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Simulating the Barrier Heights Impact on the Performance of Dissimilar Electrodes Metal-Insulator-Metal Diode

***Abstract**. Metal-insulator-metal (MIM) tunnel diodes are desirable for applications including ultra-high frequency rectenna detectors, solar cells, and mixers due to their femtosecond-fast transmission. These applications place strict demands on the current-voltage I(V) properties of diodes. In this paper, a single insulator tunnel diode is simulated using SILVACO ATLAS software to correlate the importance of insulator interfacial stability to MIM rectification performance, which helped to analyse and develop MIM diodes with the desired properties. By keeping the Al_2O_3 insulator layer, different metals were used as electrodes of the MIM diode to achieve the desired asymmetry. Two schemes of electrode asymmetry were proposed, the first scheme is based on using a metal that produces a constant barrier height at one side of the insulator layer and different barrier heights at the other by using different metals. The second structure implicates using different metals at the sides of the insulator to achieve different barrier heights but with constant barrier differences between the metals. A voltage range of ±0.4 V was used to study electrical characteristics. It is found that the MIM structure with fixed barrier height at cathode side produces a good asymmetry with poor nonlinearity, while the results of fixed barrier height at anode side reveals that the figure of merit (FOM) strongly depends on the work function difference of the metals of the MIM structure. For the constant barrier differences, it is found that the smaller the barrier height the larger the current response produced and the lower the turn on voltage. The impact of insulator thickness on the diode FOM shows that the lowest thickness produces the highest asymmetry and nonlinearity.*

***Streszczenie.** Diody tunelowe typu metal-izolator-metal (MIM) są pożądane w zastosowaniach, w tym w detektorach prostokątnych ultrawysokiej częstotliwości, ogniwach słonecznych i mikserach ze względu na ich szybką transmisję femtosekundową. Te zastosowania nakładają surowe wymagania na właściwości prądowo-napięciowe I(V) diod. Przeprowadziliśmy symulację pojedynczej diody tunelowej izolatora za pomocą oprogramowania SILVACO ATLAS, aby skorelować znaczenie stabilności międzyfazowej izolatora z wydajnością prostowania MIM, co pomogło nam przeanalizować i opracować diody MIM o pożądanych właściwościach. Zachowując warstwę izolatora Al_2O_3, zastosowano różne metale jako elektrody diody MIM w celu uzyskania asymetrii elektrody. Zaproponowano dwa schematy asymetrii elektrod, pierwszy schemat opiera się na zastosowaniu metalu, który wytwarza stałą wysokość bariery po jednej stronie warstwy izolatora i różne wysokości bariery po drugiej, przy użyciu różnych metali. Druga struktura implikuje użycie różnych metali po bokach izolatora w celu uzyskania różnych wysokości bariery, ale przy stałych różnicach bariery między metalami. Do badania charakterystyk elektrycznych wykorzystano zakres napięcia ±0,4 V. Stwierdzono, że struktura MIM ze stałą wysokością bariery po stronie katody daje dobrą asymetrię ze słabą nieliniowością, podczas gdy wyniki ze stałą wysokością bariery po stronie anody pokazują, że liczba zasług (FOM) jest silnie zależna od różnicy pracy wyjścia posiłki struktury MIM. Stwierdzono, że dla stałych różnic barierowych im mniejsza wysokość bariery, tym większa odpowiedź prądowa i niższe napięcie włączenia. Wpływ grubości izolatora na diodę FOM pokazuje, że najmniejsza grubość izolatora powoduje największą asymetrię i nieliniowość. (**Symulacja wpływu wysokości bariery na działanie różnych elektrod Metal-izolator-metalowa dioda**)*

Keywords: MIM diode, tunnelling, electrode asymmetry, SILVACO ATLAS.
Słowa kluczowe: Dioda MIM, tunelowanie, asymetria elektrod, SILVACO ATLAS.

Introduction

An electron can undergo quantum mechanical tunneling when its kinetic energy is exceeded by a potential barrier. in recent years this cycle was habitually utilized in various types of gadgets from a passage diode to an examining magnifying lens, and it has been widely contemplated both tentatively and hypothetically for nearly 100 years [1,2]. Still, new boundary nanostructures with various materials and tunneling related peculiarities are continually being researched. In a layered nanostructure, a straightforward tunnel junction consists of a thin insulating barrier between two conducting electrodes [3]. In the cutting-edge mechanical period, semiconductor electronic gadgets have turned into a critical establishment in the development and organization of canny framework operating at rapid and high frequency. The development of this nano semiconductor field is a direct result of enormous efforts made simultaneously in a variety of fields. New device structure concepts and functionalities, as well as their physical aspect and interactions with electrons, photons, and phonons in low-dimensional systems, and impressive progress in experimental setup and spectroscopic systems, are among these [4].

The advances in this field are owed a lot to the original work of Esaki and Tsu who investigated novel quantum structures as they designed the bandgap devices by stacking layers of various semiconductors [5,6]. Thus, noticeable impacts of quantum wells and the development of superlattice semiconductors began flourishing during the 1980s [7]. The most important hypotheses regarding the physics of electrons in semiconductor heterostructures were established at that time. This was the groundwork for laying out the vital idea of quantum restriction in semiconductor gadgets.

Tunnel diodes are fabricated in a similar way to the other semiconductor diodes used for rectification, mixing, switching, parametric amplification, and voltage reference in that it has a p-n junction with electrodes attached to each region. In each of the latter situations, the p-n junction geometry and the physical features of the semiconductor material are controlled in order to maximize the diode characteristics for a specific application. The p-n junction of the tunnel diode, called PIN, must have two properties in order to function properly: it must be narrow (i.e., the charge transition from n-type to p-type regions must be abrupt), and both of its regions must be degenerated. Metal-Insulator-Metal diodes (MIM) are a type of tunnelling diodes. MIM diode is a nano-electronic device that consists of two metal contacts and a thin layer of insulating. Although the interest in Metal-Insulator-Metal (MIM) devices started about 50 years ago [8-9], however, in the last few years they attracted the attention again due to their use in many applications such as the rectifying antenna-coupled diodes (rectennas), infrared /terahertz detectors [10-11] and resistive random access memory (RRAM) [12-13]. Since the MIM structure is very simple and can be fabricated at low temperature, the researchers focused their attention to use this device in the area of microelectronics [14-15]. The characteristics of the MIM diode depend greatly on the choice of metals, insulator materials and insulator thickness. The thickness of the insulator should be kept below 10 nm to keep the tunneling current as the main transport mechanism in a MIM diode current conduction processes [15]. The work function difference between the electrodes ($\Delta\varphi_m$), the barrier heights at both metal-insulator interface, and the process of charge transport through the insulator all serve to limit the rectification performance in MIM diodes. The insulator barrier's barrier heights on both sides are affected by whether the metals on the two sides are similar or dissimilar [16-17], and this feature is accomplished by utilizing different metals. The barrier heights are defined as the difference between the work function of the metal and the insulator's electron affinity at metal-insulator interfaces. There will be two different potential barrier values between metal one and the insulator, as well as between metal two and the insulator if just one insulator is employed. These two interfaces affect the forward-to-reverse current ratio (asymmetry) or a sharp turn-on (nonlinearity) depending on the work functions of the metals.

According to the experimental study by P. Periasamy et al. [18], they found that a low barrier height, which has the work function of one of the metals and the insulator's electron affinity value should be close to each other, results in a MIM device with the necessary maximal asymmetry and nonlinearity rectification properties while minimizing turn-on voltage. The MIM diode performances can be improved by increasing nonlinearity. Moreover, a significant tunneling current asymmetries allows for non-biasing detection of incident waves . Using different electrodes is a common strategy for achieving strong nonlinear and asymmetric currents on MIM diodes. In the present work, MIM diode simulated to investigate the impact of the asymmetric barrier formation between the metals at both sides of the MIM structure on the diode performance characteristics. The study involves two structures to achieve the asymmetry between the metals at both sides of the insulator; the first one comprises using a constant barrier height at one side of the insulator layer while the second structure implicates using different metals at the both sides of the insulator to achieve different barrier heights but with constant barrier differences between the metals.

Simulation Parameters

The MIM diode was simulated using Silvaco TCAD software with different structures at standard conditions to investigate the impact of barrier height on the electrical properties of the MIM diode. The first structure involved setting a fixed insulator material and a metal of one side (cathode) of the MIM structure. Aluminum oxide (Al_2O_3) with electron affinity of 1.35 eV was used as an insulator layer. The thickness of this layer was fixed at 2 nm. To achieve the electrodes dissimilarity one metal (aluminum with work function of 4.26 eV) was used as reference cathode on left side of the MIM structure. This metal will produce a constant barrier height with an insulator with φ_C=2.91 eV. At the right side of the MIM structure, different metals were employed individually as anodes with diverse work functions. These metals are Cd, Ag, Co, Au, and Pt with work function 4.08, 4.65, 5.0, 5.31, and 5.65 eV, respectively.

The asymmetric barrier formation between the metals at the sides of the MIM structure allows tuning electrodes dissimilarity. Table 1 summarizes the parameters of aforementioned structures.

The second structure comprised setting a fixed same insulator material of the previous case and metal on one side (anode) of the MIM structure. In contrast, the metal on the other side (cathode) was individually changed to achieve the electrodes dissimilarity.

In this case, Ni with work function of 5.22 eV was used as anode while the cathode materials were Ba, Ta, La, Zn, and Nb with work function of 2.52, 3, 3.5, 3.63, and 3.95 eV respectively. The Ni produce a constant barrier height with an insulator with φ_R=3.87 eV. Table 2 summarizes the parameters of the second structures.

Table 1. The structures of MIM diodes with fixed cathode metal [17,18]

Structures	φ_C eV	φ_A eV	$\Delta\varphi_m$ eV
Al- Al_2O_3-Cd	4.26	4.08	0.18
Al-Al_2O_3-Ag	4.26	4.65	0.39
Al- Al_2O_3-Co	4.26	5.0	0.74
Al- Al_2O_3-Au	4.26	5.31	1.05
Al- Al_2O_3-Pt	4.26	5.65	1.39

Table 2. The structures of MIM diodes with fixed anode metal [17, 18]

Structures	φ_C eV	φ_A eV	$\Delta\varphi_m$ eV
Ba- Al_2O_3-Ni	2.52	5.22	2.7
Ta- Al_2O_3-Ni	3.0	5.22	2.22
La- Al_2O_3-Ni	3.5	5.22	1.72
Zn- Al_2O_3-Ni	3.63	5.22	1. 59
Nb- Al_2O_3-Ni	3.95	5.22	1.27

The third structure included setting a fixed same insulator material of the previous cases and a constant $\Delta\varphi$ between the metals on both sides of the MIM structure but with different barrier height. In this case the individual metal pairs were used at the both side of the Al_2O_3 insulator material are (Ba and Ag), (Ta and Cu), (La and Pt), (Zn and Ir), and (Nb and Pt). These metals provide a constant barrier potential $\Delta\varphi_m$=2.1 eV with different barrier height. Table 3 summarized the parameters of the third structures.
To optimize the figure of the merit of the MIM device, the last structure was used. This structure involved the impact of the insulator thickness on the MIM diode figure of merit. A voltage range of ±0.4 was used to study the electrical characteristics for all the structures.

Table 3. The structures of MIM diodes with constant barrier potential [17,18]

Structures	φ_C eV	φ_A eV	$\Delta\varphi_m$ eV
Ba- Al_2O_3-Ag	2.5	4.6	2.1
Ta-Al_2O_3-Cu	3.0	5.1	2.1
La- Al_2O_3-Pt	3.5	5.6	2.1
Zn- Al_2O_3-Ir	3.6	5.7	2.1
Nb- Al_2O_3-Pt	3.9	5.99	2.1

Results and Discussion

The main goal of the present research is to determine how the performance of MIM rectification is affected by the electrodes' dissimilarity, barriers' heights, and insulators' thicknesses. Asymmetry (f_{ASYM}), non-linearity (fNL), and turn-on voltage (TOV) are specific figures of merit (FOMs) that describe the rectification performance. These parameters can be extracted from the DC current-voltage curves.

3.1 Influence of using dissimilar electrodes:

Fig. 1 presents a set of I-V curves for the structures that produce electrode dissimilarity with a fixed cathode metal and different anode metals. The electrodes dissimilarity varied from 0.18 eV to 1.39 eV as illustrated in Table 1. Fig. 1 reveals the asymmetric in the diode current due to the asymmetry in the MIM potential. It can be seen that the change in the work function of the anode by using different metals does not produce a much difference in the tunneling current. This can be attributed to the fact that in the case of dissimilar metals, the current-voltage characteristics depend not only on the bias voltage but also on the polarity of the voltage. Conventionally, if the metal with the lower work function is positively biased and the metal with the higher work function is negatively biased, the MIM junction is said to be forward biased. When the lower work function metal is negatively biased it is reverse biased [19]. Fig. 1, also reveals that all the devices have a low turn-on voltage of around <0.1 V with a noteworthy asymmetric and non-linear response under positive bias, therefore, indicating that resonant tunneling is the predominant tunneling mechanism in this arrangement.

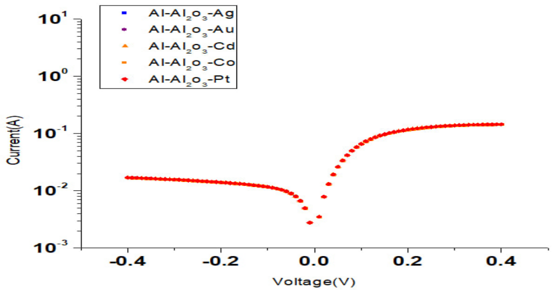


Fig.1. Current–voltage (I–V) curves for different MIM structures with electrodes dissimilar (fixed cathode)

Fig. 2 (a) and (b) show respectively the f_{ASYM} and f_{NL} FOMs for MIM structures that are summarized in table 1. These figures exhibit asymmetry and nonlinearity values of ~8 and ~1.5, respectively. It can be seen that the MIM structure with electrodes dissimilar and fixed cathode produce a good asymmetry with poor nonlinearity. Since the nonlinearity of the diode defines the sensitivity of the MIM diode, the sensitivity of the MIM structure with electrodes' dissimilarity under the condition shown in table 1 is weak.

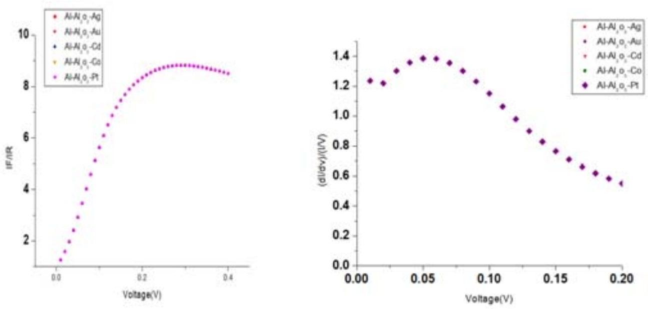


Fig.2. (a) Asymmetry (b) nonlinearity curves for different MIM structures with electrodes dissimilar (fixed cathode)

To study the impact of the barrier height variation from the cathode side on the MIM diode performance a dissimilar cathode and anode metal electrodes was simulated. Nickel was only chosen as the anode electrode and metals with different work function were chosen as the cathode electrode individually to achieve different values of electrodes asymmetric with diverse barrier potential from the anode side. Fig. 3 shows a set of I-V curves for the structures that are summarized in tables 2. At first glance, it seems that the I-V curve depends strongly on the work function difference of the meals of the MIM structure, i.e, $\Delta\varphi = (\varphi_C - \varphi_A)$, where the structures that have a large difference between the left and right work functions produce a large forward current with lower low turn-on voltage. It can be noticed in Fig. 4 that the forward current increases ~20 times when $\Delta\varphi$ increases from 1.27 to 2.7 eV while the reversed biased current is almost unaffected with $\Delta\varphi$ variation. By comparing these results with the results of the previous case it can be deduced that the MIM diode forward current is strongly dependent on the barrier height at the interface between the cathode and insulator. The Nb/Al_2O_3 and Al_2O_3/Ni interfaces have high barrier heights that limit meaningful electron transit until a bias voltage on the order of the barrier height is applied. Such bias voltage resulting an electric field across the insulator enough to breakdown the insulator as reported in [20].

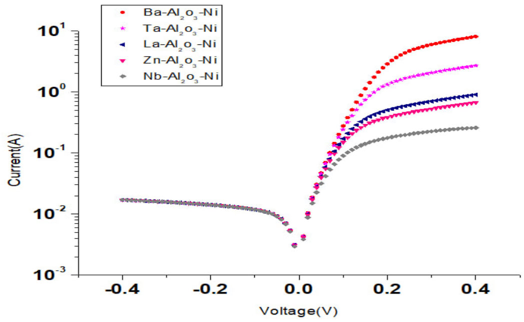
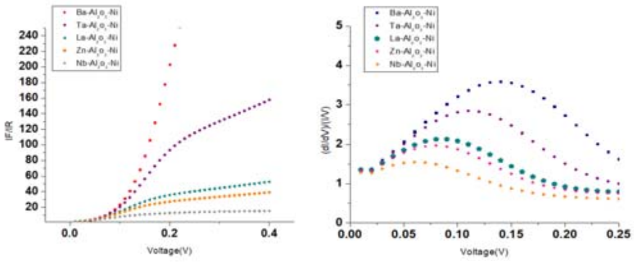


Fig.3. Current–voltage (I–V) curves for different MIM structures with dissimilar electrodes (fixed anode)

Figs. 4 (a) and (b) show, respectively the asymmetry and the non-linearity of the MIM diode structures that are given in Table 2. The Ba-Al_2O_3-Ni diode exhibits the maximum asymmetry and non-linearity.

These findings agree with the hypothesis that states the minimum turn-on voltage and maximum asymmetry and non-linearity are achieved when the electron affinity of the insulator would be close to one of the metal work function values so as to produce a low barrier height [21].



ig.4. (a) Asymmetry (b) nonlinearity curves for different MIM tructures with dissimilar electrodes (fixed anode).

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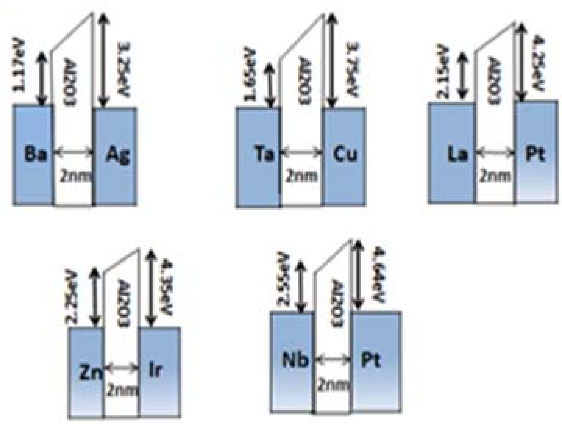


Fig.5. Energy band diagram for the structures in Table.3.

To investigate the impact of the barrier height variation on the MIM performance using Al_2O_3 as an insulator, different metals with constant work function differences $\Delta\varphi$ were chosen. The set of the chosen metals produces a work function difference of 2.1 eV. The used metals as cathode, individually, are Ba, Ta, La, Zn, and Nb that produce barrier heights of 1.15, 1.65, 2.15, 2.25, and 2.55 eV, respectively. At the same time, the corresponding anode metals are Ag, Cu, Pt, Ir, and Pt, producing barrier height from the anode interface side of 3.25, 3.75, 4.25, 4.35, and 4.64 eV respectively. Band diagrams of these MIM structures are shown in Fig. 5 and are based on the materials properties tabulated in Table 3.

Fig. 6 shows the I-V curves of the aforementioned MIM structures. Although these structures produce a fixed work function difference but Fig. 6 reveals that the I-V responses of the diodes is qualitatively related to the barrier height. The smaller the barrier height, the larger the current response and the lower the turn on voltage. This is can be explained by the fact that the electrodes' low energy barriers enable thermally activated conduction mechanisms such as Schottky emission (SE) to be effective at room temperature [22].

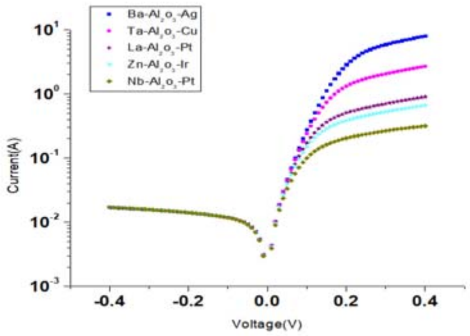


Fig.6. Current–voltage (I–V) curves for a set of the different metals that produces a difference barrier height and constant work function difference of 2.1 eV.

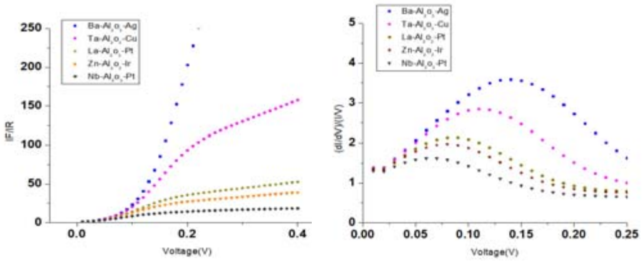


Fig.7. (a) Asymmetry (b) nonlinearity curves for a set of the different metals that produces a difference barrier height and constant work function difference of 2.1 eV.

Figs. 7 (a) and (b) show, respectively the asymmetry and the non-linearity of the MIM diode structures that are given in Table 3. The Ba-Al_2O_3-Ag diode which has a minimum barrier potential exhibits the maximum asymmetry and non-linearity. These results support the concept that a low barrier height is produced when the electron affinity of the insulator approaches one of the metal work function values, resulting highest levels of asymmetry and nonlinearity [21].

3.2 Influence of insulator thickness:

The physical properties of the insulator layer govern the performance of the MIM diode. Hence, the thickness of the insulator layer plays a vital role in controlling the characteristics of the I-V curves where the tunnelling probability affected by insulator thickness. Decreasing the thickness of the insulator layer makes higher tunnelling probability possible at lower voltages. The turn-on voltage can be close to zero volts in MIM diodes with a very thin insulator layer [23-24]. From the previous results, it can be seen that the Ba-Al_2O_3-Ag gives the highest levels of asymmetry and nonlinearity, so in this section, this structure is selected to study the impact of the thicknesses of the insulator layer on the MIM diode FOM. Simulations are launched from 1.0 nm insulator thickness to 3.0 nm insulator thickness with steps of 0.5 nm. The simulation results in Fig. 8 reveals that the increasing in the insulator thickness reduces the forward current, thus it can be noted that the asymmetrical in (I-V) curves decreases with the increase of the thickness. As shown in Fig. 9, the asymmetry reaches the peak at the lowest thickness and it is almost the same at 5 nm and 6 nm. The highest nonlinearity is reached the highest value at 1 nm.

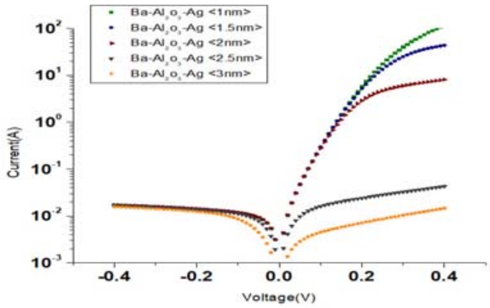
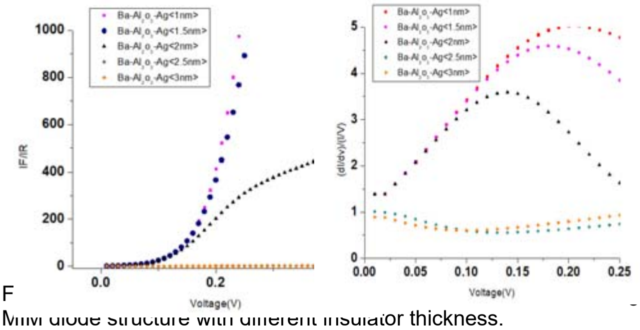


Fig.8. Current–voltage (I–V) curves for a set of Ba-Al_2O_3-Ag MIM diode structure with different insulator thickness.



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MIM diode structure with different insulator thickness.

Conclusion

The effect of tuning the barrier height of the metal-insulator interface of a MIM diode and insulator thickness was investigated using SILVCAO software as a possible technique to obtain a good figure of merit and decrease the diode resistance. The devices' I-V characterization revealed their capabilities as rectifiers in terms of asymmetry and non-linearity, which affected the devices' sensitivity. It is found that the tunneling current density does not significantly affected by barrier height at the anode-insulator interface, whilst the variation of the barrier height at cathode –insulator interface produces a significant impact on FOM. The large barrier height difference between the metals produces a large forward current with a lower low turn-on voltage. Our findings showed that the barrier height at the cathode-insulator interface has a significant impact on the MIM diode forward current. In addition to that, using a fixed work function difference between the metals at the sides of the insulator with varying barrier height is critical in determining MIM diode performance. The thickness of the insulator is a prominent additional factor that has a significant impact on the tunneling current. It was found the less thickness of the insulator produces a relatively high forward current with a noticeable increase in the asymmetric and nonlinearity propoerties.

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