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Research paper

Metal-insulator-metal diodes with sub-nanometre surface roughness for energy-harvesting applications

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For ambient radio-frequency (RF) energy harvesting, the available power levels are quite low, and it is highly desirable that the rectifying diodes do not consume any power at all. Contrary to semiconducting diodes, a tunnelling diode – also known as a metal-insulator-metal (MIM) diode – can provide zero-bias rectification, provided the two metals have different work functions. This could result in a complete passive rectenna system. Despite great potential, MIM diodes have not been investigated much in the GHz-frequency regime due to challenging nano-fabrication requirements. In this work, we investigate zero-bias MIM diodes for RF energy-harvesting applications. We studied the surface roughness issue for the bottom metal of the MIM diode for various deposition techniques such as sputtering, atomic layer deposition (ALD) and electron-beam (e-beam) evaporation for crystalline metals as well as for an amorphous alloy, namely ZrCuAlNi. A surface roughness of sub-1 nm has been achieved for both the crystalline metals as well as the amorphous alloy, which is vital for the reliable operation of the MIM diode. An MIM diode comprising of a Ti-ZnO-Pt combination yields a zero-bias responsivity of 0.25 V−¹ and a dynamic resistance of 1200 Ω. Complete RF characterisation has been performed by integrating the MIM diode with a coplanar waveguide transmission line. The input impedance varies from 100 Ω to 50 Ω in the frequency range of between 2 GHz and 10 GHz, which can be easily matched to typical antenna impedances in this frequency range. Finally, a rectified DC voltage of 4.7 mV is obtained for an incoming RF power of 0.4 W at zero bias. These preliminary results of zero-bias rectification indicate that complete, passive rectennas (a rectifier and antenna combination) are feasible with further optimisation of MIM devices.

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1. Introduction

Radio-frequency energy harvesting is becoming a popular source of renewable energy for the smart environment, where a large number of sensors and devices are connected to deliver useful information, for example, the Internet of Things (IOT). There is also much interest in powering the systems remotely using far-field RF technology. This is particularly important for many applications, such as small, smart dust sensors [\[1\]](#page--1-0) or implantable sensors [\[2\]](#page--1-0). For remote, wireless powering, a dedicated RF source is used, which can provide sufficient power to operate these sensors, unlike the RF energy-harvesting approach where ambient RF energy is used to power the devices. In the latter case, RF power is low, and thus places many constraints on the efficiency of the system. In both cases, however, a diode is required to rectify the incoming signal from the antenna to obtain a useful DC output.

For energy-harvesting applications, it is highly desirable that the diode does not draw any power for its operation. The process, known as a zero-bias operation [\[3,4\],](#page--1-0) is typically not feasible with

⁎ Corresponding author. E-mail address: atif.shamim@kaust.edu.sa (A. Shamim). semiconductor-based diodes as they require bias for their operation, and thus consume power. On the other hand, MIM diodes, which work on the principle of electron tunnelling through a thin insulator between the two metals, can be used without being biased as long as metals with different work functions are used [\[5,6\]](#page--1-0). For rectification purposes, these diodes can be integrated with an antenna [\[7\]](#page--1-0) to form a completely passive rectenna system as shown [Fig. 1.](#page-1-0) Their ability to operate under zero-bias conditions and their fast response times as well as the possibility of their realisation through low-cost additive technologies [\[8\]](#page--1-0) make them attractive for high-frequency applications where typical semiconductor-based devices cannot operate [\[9\]](#page--1-0).

Though the real advantage of MIM diodes is high frequencies (THz range), their zero-bias rectification ability can also be beneficial for harvesting and wireless powering at RF frequencies [\[10\]](#page--1-0). The trade-off, however, is its poor non-linearity, and subsequently, poor responsivity and rectification ability at present. Moreover, due to the tunnelling operation, it offers high DC resistance. For its realisation, there are two major challenges: firstly, it needs a thin insulator (typically a few nanometres of thin oxide) to ensure electron tunnelling, and secondly, low surface roughness is required, particularly for the bottom metal, to produce reliable and repeatable devices.

Fig. 1. A schematic of a rectenna device. The frequency received by the antenna is rectified by the MIM diode, which is then further smoothened by the DC filter before being delivered to the load.

Previously reported works on MIM diodes used crystalline metals as the bottom electrodes, without investigating any issues related to the surface roughness of the bottom metal. However, recent work [\[11\]](#page--1-0) dealt with this issue, and reported that crystalline metals show high surface roughness; therefore, they are not suitable for the bottom electrodes of MIM diodes. That work [\[11\]](#page--1-0) recommends amorphous alloy films instead of crystalline metals to achieve low surface roughness, but at the cost of much lower conductivities. It is worth mentioning that in [\[11\],](#page--1-0) the surface-roughness data were collected for different film thicknesses without providing any details on the exact thickness of the films, making it difficult to establish whether the surface roughness is due to the crystalline nature of the metals or because of the thicker crystalline films, as compared to the amorphous alloy films. In this work, we have tried to address this issue, and have provided a detailed comparison between various fabrication methods, crystalline metals and amorphous alloys. This work also presents the achieved surface-roughness values and their effect on the performance of MIM diodes.

Furthermore, most of the work on MIM diodes focuses on high frequencies (THz range) [\[5,6,12\]](#page--1-0). There are only a handful of papers that reported on MIM diodes operating in the RF range, and most of them have serious limitations as far as RF characterisation of the MIM diodes is concerned. In [\[13\]](#page--1-0), an MIM diode has been measured for its rectification abilities by impinging RF waves directly on the diode using a commercial antenna; however, the major problem is that the diode has not been characterised for its impedance performance using S-parameter measurements, which mean that its efficiency cannot be calculated accurately due to the unknown mismatch loss. Furthermore, in the absence of the input impedance of the diode, it is not possible to efficiently integrate it with an RF antenna with appropriate matching. Finally, the authors had operated the diode at non-zero bias voltages, which could result in poor efficiency of the device. Similar works have been reported in [\[14\]](#page--1-0) and [\[15\]](#page--1-0), where the authors have provided better RF characterisation of the device. In [\[14\]](#page--1-0), the diode was characterised for its S-parameter measurements using a vector-network analyser (VNA). However, it was never measured for its rectification ability, which is performed by measuring the DC output voltage across a load when the diode is excited by an RF signal. Also, the design that is presented in this work was principally for the THz range of operation; however, due to the lack of measurement equipment at such high frequencies, the authors restricted their characterisation in the GHz range. In [\[15\],](#page--1-0) the authors characterised the fabricated diode for its input impedance and RF-to-DC conversion abilities. However, the diodes' rectification has been shown with applied bias. From the above literature review, it can be said that both the RF characterisation of an MIM diode and its application at a zero-bias condition still require considerable work and investigation for energy-harvesting applications.

Based on the observations made above, the work presented in this paper reports a systematic study of MIM diodes for RF applications. In addition to the above-mentioned surface-roughness study, we also provide complete DC/RF characterisation. Moreover, RF-to-DC rectification at zero bias is also demonstrated in this work for the first time. In Section 2, we describe the operating principle and characteristics of MIM diodes. The investigation of surface roughness for the bottom electrode of MIM diodes, along with the fabrication process and DC response of the diodes, has been summarised in [Sections 3 and 4.](#page--1-0) The RF characterisation of MIM diodes is covered in [Section 5](#page--1-0).

2. Metal-insulator-metal diodes

A pn-junction diode can be forward or reverse biased, depending on the polarity of the applied voltage [\[16\].](#page--1-0) However, in the absence of any applied voltage, the pn-junction diode will ideally act as an open circuit for any incoming signal. The MIM diode, on the other hand, is a tunnelling device, which is formed by two metal electrodes separated by a thin film of the insulating layer. It works on the principle of quantum-mechanical tunnelling, where electrons tunnel between the two electrodes through an appropriate bias applied across the diode [\[17\]](#page--1-0). However, by choosing metals that have different work functions, and by separating them with a suitable insulator, electrons can tunnel without any applied bias [\[18\]](#page--1-0). The important parameters for the operation of an MIM diode include the work function of the metals, the electron affinity, the dielectric constant and the physical thickness of the insulator. For our specific MIM diode, the structure is composed of Pt/ZnO/Ti, where Pt has a work function of 5.65 eV and Ti 4.33 eV [\[19\].](#page--1-0) The reason for choosing Pt and Ti is to have a higher work-function difference, since a high difference enhances the electron tunnelling [\[20,21\]](#page--1-0). The electron affinity of ZnO varies between 2 eV and 2.2 eV, and is taken to be 2.02 eV in our experiment [\[22](#page--1-0)–24]. The conduction-band offset diagram is depicted in [Fig.](#page--1-0) [2](#page--1-0)(a). [Fig. 2](#page--1-0)(b) illustrates the built-in electric field created from the Ti top electrode to the Pt electrode in thermal equilibrium due to the work-function difference between the Ti and Pt electrodes [\[25\].](#page--1-0) When a positive voltage is applied to the top electrode, an external field is created from the Ti electrode to the Pt electrode, as demonstrated in [Fig.](#page--1-0) $2(c)$ $2(c)$ [25–[27\].](#page--1-0) The applied electric field causes the electrons to flow from Pt to Ti. When a negative voltage is applied to the Ti top electrode, an external electric field is created from the Pt electrode to the Ti electrode, as illustrated in [Fig. 2](#page--1-0)(d). The flow of current in this direction will be opposite to the case shown in [Fig. 2\(](#page--1-0)c). From [Fig. 2](#page--1-0), it is evident that the difference in the work functions creates a Fermi-level gradient on the both sides of the potential barrier, facilitating electron tunnelling through the oxide layer.

The probability of electron tunnelling depends on the thickness and the height of the insulator barrier [\[28\]](#page--1-0). It is important to compute the number of possibilities that an electron (of given energy) from a metal electrode can tunnel to the empty states of another metal electrode through the insulator. A decrease in the tunnelling distance results in an increase in tunnelling current, and vice versa. However, a physical thickness of the insulator layer is required to isolate the two metal arms. This equates to the non-linear dependence of the tunnelling current on the applied voltage and diode characteristics. Simmons et al. derived a formula for the tunnelling behaviour of electrons through a barrier of any arbitrary shape [\[28,29\]:](#page--1-0)

$$
J = \frac{1.1 \ q^2}{4\pi h} \frac{1}{\varphi_b} \left(\frac{V + \Delta \varphi_b}{S}\right)^2 \times \ \exp\left(\frac{-23\pi \sqrt{qm}}{6h} \varphi_b^{\frac{3}{2}} \left(\frac{S}{V + \Delta \varphi_b}\right)\right) \tag{1}
$$

where q is the electric charge, h is Plank's constant, V is the applied bias, φ_b is the barrier height of the electrode-insulator interface from which electrons are tunnelling, $\Delta\varphi_b$ is the difference in barrier heights between the interfaces of the insulator with the top and bottom electrodes (φ_b = the work function of metal-electron affinity of oxide [\[17,28\]\)](#page--1-0), m is the effective electron mass, S is the tunnel barrier thickness and I is the tunnelling-current density. Based on Eq. (1), the device will have a nonzero current density even if V is zero, unlike a pn-junction diode. Also, it is evident that the current density decreases with an increase in the tunnel-barrier thickness, and a work-function difference between the two electrodes is required to achieve the tunnelling phenomenon.

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