A simulation study of multi-junction insulator tunnel diode for solar energy harvesting applications

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Abstract

There has been an ongoing demand of clean and inexpensive energy source for the sustainable growth of humanity. However, depletion of fossil fuels and fluctuation in oil prices have resulted in a global crisis for increasing the demand of clean and green energy. The world total energy consumption is currently higher than 55,235 TWh, and it grows at a rate of 2.5% annually. The increase in energy demand and decrease in energy supply signifies the urgent need to limit the dependency on fossil fuels and seek renewable sources of energy. The scientific communities and researchers are seeking alternative sources of renewable energy. Infrared (IR) energy harvesting is a promising contribution to sustainable energy demand. There is abundant IR energy available in the environment in the spectrum range from 2 to 11 μm (in wavelength), having maximum intensity at 10.6 μm (28.3 THz). The idea is to treat the waste heat as very high oscillating electromagnetic waves, which can be grabbed by a nanoantenna and further rectified by a diode into useful energy. This combination of nanoantenna and diode is known as ‘Rectenna system.’ Multilayer insulator diodes, which operate on the principle of electron tunneling, are one of the few candidates for such high-frequency operation. In this article, different combinations of the metal–insulator–insulator–metal (MII1I2M2) diode are studied for operation at high frequency (28.3 THz or 10.6 μm). The thickness of varying insulator layers with different dielectric constants is simulated and optimized to have the best resistor–capacitor time constant matching and an enhanced rectification. To the best of our knowledge, this is the first comprehensive and systematic study of the MII1I2M2 diode-based rectenna system for energy harvesting applications at 28.3 THz.

1. Introduction

Energy usage increases daily because of the high demands due to emerging technologies, industrial developments, and an increasing population. The Internet of things has increased the energy consumption of an individual by more than 50% in the last few decades [1, 2]. However, the production of clean and green energy to meet this growing demand is lagging, which has resulted in the scientific communities seeking alternative ways of producing low-cost biofriendly energy. So far, solar energy harvesting is a promising source for sustainable power generation. The traditional photovoltaic panels, which are available in the market, can mostly harvest energy from the visible spectrum (400–750 nm), leaving most of the infrared (IR) range unused. The IR energy is also available in the surroundings in the form of waste heat, which comes from metal heating, fluid heating, and steam generation. This IR energy fluctuates between the temperature range of 400 and 2,000 K, and wavelength varies in mid-IR from 2 to 11 μm, with the maximum intensity at 10.8 μm (28.3 THz) [3–5]. The idea is to treat the waste heat as high-frequency (THz) electromagnetic waves, which can be collected and rectified by a rectenna system (a combination of a nanoantenna and a diode) (figure 1).
When exposed to IR sources, antennas generate a strong electric field due to the highly localized surface plasmon at the arms of nanoantennas. [6]. Converting these localized THz waves to direct current (DC) signals is challenging but can be achieved with the help of a metal–single-insulator–metal (MIM) tunneling diode [7–10]. Researchers have demonstrated MIM diode-based rectenna systems. One of the significant issues in the previously reported works was the reduced efficiency of the rectenna systems, mainly due to the minimal nonlinearity of the MIM diode [6, 11, 12].

For rectenna applications, it is essential to have a diode with high nonlinearity, which can subsequently lead to higher rectification ability [13–15]. It is expected that higher nonlinearity can be achieved by incorporating multiple insulating layers between the metal arms, i.e., metal–insulator–insulator–metal (M1I1I2M2) diodes [16–19]. Hegyi et al [20] have shown that M1I1M2 devices could have better responsivities than the single insulator case. However, the study of M1I1I2M2 diodes is inadequate owing to nanoscale fabrication challenges [21, 22]. The experimental cost and overtaken effort can be reduced by simulating data for different types of insulators and proposing the potential candidates to the scientific community. Moreover, in the previously published works, the DC results were obtained by applying a bias to the rectenna system, which is not an ideal case for energy harvesting applications [23–28]. In this study, simulation results show that it is possible to realize a passive rectenna system using M1I1I2M2 diode by carefully selecting the metals and insulating layers. Additionally, a systematic simulation study on different types of M1I1I2M2 diodes to verify the superior performance of multi-insulating layer diodes over their single insulator counterparts is presented. Additionally, we have shown that the best resistor–capacitor (RC) time constant matching can be achieved by selecting the right combination of oxide thickness with a proper dielectric constant. Further, we study the various possible combinations of oxide materials and optimized thickness to obtain a high operating cutoff frequency. Moreover, we have shown that it is also possible to capture other wavelength ranges of the waste heat spectrum by carefully selecting the different oxide materials with the right thickness. To the best of our knowledge, this is the first demonstration of a systematic study of the M1I1I2M2 diode. The enhanced nonlinearity and high zero bias tunneling ability at 28.3 THz make the M1I1I2M2 diode a potential candidate for rectenna and energy harvesting applications over the single insulator-based rectenna system.

### 2. Theory of MIM and M1I1I2M2 tunnel diodes

The following parameters give the characteristics of tunnel diodes: (1) differential resistance of the diode, (2) diode responsivity, (3) nonlinearity of diode, and (4) diode cut off frequency. A differential or dynamic resistance ($R_d$) is obtained by differentiating the current ($I$) on the applied voltage ($V$). It is given by equation (1).

To have a proper impedance matching between diode and antenna, a low value of ($R_d$) is essential [29–31].

$$R_d = \frac{1}{\frac{dI}{dV}}$$  \hspace{1cm} (1)

The second parameter is the diode responsivity; the diode tunneling ability can be determined using this parameter. Diode responsivity can be expressed as follows:

$$\text{Responsivity} = \frac{1}{2} \left( \frac{d^2I}{dV^2} \right)$$ \hspace{1cm} (2)

Diode responsivity determines the alternating current (AC) to DC conversion capability of a diode. A high diode responsivity means a tremendous rectification ability for the diode [21].

![Figure 1. A schematic of a rectenna system consisting of an antenna and a rectifying diode. After rectification, the final output is the direct current, which is transferred to the load.](image)
The third parameter is diode nonlinearity, which can be defined through the nonlinear factor given by

\[
\text{Nonlinear factor} = \frac{I(V_{\text{read}})}{I\left(\frac{V_{\text{read}}}{2}\right)},
\]

where \(V_{\text{read}}\) is the reading voltage. In the linear case, the ratio of the current level at \(V_{\text{read}}\) to that at \(\frac{V_{\text{read}}}{2}\) is less than 2. If this ratio is \(\leq 2\), the response is termed as nonlinear behavior \[32\].

The last parameter, diode cutoff frequency—is expressed as follows:

\[
f_c = \frac{1}{2\pi R_c C},
\]

\[
C = \varepsilon_0 \varepsilon_r \frac{A}{d},
\]

where \(R_c\) is the equivalent resistance of the diode and antenna, \(C\) is the diode capacitance, \(\varepsilon_0\) and \(\varepsilon_r\) are relative permittivity and dielectric constant of an oxide material, \(A\) is the overlap/junction area of the oxide layer in the diode, and \(d\) is the oxide thickness, respectively.

To understand the behavior of a diode and its nonlinear characteristics, it is essential to study the systematic band diagram (figure 2). The nominal thickness of an oxide and work function of metal electrodes were considered in figure 2. To explain the concept of a single insulator tunneling diode, we considered aluminum oxide (\(\text{Al}_2\text{O}_3\)) as an insulator because of its low dielectric constant and gold (Au) and titanium (Ti) as metal layers, considering the high work function difference between them.

As shown in figure 2(b), a built-in electric field is created from the top metal electrode toward the bottom metal layer due to the difference between the Ti and Au metal work function. When the positive voltage was connected to the top metal, an external field was generated from the Ti electrode toward the Au electrode. The
applied field and the internal field of the diode were parallel, thus a resultant increase in the electric field was observed (figure 2(c)).

Besides, when the top metal (Ti) was connected to the negative voltage, an external electric field was created from the bottom metal layer (Au) toward the Ti metal layer. Fields were in the opposite direction, hence a small value of the electric field was generated in the Al₂O₃ layer (figure 2(d)) [33, 34].

Additionally, owing to the difference in the work function, there was electron migration from Ti to Au, even in the absence of any applied bias (figure 2). So, if the thickness of the oxide layer is small, there is a possibility of current flow in the diode, even in the absence of bias known as the zero-bias performance of a tunnel diode, which translates into zero-bias responsivity.

The feasibility of electron tunneling depends on the thickness and energy barrier height of the insulator. The essential factor is to compute the possibility of electron migration between metal electrodes through thin insulator layers. The thickness of the insulator layers determines the tunneling distance and is inversely proportional to the tunneling current. In any case, a substantial thickness of the insulator layer is needed to separate the two metal electrodes. The thickness of the insulator layers plays a crucial role in computing the nonlinear dependence of the tunneling current on the applied voltage and diode characteristics. The equation to determine the tunneling performance of electrons through any randomly shaped barrier was derived by Simmons et al [35] and is given as follows:

\[
J = \frac{1.1q^2}{4\pi h} \left( \frac{V + \Delta \varphi_b}{\varphi_b} \right)^2 \times \exp \left( \frac{-23\sqrt{qm}}{6h} \varphi_b \frac{S}{V + \Delta \varphi_b} \right),
\]

where \( q \) is the electric charge of the electron, \( h \) is the Planck’s constant, \( V \) is the applied bias, \( \varphi_b \) is the barrier height of the electrode insulator interface from which electrons are tunneling, \( \Delta \varphi_b \) is the difference in barrier heights between interfaces of the insulator with the top and bottom electrodes (barrier height is the difference of work function and electron affinity of the oxide), \( m \) is the effective electron mass, \( S \) is the tunnel barrier thickness, and \( J \) is the tunneling current density. Unlike the PN-junction diode, it is evident from equation (6) that even for \( V = 0 \), we will get a nonzero current density. Notably, from equation (6), it is mandatory to have a work function difference between the two metal electrodes to initiate the tunneling process. Besides, with an increase in the tunnel barrier, the current density continues to decrease. The MIM is generally governed by the Fowler–Nordheim and direct tunneling mechanisms [36, 37]. However, as mentioned above, the current density decreases with the oxide thickness. To overcome this, an alternative approach is to have resonant tunneling [38]. This can be achieved by having a multilayer tunneling structure, commonly known as the M₁I₁I₂M₂ diode (figure 3). There is an extra barrier at the interfaces of the two insulators because of the differences in the electron affinity, which leads to a more significant change in resistance, thereby resulting in enhanced asymmetry and nonlinearity. Moreover, the two insulator layers also enable step tunneling. The step tunneling allows more
precise control of the diode asymmetry and its rectification capabilities at low voltages\cite{39, 40}. Additionally, owing to the large change in resistance, the responsivity of the diode also increases. Thus, adding an extra insulator layer enables realizing M1I1I2M2 diodes with higher responsivity and lower differential resistance than MIM diodes with similar current densities.

3. Results and discussion

To better access the tunneling behavior and current–voltage (I–V) behavior of the M1I1I2M2 diodes, it is essential to perform a simulation study. To predict the I–V response of an M1I1I2M2 diode, based on equation (6), we developed a quantum mechanical simulator. Before proceeding with the M1I1I2M2 diode simulation, a validation test was performed to compare the outcomes of the simulation with published results. Fowler–Nordheim, resonant tunneling, transfer matrix, step tunneling, and the shape of the tunnel barrier for different voltages were employed in the simulation model to compute the tunneling probability\cite{41, 42}.

The M1I1I2M2 diode uses two adjacent insulators sandwiched between the metal electrodes. These two insulators have different electron affinities, which results in a discontinuity at their interfaces. Our simulation stack and its equivalent energy band diagram are shown in figure 4. As mentioned above, the waste heating varies from 2 to 11 $\mu$m, having a maximum intensity at 10.6 $\mu$m (28.3 THz). To start, first, we calculated the diode cutoff frequency of the diode using equation (5). The cutoff frequency of the M1I1I2M2 diode was inversely proportional to its overlap area, thus the application of these diodes at high frequencies required the ultrasmall overlap area to match the RC time constant. In the simulation model, we used an overlap area of 100 nm$^2$ and assumed a standard antenna impedance of 50 $\Omega$\cite{43}. Possible combinations of oxides matching the peak frequency range of the waste heat are illustrated in table 1. The value of the dielectric constant was taken from the standard database\cite{44–47}. The simulation model gave the current values for different voltage ranges. In the simulation model, the voltage sweep range was set from $-1$ to 1 V.

| Oxide         | Dielectric constant | Thickness (nm) | Calculated frequency from equation (4) (THz) |
|--------------|---------------------|----------------|---------------------------------------------|
| Al$_2$O$_3$–TiO$_2$ | 0.304–1.34          | 2              | 29.3                                        |
| Al$_2$O$_3$–ZnO  | 0.304–3.57          | 2–3            | 27.0                                        |
| Al$_2$O$_3$–HfO$_2$ | 0.304–3.92         | 2              | 25.9                                        |
| TiO$_2$–ZnO    | 1.34–3.57           | 2–3            | 10.1                                        |
| TiO$_2$–HfO$_2$ | 1.34–3.92           | 2–3            | 9.88                                        |
| ZnO–HfO$_2$    | 3.57–3.92           | 2–3            | 4.88                                        |

Figure 4. (a) Simulation stack up. M$_1$ and M$_2$ represent the metals at top and bottom and I$_1$ and I$_2$ represent the different oxide layers of the diode. (b) Energy band diagram of an M$_1$I$_1$I$_2$M$_2$ diode with different barrier heights.

Table 1. Various combinations of oxide layers and optimized thickness to match the peak intensity frequency range of waste heat.
Since our main objective is to study the effect of different oxide combinations on the M₁I₁I₂M₂ diode performance, we fixed the bottom and top metals. We chose platinum (Pt; work function = 5.65 eV) as the bottom metal and titanium (Ti; work function = 4.33 eV) as the top metal. These metals were selected to realize a high work function difference. As per equation (6), a high work function difference enhances the current density in the M₁I₁I₂M₂ diode.
The I–V response for different M1I1I2M2 diodes is shown in figure 5. We extracted the dynamic resistance and responsivity from the I–V response using equations (1) and (2). Since our primary goal is to study the zero-bias performance, we focused on extracting responsivity and dynamic resistance at zero bias (table 2). The zero bias resistance and zero bias responsivity is shown in figures 6(a)–(b). We realized that the I–V response and responsivity were very sensitive to the arrangement of individual oxide layers.

From table 2, for the oxide combination where the difference in electron affinity was more significant, resonant tunneling and built-in asymmetry were enhanced, leading to higher responsivity. In addition, owing to the difference in the electron affinities between the two insulator layers, there was an extra barrier at the interfaces of the oxide, which enhanced the asymmetry and increased the nonlinearity properties. The nonlinearity was directly related to the responsivity of the M1I1I2M2 diode. A high nonlinearity enhanced the responsivity of the M1I1I2M2 diode. The M1I1I2M2 diode with high responsivity has excellent rectification and tunneling ability, which is one of the most significant outcomes of this study.

Besides, we computed the nonlinear factor of the simulated diode using equation (3). It is evident from table 2 that we realized a nonlinear factor of $\geq 2$ for all oxide combinations, which is another significant result of this study, as it showed that different oxide combinations could be useful in realizing high nonlinearity M1I1I2M2 diode for a high-efficiency rectenna system. By comparing the simulation results, the M1I1I2M2 diodes had higher dynamic resistance than MIM diodes for the same overlap area and comparable thickness. The nonlinearity and responsivity were more pronounced in M1I1I2M2 diodes. The simulation results indicated that M1I1I2M2 diodes were superior to MIM diodes in terms of their rectification capability.

4. Conclusion

In this article, we presented a systematic study of different types of M1I1I2M2 diodes for THz energy harvesting applications. Additionally, different oxide combinations of M1I1I2M2 diodes were investigated to match the cutoff frequency and enhance the rectification ability. It is concluded that insulators with a significant difference in electron affinity enhance the responsivity of the M1I1I2M2 diode. Our simulation results are promising and can be useful to the scientific community working in this domain in planning their fabrications and experiments. The simulation model can be further optimized to study M1I1I2M2 diodes with different metal combinations.

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Data availability statement

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

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