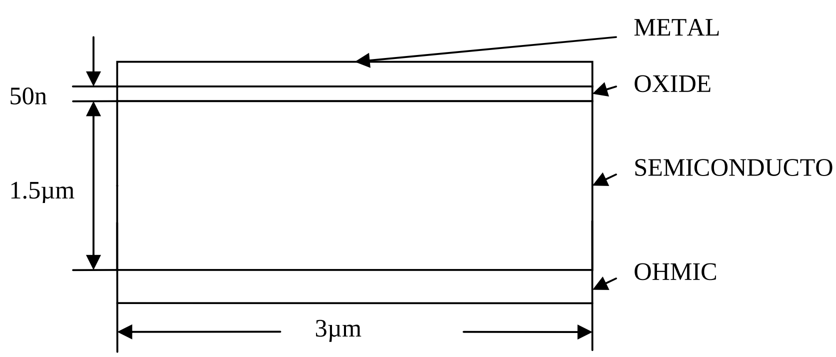

Fig. 1. Simulated MOS capacitor structure

3. Simulations

The MOS capacitor structure was simulated using 2D Taurus Medici from Synopsys [5]. Both Si and 3C-SiC structures were studied. A fixed oxide charge and an oxide-semiconductor interface states charge were considered. For Si-MOS, an oxide charge of 1.82 x 10^{10} cm^{-2} and an interface states charge of 10^{10} cm^{-2}/eV were used [6]. For SiC-MOS, the trapped oxide charge is 10^{12} cm^{-2} and the interface states charge is 10^{12} cm^{-2}/eV [7].

The effects of the trapped oxide charge and the interface charge on the structure's C-V characteristic was investigated. Also, the operating temperature domain was determined in an inert environment. The influence of a hydrogen environment on structures' behavior was analyzed too. The study implied the simulation of structures' C-V characteristic.

4. Results

4.1. Fixed oxide charge and interface states charge

In order to evince the influence of fixed oxide charge and interface states charge on the C-V characteristic, three types of structures were considered and simulated for the devices based on Si and SiC. The first one represents an ideal MOS structure, with no trapped oxide charges and no interface states charges. The second structure has only a fixed oxide charge and the third one signifies a real MOS structure, with both fixed oxide charge and interface states charge.

The C-V characteristics for Si-MOS and SiC-MOS devices are illustrated in Figs. 2-3.

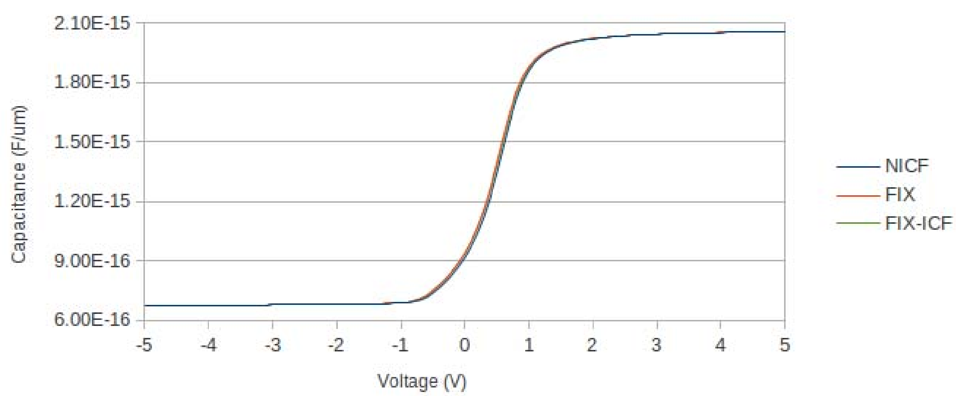

Fig. 2. Si-MOS structure's C-V characteristics – (a) NICF – no oxide and interface states charges, (b) FIX – fixed oxide charge, (c) FIX-ICF – fixed oxide charge and interface states charge

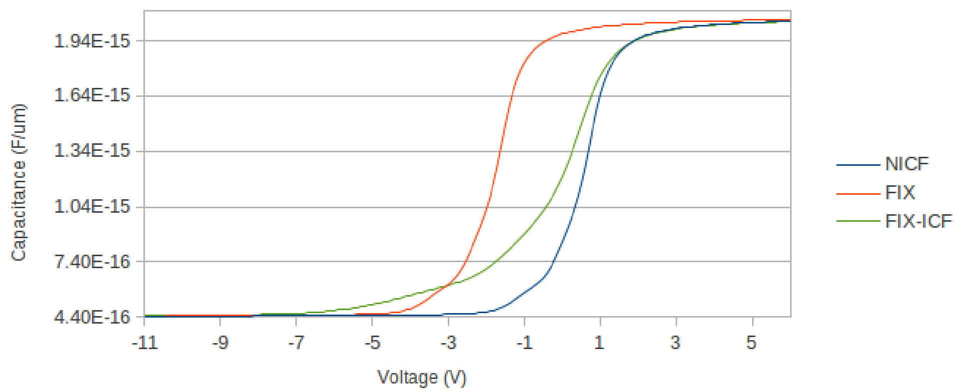

Fig. 3. SiC-MOS structure's C-V characteristics – (a) NICF – no oxide and interface states charges, (b) FIX – fixed oxide charge, (c) FIX-ICF – fixed oxide charge and interface states charge

It can be observed that the fixed oxide charge produces a parallel shift of the C-V characteristic towards negative voltages. This is due to the fact that the charges trapped into the oxide are positive, thus reducing the *flat-band* voltage of the capacitor, and they also do not change with the bias voltage [8]. The interface states charge varies with bias voltage. Also, it diminishes the dependence of the depletion region's charge with bias voltage. Thus, in order to pass the MOS capacitor from accumulation to inversion, a larger voltage interval is required (Figs. 2(c) – 3(c)) [8].

For Si-MOS structure, the variation of C-V characteristics is very small. For SiC-MOS, the changes are significant. This is caused by the greater concentration of charges in the oxide and at the oxide-semiconductor interface and by the larger band gap of SiC (2.39eV for 3C polytype) in comparison with Si (1.12eV). Thus, it can be stated that the structure defects are important only for SiC-MOS structure.

4.2. Operating temperature range

In order to determine the operating temperature range for the real Si-MOS and SiC-MOS structures, an inert environment was considered. Thus, the only parameter that was varied during simulations was the temperature of the structure.

4.2.1. Si-MOS

The Si-MOS structure was simulated in the temperature range of 300-500K. The C-V characteristics are illustrated in Fig. 4.

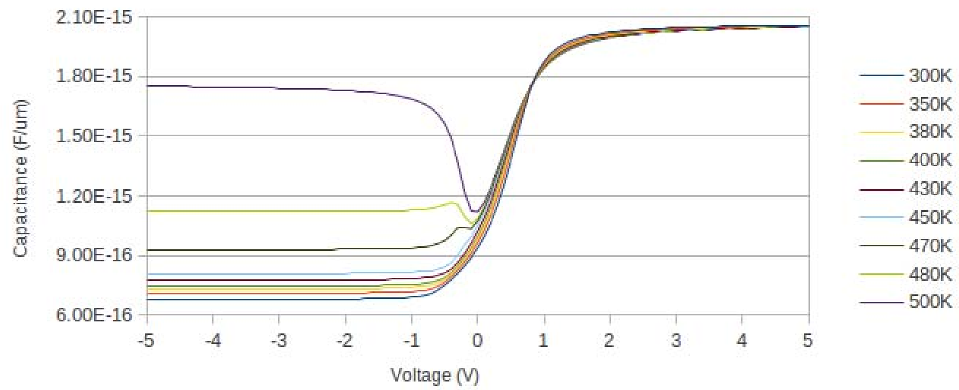

Fig. 4. Si-MOS structure's C-V characteristics in the 300..500K temperature range

It can be observed that the maximum operating temperature for the Si-MOS structure is 430K. Over this temperature, the C-V characteristics are distorted. As the temperature increases, the slope of the depletion region decreases and the inversion region's capacitance increases. These are caused by the enhancement of the electron's thermal energy, which produces an increase in the interface states charge and a reduction of the depletion region's width.

4.2.2. SiC-MOS

The SiC-MOS structure was simulated in the temperature range of 700-1300K. The C-V characteristics are illustrated in Fig. 5.

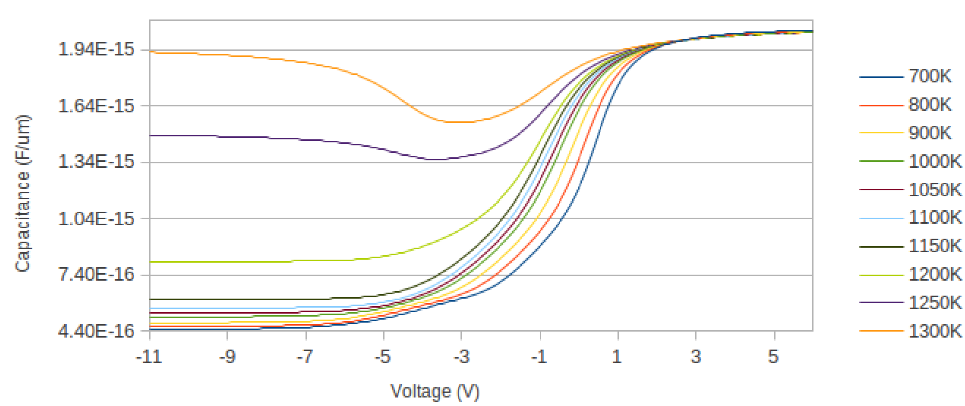

Fig. 5. SiC-MOS structure's C-V characteristics in the 700..1300K temperature range

It can be stated that the maximum operating temperature for the SiC-MOS structure is 1150K. Over this temperature, the C-V characteristics are distorted. As already shown for the Si-MOS, the increase of temperature causes a decrease in the depletion region's slope and an increase in the inversion region's capacitance. For SiC-MOS, it can also be observed that the C-V characteristic shifts towards the negative voltages. This is caused by the fact that the increased number of thermally generated electrons in the semiconductor reduces the structure's *flat-band* voltage. At 1300K, the inversion region's capacitance equals the accumulation region's capacitance. This signifies that in inversion conditions, the depletion region of the structure is eliminated.

4.3. Hydrogen environment

MEDICI does not offer the possibility to simulate different gas concentrations in the external environment. Thus, the magnitude of the metal work function's reduction and of the interface states' passivation in a hydrogen environment cannot be determined. The purpose of the study was only to analyze the effects of a hydrogen environment on the MOS capacitor's C-V characteristic, not to determine their magnitude.

4.3.1. Si-MOS

As shown before, the maximum operating temperature of the Si-MOS structure is 430K. When the sensor is introduced in a hydrogen environment, the metal work function is reduced and the C-V characteristic is shifted towards negative voltages. In this range of temperatures, there is no passivation of interface states [4].

In order to simulate different hydrogen concentrations, the metal work function (WF) was varied between 5.12eV, the value for Pd in inert environment, and 4.70eV, the value associated to the maximum concentration of hydrogen considered for this study. The simulations were performed at different temperatures in the 300-430K range. A fixed oxide charge of 1.82×10^{10} cm^{-2} and an interface states charge of 10^{10} cm^{-2}/eV were employed [6].

The C-V characteristics of the Si-MOS structure in a hydrogen environment, at different temperatures, are illustrated in Figs. 6-8. It can be observed that as the hydrogen concentration increases, the metal work function decreases and the C-V characteristic shifts to the left. Also, when the temperature increases the slope of the depletion region diminishes. This phenomenon was explained in 4.2.1. The voltage shifts are similar for all operating temperatures. This signifies that the temperature does not influence the sensor's response when considering the same hydrogen absorption (WF=5.12..4.70eV).

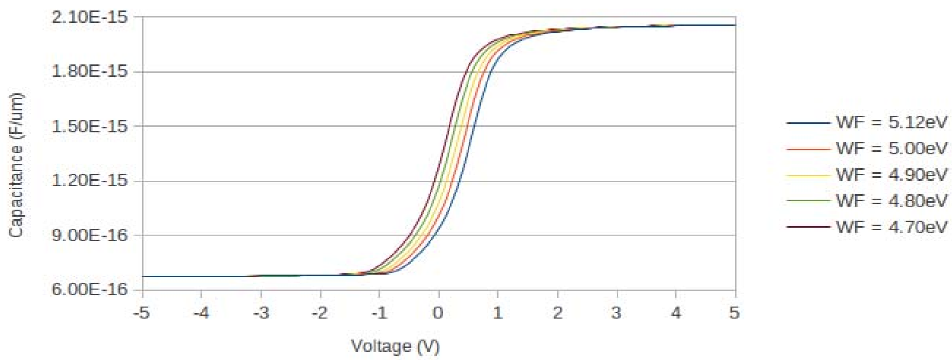

Fig. 6. Si-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 300K

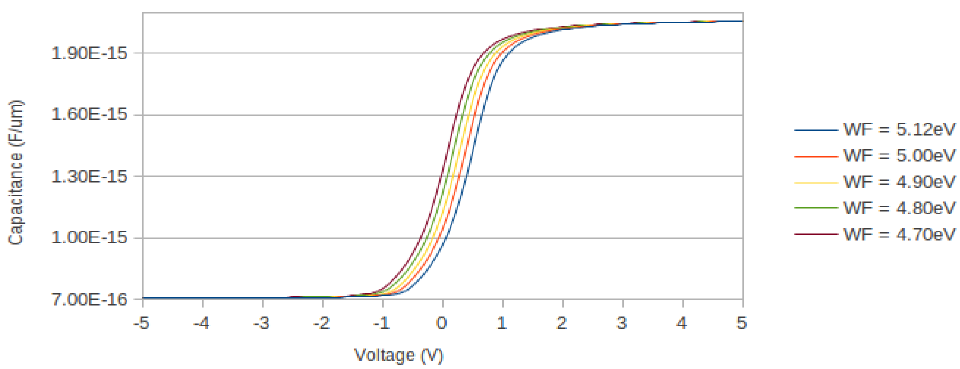

Fig. 7. Si-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 350K

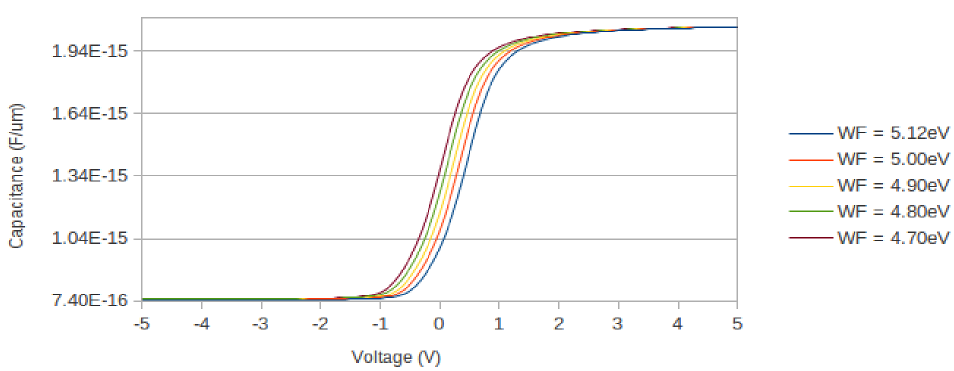

Fig. 8. Si-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 400K

4.3.2. SiC-MOS

The SiC-MOS structure has a maximum operating temperature of 1150K. When the sensor is introduced in a hydrogen environment, the metal work function is reduced and the C-V characteristic shifts towards negative voltages. At temperatures over 700K, the interface states are passivated [4]. The passivation process diminishes the charge density at the oxide-semiconductor interface, reducing the transition from accumulation to inversion for the SiC-MOS structure.

To account for different hydrogen concentrations, the metal work function (WF) was varied between 5.12eV and 4.70eV, as in the Si-MOS case. Also, the interface states charge (ICF) was modified from 10^{12} cm^{-2}/eV to 6 x 10^{10} cm^{-2}/eV. The simulations were performed in the temperature range of 700-1050K, where the passivation process takes place. An oxide charge of 10^{12} cm^{-2} was used [7].

The C-V characteristics of the SiC-MOS structure in a hydrogen environment, at different temperatures, are illustrated in Figs. 9-11.

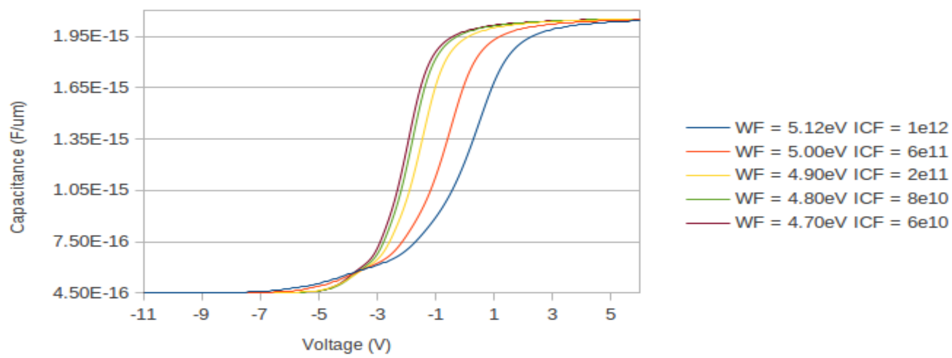

Fig. 9. SiC-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 700K

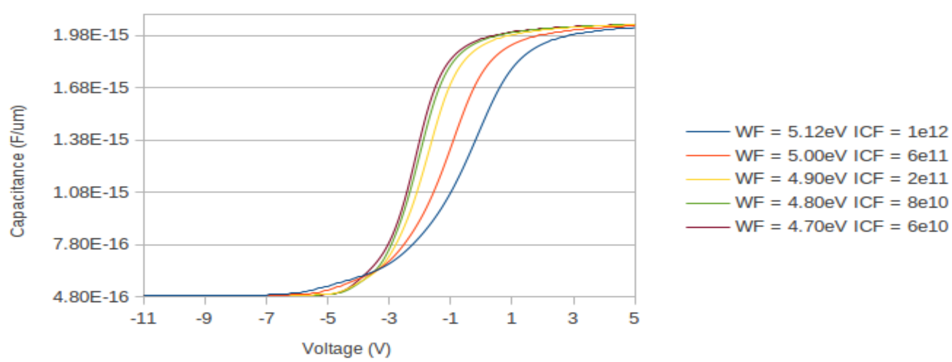

Fig. 10. SiC-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 900K

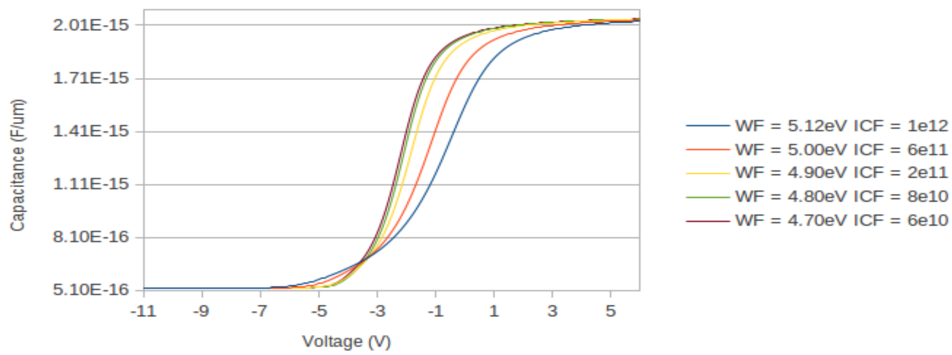

Fig. 11. SiC-MOS structure's C-V characteristics in a hydrogen environment with different gas concentrations, at a temperature of 1000K

As the hydrogen concentration increases, the metal work function decreases and the C-V characteristic shifts towards negative voltages. The interface states concentration decreases too, increasing the slope of the transition from accumulation to inversion. Also, when the temperature increases, the variation of the C-V characteristic with hydrogen concentration diminishes. As seen in 4.3.1. for the Si-MOS structure, the temperature does not influence the parallel voltage shift of the C-V curve. Thus, it can be stated that when the temperature increases, only the variation of the C-V characteristic with interface states concentration is reduced.

5. Conclusions

A MOS capacitor structure used as hydrogen sensor was simulated extensively. Both Si and SiC were employed for the semiconductor layer. The influence of the fixed oxide charge and of the interface states charge on the structure's C-V characteristic was analyzed. Also, the structure's maximum operating temperature and the influence of a hydrogen environment on the C-V characteristic were investigated.

Results showed that the fixed oxide charge and the interface states charge have a larger impact on the SiC-MOS structure. Also, the voltage interval needed to pass the SiC-MOS capacitor from accumulation to inversion is larger than the one for Si-MOS. These results are caused by the greater number of defects at the SiO_2-SiC interface.

The performed simulations also showed that the Si-MOS structure can operate at temperatures up to 430K. In this temperature range, the only effect of hydrogen is a parallel voltage shift of the C-V characteristic. The SiC-MOS structure has a maximum operating temperature of 1150K. Over 700K, an additional effect is observed: an increase in the C-V characteristic's depletion region slope.

The gap between the maximum operating temperatures of Si-MOS and SiC-MOS is caused by the difference between the band gaps of Si (1.12eV) and SiC (2.39 for 3C polytype). Following the obtained results it can be stated that the SiC-MOS structure is suited for hydrogen detection at high temperatures up to 1150K. Due to a reduced concentration of interface states, the Si-MOS structure's C-V characteristic showed a smaller variation with temperature. This offers a better stability for the hydrogen sensor. Thus, the Si-MOS structure is preferred as a hydrogen sensor at temperatures up to 430K.

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