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Investigation of Leakage Current in Micro M-I-M Structure Using Multilayer High-K Dielectric Materials with COMSOL Multiphysics

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***Abstract*—Micro Metal-Insulator-Metal (M-I-M) capacitor structures are well-known passive components that have been broadly used in integrated circuits, Radio Frequency (RF) decoupling, Micro Electro Mechanical Systems (MEMS) sensors, and health monitoring systems. Thanks to its small dimensions, it can be easily integrated into microelectronics. With the acceleration of the scalling dawn of integrated circuits and systems, the size of the capacitor and other components must be reduced. It has become challenging to fabricate a micro M-I-M capacitor with low leakage current and high-capacity density since the leakage current and depletion effect are reported as the main factors of the gradual loss of electrical energy in the micro-M-I-M capacitor. Thus, minimizing the leakage current and the depletion effect became a new research trend. This paper presents a penta-layer high-K dielectric between the electrodes to reduce the leakage current in the micro-M-I-M capacitor. For this purpose, various dielectric materials were investigated. It was found that niobium pentaoxide (Nb_2O_5) and hafnium dioxide (HfO_2) as penta-layer dielectric materials provide the lowest leakage current between the two electrodes. The recorded values of leakage current density are reduced to a mere 0.95 µAmps/mm^2 from several µAmps/mm^2 at the operating voltage of 1 V. The reported micro-M-I-M capacitor has potential application as an energy storage device.**

***Index Terms*—Energy storage; High-K dielectrics; Leakage current; MEMS; Metal-insulator-metal.**

I. INTRODUCTION

In recent years, the micro Metal-Insulator-Metal (M-I-M) capacitor has gained commercial and research considerations due to its tremendous utilization in the fabrication of digital and mixed analog devices. Due to its micro dimension, it can be easily integrated into microelectronics. In Radio Frequency (RF) circuits, micro M-I-M capacitors serve as filters, oscillators, and tuning elements. For example, the M-I-M filter is used with a half-wave or full-wave rectifier to eliminate ripple [1]–[3].

Similarly, in the field of medicine, the conventional health monitoring service, which is time-consuming, can be replaced by a convenient and handy wearable health monitoring system [4], [5]. A flexible capacitor-based sensor is a crucial device to detect strain and pressure [6]. Moreover, in Complementary Metal Oxides Semiconductor (CMOS) technology, micro M-I-M capacitors with low leakage current are considered the fundamental block in producing various integrated circuit devices [7], [8]. They are also used to fabricate different energy harvesting and mixed analog devices due to their low electrode resistivity [9]. Moreover, dielectric capacitors are currently the best energy storage (ES) devices since they have the highest power density and the longest lifetime [10], [11]. A micro M-I-M capacitor is a passive two-terminal component made up of two conducting parallel plates separated by a dielectric insulating substance. High dielectric (K) insulators have been extensively investigated as dielectrics for storage, flash memory, Metal-Oxide-Semiconductor Field-Effect Transistor (MOSFET), and dynamic random access memory, as well as as a channel for Oxide Thin Film Transistor (oxide-TFT) [12].

Hafnium dioxide (HfO_2), niobium pentoxide (Nb_2O_5), and zinc oxide (ZnO) are some of the high-K dielectrics that have attracted much attention in micro M-I-M structures to obtain large storage cell capacitance because they provide strong electric breakdown strength and extremely low leakage current [10]–[13]. However, as the size of the

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devices shrinks, achieving these properties becomes more challenging. Due to the small dimension, the structure of the device also causes additional problems such as doping [14]. However, the effects of fundamental forces are reduced [15]. The variation in fundamental forces for the scaling factor is illustrated in Fig. 1.

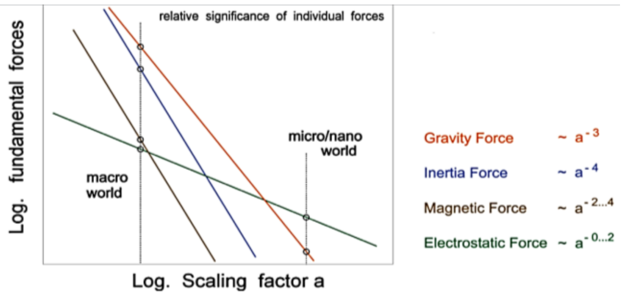


Fig. 1. Variation in fundamental forces for the scaling factor, original figure from [16].

It can be concluded from Fig. 1 that as the size of the devices decreases (Log. Scaling factor an on the x-axis), the acting forces, i.e., gravity, inertia, and magnetic (fundamental forces of the y-axis), become negligible while the electrostatic force, which is used in capacitor principle, remains dominant; therefore, mechanical strength and lifetime increased [17], [18].

II. RELATED WORKS

Previously, in the Very Large-Scale Integration (VLSI) technology, the capacitive structure was based on polysilicon insulator polysilicon (PIP). The depletion effect was found using silicone as a substrate and polysilicon as an electrode that gives an undesirable dependence of capacitance on voltage [19]. Metal electrodes are recommended for micro M-I-M capacitors to acquire a high-quality factor and a negligible depletion effect [20]. Thin films of silicon dioxide (SiO_2) possessing good dielectric properties deposited by the Plasma Enhanced Chemical Vapor Deposition (PECVD) are preferred due to their low temperature deposition [21]. However, traditional dielectrics, such as silicon nitride (Si_3N_4) and silicon dioxide (SiO_2)-based micro capacitors, possess a low capacitance density [22], [23]. The thickness of the dielectric material can be reduced to optimize the capacitance density. Furthermore, the leakage current can also increase to a value that makes it essential to replace the oxides or nitrides of a silicon-based micro capacitor with a high-K dielectric material [24]. Zirconium dioxide (ZrO_2) is utilized as a dielectric material for flexible and transparent capacitors that provides a good quality factor of 82 [25]. At the same time, ZnO is preferred as a dielectric material due to its high stability and reliability under ambient conditions [26]. In this research work, a conventional single-layer dielectric M-I-M capacitor has been replaced and compared with a penta-layer dielectric material to reduce the leakage current.

In a capacitor, the electrical energy stored between the parallel conducting electrodes depends on the capacitance of the capacitor when connected to an external DC source [27]. Second-order polynomials used to estimate the capacitor dependence on voltage are shown in (1)

$$C(V)/C_0 = \alpha V^2 + \beta V + 1. \tag{1}$$

C_0 and $C(V)$ are the capacitance measured at zero bias and V bias, while α and β are two appropriate parameters known as the quadratic and linear coefficients of the capacitance. As a result of the existence of impurities and imperfections in materials, dielectrics are not ideal insulators, allowing a small current to pass between the two conducting electrodes. The leakage current is a critical drawback that suffers the holding capability of the micro M-I-M capacitor [28]. It wrecks the dielectric insulation between the plates and causes energy loss. The relation of leakage current is shown in (2)

$$I_e = V/R, \tag{2}$$

where the leakage current is denoted by I_e due to resistance R and applied voltage V. In various studies, leakage current was revealed to be caused by a variety of conduction mechanisms, including Poole-Frenkel (P-F) emission, trap-assisting tunneling methods, and ionic conduction [27]. Thin film high-K dielectrics between the electrodes can reduce the leakage current [29]. Moreover, the leakage current density is an essential feature of a micro M-I-M capacitor and can be expressed using a modified Richardson-Schottky formula, as shown in (3)

$$J = \alpha T^{\frac{3}{2}} \mu E \left(\frac{m_e^*}{m_0}\right)^{\frac{3}{2}} e^{\left[\frac{-q\phi_B}{kT} + \frac{q}{kT}\sqrt{\frac{qE}{4\pi\varepsilon_0\varepsilon_r}}\right]}, \tag{3}$$

where α is the Richardson constant, μ denotes the mobility of electrons in dielectric materials, E is the strength of the electric field, m_e^* and m_0 are the effective mass and rest mass of the electron in dielectric materials, q is the charge of the electron, ϕ_B is the barrier height at the injection interface, k is the Boltzmann constant, T is the temperature, ε_0 and ε_r are the permittivity in a vacuum and the relatively permittivity of the dielectric. It is preferable to use high-K dielectric materials to reduce the leakage current density while enhancing the capacitance density [30].

In a micro M-I-M capacitor, the top and bottom electrodes are typically composed of the same material. In many investigations, researchers used various materials for either electrode. The electrode materials have a considerable impact on the performance of the micro M-I-M capacitor. In this research work, we have used Aluminum with a high working function of 4.2 eV metal electrodes that provide a smaller leakage current [31]. Although the dielectric material mainly determines the performance of a micro M-I-M. A single-layer dielectric insulating system with a breakdown effect is demonstrated in Fig. 2. Charges moving from the top to the bottom are trapped in the insulation layer with the applied voltage across the electrodes.

With an increase in applied voltage, the resistance of the insulating layer reduces rapidly. As a result, the leakage current increases, permanently destroying the insulation layer [32]. This effect can be minimized by replacing the single-layer insulation with the penta-layer high-K dielectric insulation. The multiple layers in the insulation provide additional resistance for the current as a result of the surface nonlinearity between the interfaces. Various investigations have been carried out to minimize the leakage current by increasing the thickness of the dielectric material, enhancing the deposition method, and utilizing different dielectric materials. However, increasing the dielectric thickness also decreases the capacitance, as shown in (4)

$$C = \varepsilon A / h, \tag{4}$$

where ε, A, and h denote permittivity (dielectric constant K), area, and thickness of the insulating material, respectively. Hence, the capacitance can be increased by increasing the area of conductive parallel plates, minimizing the thickness of the dielectric (distance), or using high permittivity (High-K) materials [33]. Leakage current and depletion effect are critical factors that affect the performance of micro M-I-M capacitors. This paper proposes an optimum penta-layer high-K dielectric structure with the metal electrode to minimize leakage current, high capacitance density, and low depletion effect. Moreover, a single-layer dielectric material is replaced by a penta-layer high-K dielectric material to provide many interface resistances in the flow of electric charges.

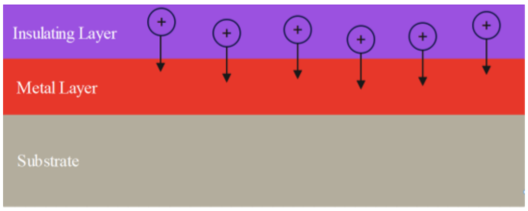


Fig. 2. Leakage current of a single-layer insulating system.

A. Single-Layer Insulating Structure

Figure 3 shows a model of a typical single-layer insulating system for a micro M-I-M capacitor, which comprises of two conducting metal plates insulated by a single-layer dielectric material. The top and bottom electrodes are made of aluminum and have a length (L) of 5 µm and a width (W) of 3 µm. The area is 5 µm × 3 µm, and the dielectric thickness is 150 nm.

Different materials, such as Nb_2O_5, HfO_2 and zinc oxide (ZnO), were used as a single-layer dielectric. The results demonstrate that single-layer insulation has a higher leakage current density than penta-layer insulation due to a single interface in the current flow.

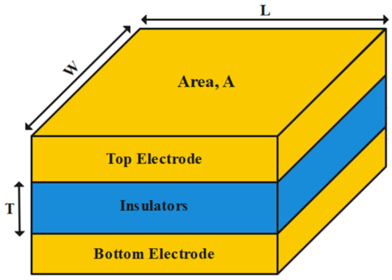


Fig. 3. Schematic of typical micro M-I-M capacitor with single-layer dielectric material sandwiched between metal plates with dimensions.

B. Proposed Penta-Layer Insulation Structure

This section introduces a penta-layer insulation structure for micro M-I-M structure, as shown in Fig. 4. A single-layer dielectric is replaced by a penta-layer dielectric structure. The length (L) of the device is 5 µm, and the width (W) is 3 µm. The thickness (T) of the dielectric layer is 150 nm.

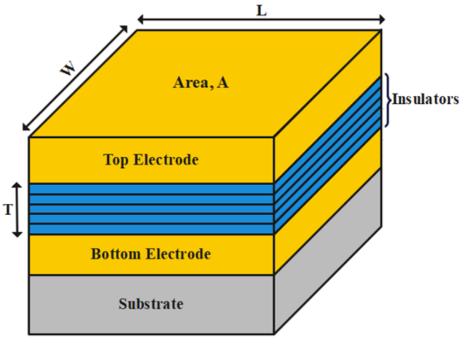
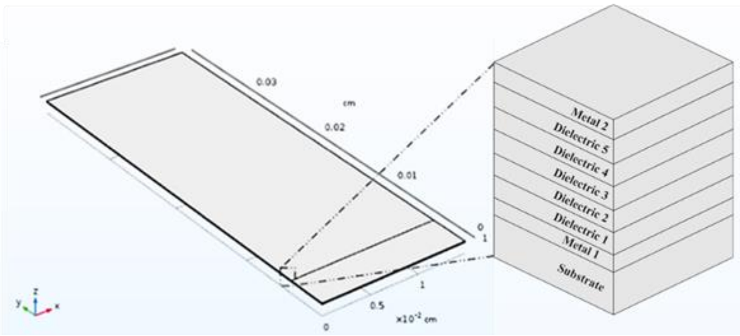


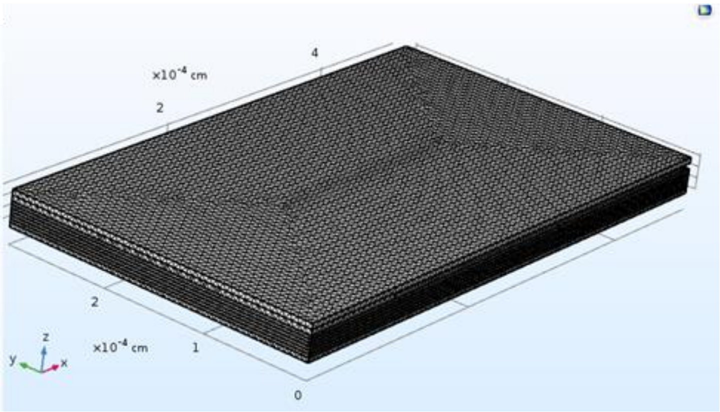
Fig. 4. Schematic of the proposed structure of the micro M-I-M capacitor with penta-layer of insulating material.

The proposed structure design in COMSOL Multiphysics is illustrated in Fig. 5(a). The dielectric materials are placed as insulation after the aluminum layer is designed as the bottom metal on a glass substrate. In the end, the top metal layer of aluminum is defined in COMSOL Multiphysics software. The electrical conductivity, thermal conductivity, relative permittivity, and surface roughness of the materials are assigned to individual layers of the M-I-M capacitor based on fabrication techniques. The surface roughness of HfO_2 is 2 nm when it is deposited at 175 °C by atomic layer deposition [34].

According to the practical result of the surface roughness of the materials, the meshing is performed. Meshing divided the entire structure into small fragments and was carried out via a built in mesh module.



(a)



(b)

Fig. 5. (a) M-I-M-capacitor designed in COMSOL Multiphysics with dimensions, i.e., Top metal (aluminum as an electrode) with area 5 µm × 3 µm, the thickness of 30 nm, Insulator (penta-layer) with each layer's area 5 µm × 3 µm and thickness of 30 nm, aluminum Bottom Metal; (b) Side view of Normal Mesh of the micro M-I-M capacitor.

In the mesh category, the element size can be selected from highly coarse to exceptionally fine quality to make the conclusion more perfect and precise depending upon the surface roughness requirement. The V-I characteristic curve is examined in the "Results" module. Normal meshing is applied to the structure after selecting the material to layers, as shown in Fig. 5(b). The AC/DC physics module is used to examine the leakage current vs. applied voltage trend. Multiple DC voltages are applied to the passive circuit using parametric sweep.

III. RESULTS AND DISCUSSION

Leakage currents measured throughout a DC bias voltage range of 0.1 V to 1 V for three different micro M-I-M capacitors are depicted in Fig. 6. A single-layer dielectric, such as HfO_2, Nb_2O_5, and ZnO, is used between the electrodes. At 1 V voltage, the highest leakage current for single-layer HfO_2 is 23.5 nAmps, for Nb_2O_5 - 9.24 nAmps, and for ZnO - 7.8 nAmps. The leakage current measured at the operating voltage (1 V in this example) is caused by trapped charges in the dielectric insulation layer. Because of a single interface, trapped charges can easily find the path from the top electrode to the bottom electrode, causing a high leakage current [34].

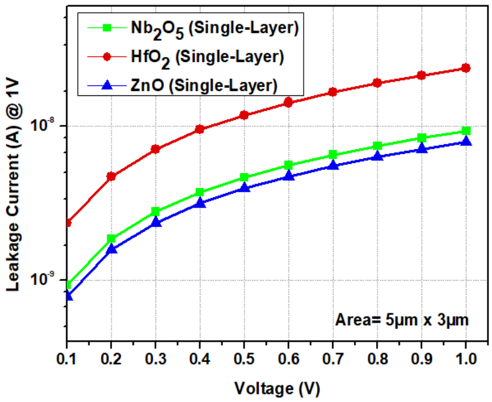


Fig. 6. V-I characteristic curve for typical single-layer dielectric system of micro M-I-M capacitor.

A renewed penta-layer high-K insulating system is proposed to reduce the leakage current. In the proposed method, a single-layer dielectric is replaced by a penta-layer while the overall thickness of the insulation layer remains same. The penta-layer arrangement provides multiple interfaces between the electrodes. Each layer is 30 nm thick and was formed at different temperatures, resulting in variations in surface roughness, decreased electrical discharge, and good mechanical strength. The change in surface roughness effectively blocks the passage of trap charges [36]. The meshing of the structure is done according to the surface roughness specified in [35]. Another reason to use HfO_2 and Nb_2O_5 is the high capacitance density and low leakage current. Furthermore, both have high relative permittivity values of around 25 and 40, respectively, making the insulation layer a very good insulator compared to silicon dioxide (SiO_2) previously used [36].

The improved structure of the high-K penta-insulating layer system is analyzed and tested successfully. The leakage current is minimized without decreasing the capacitance of the micro M-I-M capacitor. The V-I characteristic curve of the high-K insulating material of the penta-layer is demonstrated in Fig. 7. The observed leakage current through the penta-layer insulating system for Nb_2O_5 is 0.07 nAmp, while for HfO_2, it is 0.61 nAmp, and for the ZnO penta-layer insulating system, 9 nAmp is measured at an operating voltage of 1 V.

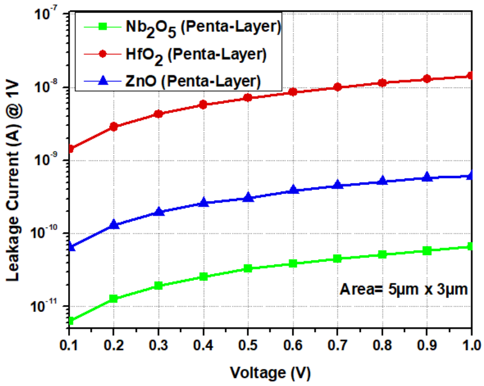


Fig. 7. Leakage current vs. voltage measurements of micro M-I-M capacitor for the proposed penta-layer insulator system for different dielectric materials.

In the literature, similar M-I-M-based structures were fabricated for multiple applications, such as in [37], two types of M-I-M capacitors with $ZrO_2/Al_2O_3/ZrO_2$ and $ZrO_2/Al_2O_3/TiO_2$ as insulation layer were examined. A leakage current density of 0.5 µAmps/mm^2 was reported in

[37] at 1 V. Leakage current is regulated through the thickness of the oxides, making the method process costly and complicated. Furthermore, in [38], Al_2O_3-based M-I-M was studied for a secondary power application. The current density of 10 µAmps/mm^2 was measured. Similarly, Kim, Bae, and Kim [39] proposed an AlO_x-based M-I-M capacitor. A leakage current density of 10 µAmps/mm^2 was reported at an operating voltage of 23.8 V [39].

Compared to recent research, our proposed penta-layer high-K dielectric-based M-I-M capacitors provide a satisfactory low leakage current density of 40 nA/mm^2, 46 nA/mm^2, and 0.93 µA/mm^2 at operating voltage of 1 V using Nb_2O_5, ZnO, and HfO_2, respectively. The dialectric penta-layer provides multiple interfaces that act as a barricade for trap charges, preventing them from reaching the bottom electrode and increasing the dielectric strength of the dielectric layer as the materials were deposited using the PECVD technique, which is the most popular and quickest method of deposition. It is inexpensive, can be performed at low temperatures (60 °C to 300 °C), and provides reasonable thickness control compared to atomic layer deposition (ALD).

The leakage current density is significantly reduced to 4.6 nA/mm^2 (35 % to 60 %) using penta-layer high-K dielectric materials compared to previous studies. Our proposed multilayer high-K dielectric structure can be broadly used as an energy storage device and integrated into integrated circuits. A brief comparison is shown in Table I.

In future work, the energy density of the M-I-M capacitor may be investigated for composite penta-layer high-K materials. In addition, the influence of the residual stress of the material on the electrical and mechanical characteristics of the M-I-M capacitor can also be studied for micromirror applications and secondary power supply.

TABLE I. COMPARISON OF LEAKAGE CURRENT WITH RELATED RESEARCH WORKS.

Materials	**Dielectric Deposition Method**	**Leakage Current at 1 V**	**Leakage Current density at 1 V**	**Active Area**	**Reference**
Nb_2O_5	PECVD	0.07 nAmps	4.6nAmps/mm^2	5 um × 3 um	Proposed Work
ZnO	PECVD	0.61 nAmps	40 nAmps/mm^2		
HfO_2	PECVD	9 nAmps	6 µAmps/mm^2		
Polyethylene naphthalate (PEN)-Substrate	PECVD	3500 µAmps at 90 V	3.5 µAmps/mm^2 at 90 V	10 cm × 10 cm	Amirzada [18]
SiO_2 and Si_3N_4 Insulation Layer					
Al-Electrodes					
Glass-Substrate	PECVD	1800 µAmps at 40 V	1.8 µAmps/mm^2 at 40 V	10 cm × 10 cm	Amirzada [18]
SiO_2 & Si_3N_4 Insulation Layer					
Al-Electrodes					
TiN-Electrode	Atomic layer Deposition (ALD)	Not given	0.5 µAmps/mm^2 at 1 V	Not given	Cha *et al.* [37]
$ZrO_2/Al_2O_3/ZrO_2$ Insulation Layer					
Silicon Substrate	Atomic layer Deposition (ALD)	Not given	10 µAmps/mm^2 at 23.8 V	10 mm × 10 mm	Mu, Chou, Ma, He, and Xiong [38]
Al_2O_3 Insulation Layer					
W/TiN-Electrode					
Glass-Substrate	Atomic layer Deposition (ALD)	1 µAmps at 1 V	1 µAmps/mm^2 at 1 V	1 mm × 1 mm	Kim, Bae, and Kim [39]
AlO_x Insulation Layer					
Al-Electrodes					

IV. CONCLUSIONS

The authors of this paper modeled and tested the optimum structure of penta-layer high-K dielectric materials for micro M-I-M capacitor using the COMSOL Multiphysics finite element method (FEM) numerical method. High-K dielectric materials are used to enhance the capacitance density. The leakage current is minimized by about 35 % to 60 % using penta-layer high-K dielectric materials compared to single-layer structure. The penta-layer high-K dielectric system has high resistance to electric charge passage. Finally, a high-K dielectric such as Nb_2O_5 is recommended to achieve a low leakage current density of 4.6 nAmps/mm^2 at a 1 V operating voltage.

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CONFLICTS OF INTEREST

The authors declare that they have no conflicts of interest to report regarding the present study.

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