

## Barrier tuning of atomic layer deposited Ta<sub>2</sub>O<sub>5</sub> and Al<sub>2</sub>O<sub>3</sub> in resonant tunneling diodes for terahertz electronics

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### Abstract

The performance of double dielectric (*MIIM*) resonant tunneling diodes using atomic layer deposited oxides of low (Al<sub>2</sub>O<sub>3</sub>) and high (Ta<sub>2</sub>O<sub>5</sub>) electron affinity ( $\chi$ ) is investigated. Varying the individual layer thickness of Ta<sub>2</sub>O<sub>5</sub> with a 1 nm thick Al<sub>2</sub>O<sub>3</sub>, evidence for resonant tunneling is observed and related to the bound states in the quantum well established between the oxide layers. The results show good rectifying capability of resonant tunneling diodes at low turn-on voltage enabling their potential use for terahertz applications.

### 1. Introduction

Diodes based on tunneling through one or more insulator layers are attractive rectifying devices for electronics and energy harvesting applications at terahertz (THz)<sup>1</sup> and infrared (*IR*) frequencies<sup>2</sup>. The main challenges remain in achieving sufficient non-linearity, high asymmetry, and low dynamic resistance<sup>3</sup> to attain efficiency when incorporated into these applications. Resonant tunneling (*RT*) serves to bring further enhancement to the current asymmetry and non-linearity<sup>4</sup>. *RT* can occur in double dielectric structures, where a quantum well is formed in the inter-barrier space allowing the formation of bound states<sup>5</sup>. The aim is to develop diodes with sufficiently non-linear and asymmetric current-voltage (*J-V*) characteristics at low turn-on voltage ( $V_{ON}$ ).

### 2. Experimental

Devices with lateral area of 100×100 μm<sup>2</sup> were fabricated on cleaned Corning glass substrates. The top (Al) and bottom (Cr) metal layers of 50 nm thickness were deposited by thermal evaporation through a shadow mask. The Al<sub>2</sub>O<sub>3</sub> and Ta<sub>2</sub>O<sub>5</sub> oxides were successively deposited over the bottom electrodes using atomic layer deposition (*ALD*) at a temperature of 200 °C. Four device structures are investigated with Ta<sub>2</sub>O<sub>5</sub> thickness of 1 (S1), 2 (S2), 3 (S3), and 4 nm (S4) deposited on top of 1 nm thick Al<sub>2</sub>O<sub>3</sub>. The thicknesses of the dielectric layers were measured by variable angle spectroscopic ellipsometry. The *J-V* measurements were done in the dark. Voltage was swept from 0 V with 1 mV step size under negative and positive bias. The bound

states were simulated using a previously reported model<sup>5</sup>, which defines a Hamiltonian matrix for the bound states to find their quantized energy levels using the time-independent Schrodinger equation.

### 3. Results and Discussion

The effect of varying the individual layer thickness of Ta<sub>2</sub>O<sub>5</sub> with a 1 nm thick Al<sub>2</sub>O<sub>3</sub> dielectric can be observed in the rectifying characteristics shown in *Figure 1*. Asymmetry is defined as the current ratio at positive bias to that at negative bias  $f_{asym} = J_+/J_-$ , Non-linearity as the ratio of static to dynamic resistance  $f_{NL} = (V/J)/(dV/dJ)$ ,<sup>6</sup> and the dynamic resistance as  $R_d = dV/dI$ . The abrupt increase in the *J-V* plots (*Figure 1.a*) at positive bias for the 4 nm thick Ta<sub>2</sub>O<sub>5</sub> oxide is thought to be attributed to *RT*. This possibility is supported by the band diagrams of *Figure 2* and *Figure 3* which indicate the probable occurrence of *RT* at positive polarity, when the energy of a quasi-stationary resonant state in the well is matched to the states neighboring the Fermi level of the top Al charge injecting electrode<sup>7</sup>. The quantum well becomes wider and deeper by increasing the applied voltage or thickness of the first oxide layer, lowering down the bound states towards the notch<sup>12</sup>, which provides further evidence that the noticeable improvement in asymmetry with thicker Ta<sub>2</sub>O<sub>5</sub> (*Figure 1.b*) and non-linearity (*Figure 1.c*) is associated with *RT*. Sample S1 shows inadequate non-linearity and asymmetry which could be because the width of the quantum well in the device with 1 nm thick Ta<sub>2</sub>O<sub>5</sub> is insufficient to accommodate a bound state in the range of the applied voltage (*Figure 3*). The voltage

$V_{ON}$  is defined here as the point at which the current abruptly increases or the knee in the asymmetry plots. For the 2, 3, and 4 nm thick  $Ta_2O_5$  respectively,  $V_{ON}$  is found to be 0.7, 0.5, and 0.33 V at positive bias, which is reasonable with the existence of one bound state at 0.89, 0.54, and 0.42 eV as extracted from the model. This decrease in  $V_{ON}$  is consistent with the likely increase in the depth of the quantum well at positive bias when the thickness of  $Ta_2O_5$  is increased as illustrated in simulations (Figure 3). The larger current observed at  $V_{ON}$  at positive bias indicates that the overall asymmetry is regulated by the dominance of  $RT$  at positive bias over other conduction mechanisms. The increase in non-linearity and the drop in dynamic resistance were steeper at positive bias, where  $RT$  occurs, than at negative bias, where step tunneling occurs, indicating the advantage of the prior mechanism for rectification suitable for THz electronics.

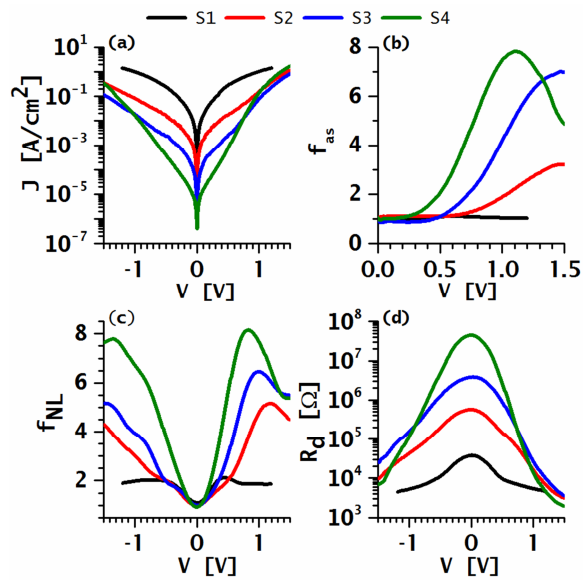


Figure 1. Rectifying characteristics of the MIIM devices showing the:  $J$ - $V$  characteristics (a), asymmetry (b), non-linearity (c), and dynamic resistance (d).

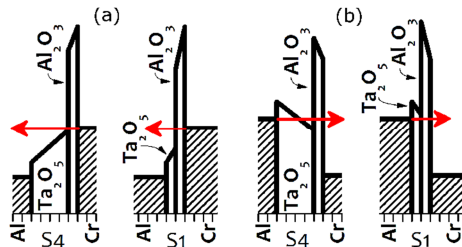


Figure 2. Energy band diagrams of S4 and S1 at  $-1$  (a) and  $+1$  V (b). Electron injection is indicated by the red arrows.

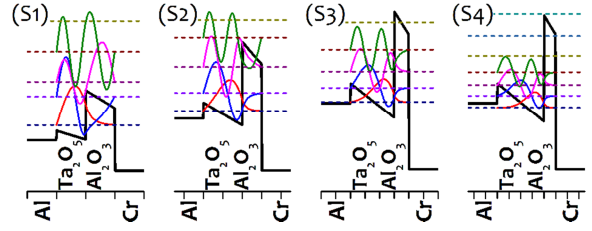


Figure 3. Simulated conduction band diagrams at  $+1.5$  V showing 0, 1, 2, and 3 bound states for S1, S2, S3, and S4, respectively.

#### 4. Conclusions

$RT$  of THz rectifying capability was demonstrated with sufficient asymmetry and non-linearity when 1 nm thick  $Al_2O_3$  layer was used with the  $Ta_2O_5$ . The effect of  $RT$  was further tuned according to the individual thickness of the  $Ta_2O_5$  layer resulting in a noticeable improvement in rectification, exceeding that of step tunneling and in agreement with theory. The rectifying characteristics were observed as a trade-off between the dynamic resistance and the asymmetry, non-linearity, and turn-on voltage. Considering the built-in voltage arising from the 0.2 eV work function difference of the electrodes, the capability of engineering  $RT$  to occur at lower  $V_{ON}$  with similar electrodes is feasible, providing scope for further enhancement towards zero-bias rectification<sup>8</sup>.

#### Acknowledgements

The work has been partly funded by EPSRC, UK, under project EP/K018930/1. The authors thank the collaborating partners: Dr J. Wrench and Prof P Chalker from the Centre for Materials and Structures for the ALD.

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