STUDY OF METAL-INSULATOR-METAL DIODES FOR 
PHOTODETECTION

Thesis
Submitted to
The School of Engineering of the
UNIVERSITY OF DAYTON

In Partial Fulfillment of the Requirements for
The Degree
Master of Science in Electro-Optics

By
Li Li

UNIVERSITY OF DAYTON
Dayton, Ohio
May, 2013
STUDY OF METAL-INSULATOR-METAL DIODES FOR PHOTODETECTION

Name: Li, Li

APPROVED BY:

Joseph W. Haus, Ph.D.
Advisor Committee Chairman
Professor
Department of Electro-Optics
Program

Partha P. Banerjee, Ph.D.
Committee Member
Professor
Department of Electrical Engineering
And Electro-Optics Program

Andrew M. Sarangan, Ph.D.
Committee Member
Professor
Department of Electro-Optics Program

John G. Weber, Ph.D.
Associate Dean
School of Engineering

Tony E. Saliba, Ph.D.
Dean, School of Engineering
& Wilke Distinguished Professor
ABSTRACT

STUDY OF METAL-INSULATOR-METAL DIODES FOR PHOTODETECTION

Name: Li, Li
University of Dayton

Advisor: Dr. Joseph W. Haus

We study the optical responsivity of metal-insulator-metal (MIM) devices using different metals, but at least one metal with displaying plasmonic resonance characteristics. We apply quantum mechanical tunneling and equilibrium electron statistics to calculate the current density for the MIM structure with forward and backward bias voltages. We also examine the tunneling properties for nanoslabs and nanorods which alter the electron density of states by laterally confining the electrons and lead to a change of the tunneling current.

To calculate the quantum tunneling current we use two methods for solving Schrödinger’s equation: Transfer Matrix Method (TMM) and Shooting method to simulate tunneling probability current through the insulating gap. Both methods are in excellent agreement. The tunneling current performance of MIM nanostructure is determined by the size and shape of insulator gap. Using the quantum results we calculate the DC and AC current of MIM nanostructures when an electromagnetic field is applied. The electrons tunnel through the
insulating gap driven by an electromagnetic field using a photon assisted tunneling expression. Finally, the results for the DC and AC current are evaluated to determine the MIM responsivity from the long wavelength infrared (IR) regime to the near IR regime.
ACKNOWLEDGMENTS

I would like to specially thank my advisor Dr. Joseph Haus, for all his help and advice in my research, for providing time and idea for this thesis. His patience, time and vast knowledge are the biggest encouragement for me. I would also like to thank my committee members Dr. Partha Banerjee and Dr. Andrew Sarangan for their encouragement, assistance and helpful comments.

Additionally, I also would like to thank Dr. Partha Banerjee, Dr. Andrew Sarangan, Dr. Andy Chong, Dr. John Loomis, Dr. Rola Aylo and Dr. Georges Nehmetallah for their great classes. I would also like to express my thanks to Dr. Cong Deng and Dr. Nkorni Katte for all their help on my research.

Finally, I would like to thank my parents and all families for their love, support and encouragement.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>iv</td>
</tr>
<tr>
<td>ACKNOWLEDGEMENTS</td>
<td>vi</td>
</tr>
<tr>
<td>TABLE OF CONTENTS</td>
<td>vii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>ix</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>xiv</td>
</tr>
<tr>
<td>LIST OF ABBREVIATIONS AND NOTATIONS</td>
<td>xv</td>
</tr>
<tr>
<td>CHAPTER I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Background</td>
<td>1</td>
</tr>
<tr>
<td>1.2 MIM Tunneling Devices</td>
<td>2</td>
</tr>
<tr>
<td>1.3 Thesis Outline</td>
<td>3</td>
</tr>
<tr>
<td>CHAPTER II. QUANTUM WAVE PROPAGATION AND THE MIM TUNNELING DIODE</td>
<td>5</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>5</td>
</tr>
<tr>
<td>2.2 Electron Tunneling</td>
<td>6</td>
</tr>
<tr>
<td>2.2.1 Transfer Matrix Method (TMM)</td>
<td>9</td>
</tr>
<tr>
<td>2.2.2 Shooting Method</td>
<td>13</td>
</tr>
<tr>
<td>2.3 Chapter Summary</td>
<td>20</td>
</tr>
<tr>
<td>CHAPTER III. TUNNELING CURRENT WITH SIDEWALL CONFINEMENT IN THE ABSENCE OF ILLUMINATION</td>
<td>22</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>22</td>
</tr>
<tr>
<td>3.2 Current Density 3D</td>
<td>23</td>
</tr>
</tbody>
</table>
3.3 Current Density 2D .................................................................26
3.4 Current Density 1D .................................................................27
3.5 Simulation Results For Lateral Confinement .........................28
3.6 Unilluminated Current Density Results For The MIM Structure ....29

CHAPTER IV. ILLUMINATED MIM CHARACTERISTICS ..................35
4.1 Introduction .............................................................................35
4.2 Weak Radiation Field ..............................................................36
4.3 Responsivity’s Radiation Field Strength Dependence ...............47
4.4 Concentrated Solar Irradiance ..................................................50
4.5 Plasmonic Enhancement ...........................................................51
4.6 Electric Field Enhancement ......................................................51
4.7 Chapter Summary ....................................................................54

CHAPTER V. CONCLUSION AND FUTURE WORK .......................56

BIBLIOGRAPHY .............................................................................59

APPENDIX A. MATERIAL PARAMETERS ........................................62
APPENDIX B. SIMULATION RESULTS ..........................................63
APPENDIX C. MATLAB CODES .......................................................69
C.1 Dark_tunneling_current_3D2D1D.m .......................................69
C.2 Shootingmethod.m .................................................................78
C.3 Responsivity_alpha_gap.m ......................................................80
C.4 Responsivity_quan_limit.m .....................................................85
Figure 1.1 A conceptual illustration of the MIM tunneling structures. On the left we have a forest of nanowires that fill a region of space. On the right we show the MIM structure with a thin insulator sandwiched between two metal nanorods. There are two different metals on each side, which give the MIM a diode tunneling current characteristic.................................................................3

Figure 2.1 The ideal energy band for an asymmetric MIM tunneling diode. Two different metals (NbN, Nb) are separated by 2nm insulator (Nb$_2$O$_5$). The Fermi level of both metals is assumed as 10eV in this case.........................................................8

Figure 2.2 Energy band diagram of a MIM diode with different metal electrodes (Metal 1 and Metal 2). (a) Forward bias: electron tunneling from metal 1 to metal 2 is dominant, (b) Backward bias: A bias voltage applied in metal 1 result in electrons in metal 2 tunnels through the barrier into metal 1. .........................9

Figure 2.3 An illustrative electronic potential (blue) with a barrier region that is characterized by a linear slope. The sub-regions of constant potential are indicated by boxes of small width and heights that are adjusted to the potential height in the region. ........................................................................................................10

Figure 2.4 The tunneling probability (log base 10) as a function of energy $E_z$ (eV) (from 9eV to 12eV) for the MIM structure shown in Figure (2.2-a)........12

Figure 2.5 The wave function magnitude plotted versus position for an energy of 12 [eV] with the same potential as in Figure (2.2-a). .................................13

Figure 2.6 An illustration of the first derivative of a function using finite differences...........................................................................................................14
Figure 2.7 Illustration of wave function for a single interface on both the left $\psi_l$ and right $\psi_r$ side. The energy band of MIM diode is same as Figure 2.3...........16

Figure 2.8 The tunneling probability as a function of energy for the energy diagram of MIM diode as same as Figure 2.3 with 0.3V applied voltage. The solution is plotted for both TMM (blue) and shooting method (red). The WKB approximation [13] is shown for comparison (green)........................................18

Figure 2.9 The tunneling probability as a function of $z$-directed electron energy and applied voltage ($V_{bias}$) for the energy diagram of MIM diode as same as Figure 2.3. The simulation result obtained by TMM..................................................19

Figure 2.10 Comparison of tunneling probability between Grover’s paper and our result. (a) Grover’s paper (b) our result for the NbN/Nb$_2$O$_5$/Nb structure with a 2 nm insulator gap....................................................................................21

Figure 3.1: Biased MIM junction with Fermi level and occupation probabilities indicated. The metal on the left side is biased by an applied dc potential...........25

Figure 3.2: Applied voltage as a function of current density for the case of MIM diode in Figure 2.3 design with gap=2nm. The lateral confinement parameters are: (a) $d_x=d_y=100$nm, (b) $d_x=d_y=50$nm, (c) $d_x=d_y=25$nm, (d) $d_x=d_y=10$nm ......29

Figure 3.3: The calculated tunneling current curve Vs. applied voltage and different gap thickness for Ag/TiO$_2$/Ti MIM diode. The tunneling current curve calculated by the TMM and plotted by surface function in Matlab.......................31

Figure 3.4: The calculated tunneling current curve vs. applied voltage and different gap thickness for Al/Nb$_2$O$_5$/Nb MIM diode..................................................32

Figure 3.5: The calculated tunneling current curve vs. applied voltage and different gap thickness for Cu/Nb$_2$O$_5$/Nb MIM diode..................................................32

Figure 3.6: The calculated tunneling current curve vs. applied voltage and different gap thickness for Au/Nb$_2$O$_5$/Nb MIM diode..................................................33
Figure 4.1: Illustration of the photon assisted tunneling process. The interaction of the electromagnetic field raises the energy of the electron to help it transition across the barrier. At single photon energies approaching the visible or near IR regime or for multi-photon cases at longer wavelengths (i.e. n>1 in this case) the electron’s energy can be larger than the barrier height.

Figure 4.2: Illuminated dc current vs. applied voltage for MIM diode Ag/TiO$_2$/Ti under small incoming field. The thickness is fixed at 2nm as an example and the photon energy is 1.4 eV. The red curve shows when alpha is equal to zero corresponding to dark current in Chapter 3.

Figure 4.3: Responsivity vs. wavelength and gap for MIM diode Ag/TiO$_2$/Ti under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.

Figure 4.4: Responsivity vs. wavelength and gap for MIM diode Al/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.1V bias applied.

Figure 4.5: Responsivity vs. wavelength and gap for MIM diode Cu/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.

Figure 4.6: Responsivity vs. wavelength and gap for MIM diode Au/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.

Figure 4.7: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0V. Quantum efficiency limit (dot).

Figure 4.8: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0.1V. Quantum efficiency limit (dot).
Figure 4.9: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0.2V. Quantum efficiency limit (dot). .................................................................45

Figure 4.10: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0.4V. Quantum efficiency limit (dot) .................................................................46

Figure 4.11: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0.5V. Quantum efficiency limit (dot) .................................................................46

Figure 4.12: Responsivity vs. wavelength and alpha for MIM diode Ag/TiO$_2$ (4.6nm)/Ti under strong incoming field, with $V_{bias}$=0V. ..................................................48

Figure 4.13: Responsivity vs. wavelength and alpha for MIM diode Al/Nb$_2$O$_5$ (4.6nm)/Nb under strong incoming field, with $V_{bias}$=0V..............................................48

Figure 4.14: Responsivity vs. wavelength and alpha for MIM diode Cu/Nb$_2$O$_5$ (4.6nm)/Nb under strong incoming field, with $V_{bias}$=0V..............................................49

Figure 4.15: Responsivity vs. wavelength and alpha for MIM diode Au/Nb$_2$O$_5$ (5nm)/Nb under strong incoming field, with $V_{bias}$=0V. ..................................................49

Figure 4.16 (a) Absorption as a function of wavelength (350nm~800nm) for different particle shape from spherical to aspect ratio 10:1. (b) Local electrical field distribution around a prolate spheroidal shaped particle at the wavelength of the surface plasmon resonance (x,z) plane.............................................52

Figure 4.17: Field intensity in the vicinity of two elliptical cross-section nanowires with major and minor axes 50nm and 10 nm respectively. The gap is 1.9 nm. (a) the two elliptic cross sections of the nanowires with field strength indicated in color. (b) a close up of the gap region with field magnitude shown on the bar. Courtesy of Domenico deCeglia.............................................53
Figure 4.18: Plot of the field intensity versus wavelength for the maximum field as a function of wavelength. Courtesey of Domenico deCeglia..................54

Figure B.1: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Ag/Cr$_2$O$_3$/Cr MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Ag/Cr$_2$O$_3$/Cr with 0.3V bias applied under small incoming field $\alpha = 0.05$. .................................................................64

Figure B.2: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Cu/Ta$_2$O$_5$/Ta MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Cu/Ta$_2$O$_5$/Ta with 0.3V bias applied under small incoming field $\alpha = 0.05$. .................................................................65

Figure B.3: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Al/Ta$_2$O$_5$/Ta MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Al/Ta$_2$O$_5$/Ta with 0.3V bias applied under small incoming field $\alpha = 0.05$. .................................................................66

Figure B.4: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Au/Nb$_2$O$_5$/NbN MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Au/Nb$_2$O$_5$/NbN with 0.3V bias applied under small incoming field $\alpha = 0.05$. .................................................................67

Figure B.5: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Cu/TiO$_2$/Ti MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Cu/TiO$_2$/Ti with 0.3V bias applied under small incoming field $\alpha = 0.05$. .................................................................68
LIST OF TABLES

Table 3.1 Expression of three different models (3D, 2D, 1D). $D_f$ is the number of degrees of freedom. $D_c$ is the number of direction confinement in the electron motion. .........................................................23

Table A.1 Material property values for metals and insulators [8, 15].. .............62
**LIST OF ABBREVIATIONS AND NOTATIONS**

<table>
<thead>
<tr>
<th>ABBREVIATIONS</th>
<th>DEFINITIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>MIM</td>
<td>Metal Insulator Metal</td>
</tr>
<tr>
<td>TMM</td>
<td>Transfer matrix method</td>
</tr>
<tr>
<td>SPR</td>
<td>Surface Plasmon Resonance</td>
</tr>
<tr>
<td>WKB</td>
<td>Wentzel, Kramers, Brillouin</td>
</tr>
</tbody>
</table>
## NOTATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hbar$</td>
<td>Planck constant by $2\pi$</td>
</tr>
<tr>
<td>$m$</td>
<td>Free electron mass</td>
</tr>
<tr>
<td>$e$</td>
<td>Electron charge</td>
</tr>
<tr>
<td>$\Psi(\vec{r},t)$</td>
<td>Time-dependent wave function</td>
</tr>
<tr>
<td>$E$</td>
<td>Total electron energy</td>
</tr>
<tr>
<td>$V(z)$</td>
<td>Longitudinal potential</td>
</tr>
<tr>
<td>$V_{\text{sidewall}}(x,y)$</td>
<td>Lateral potential</td>
</tr>
<tr>
<td>$V^2$</td>
<td>Laplace operator</td>
</tr>
<tr>
<td>$H_0$</td>
<td>Unperturbed Hamiltonian operator</td>
</tr>
<tr>
<td>$\phi_1$</td>
<td>Work function of metal 1</td>
</tr>
<tr>
<td>$\phi_2$</td>
<td>Work function of metal 2</td>
</tr>
<tr>
<td>$\phi_i$</td>
<td>Electron affinity</td>
</tr>
<tr>
<td>$\varphi_{1(2)}$</td>
<td>Potential barrier height of metal 1 or 2</td>
</tr>
<tr>
<td>$E_F$</td>
<td>Fermi energy</td>
</tr>
<tr>
<td>$\psi(z)$</td>
<td>Longitudinal wave function (z-component)</td>
</tr>
<tr>
<td>$k_{x(y)}$</td>
<td>Transverse wave vector</td>
</tr>
<tr>
<td>$\psi(x,y,z)$</td>
<td>Wave function</td>
</tr>
<tr>
<td>$z$</td>
<td>Longitudinal distance</td>
</tr>
<tr>
<td>$k_\alpha$</td>
<td>Longitudinal wave vector component for the $\alpha^{th}$ slice</td>
</tr>
<tr>
<td>$M_\alpha$</td>
<td>Transfer matrix</td>
</tr>
<tr>
<td>$T_\alpha$</td>
<td>Tunneling probability for the $\alpha^{th}$ slice</td>
</tr>
</tbody>
</table>
T  Tunneling probability current
δz  Displacement along z-axis
z  Longitudinal distance along the propagation path
V_{bias}  Applied voltage
E_z  z-directed electron energy
J^{QM}  Quantum tunneling current density
ψ*  Complex conjugate of the wave function
D_c  Dimensionality of lateral electron confinement
D_f  Number of degrees of freedom
ψ_{after}(\tilde{k})  Wave function after the potential barrier
f_1(E)  Occupation probability for an electron in metal 1
f_2(E)  Occupation probability for an electron in metal 2
E_r  Electron energy in the Lateral directions
v_x  Velocity in x- direction
v_y  Velocity in y- direction
v_z  Velocity in longitudinal direction
J^{3D}  3D Dark current density
J^{2D}  2D Dark current density
J^{1D}  1D Dark current density
d_x  x-direction quantization
d_y  y-direction quantization
V_{ac}  Ac gap voltage due to the electromagnetic field
ω  Angular frequency
\( E_{\omega} \)  Electromagnetic field amplitude

\( d \)  Thickness of insulator gap

\( E_{\text{ph}} \)  Photon energy

\( J_n(\alpha) \)  First order Bessel function with index \( n \)

\( J^{\text{dc}} \)  Dc current density

\( J^{\text{ac}} \)  Ac current density

\( \alpha \)  alpha parameter

\( \Delta J^{\text{dc}} \)  Change of dc current due to electromagnetic field

\( R \)  Responsivity

\( T \)  Lattice temperature
CHAPTER I

INTRODUCTION

1.1 Background

The combination of photonic interactions in nanoplasmas and quantum tunneling is opening a new vista for applications in energy harvesting and photon sensing. Exploiting the free electron dynamics in metals, whose response time is on a femtosecond scale [1], so that device band widths can approach 100’s THz can provide a radical departure in performance of future photonic devices.

The core of devices made from sandwiching an insulator between two different or identical metals, so-called metal-insular-metal devices (or MIM devices) have been studied for many decades, since it started in 1960s [2, 3]. The MIM diodes coupled with antenna have been used for received electromagnetic energy from a microwave beam and converted it to DC power [4]. The MIM devices showed good performance for detecting and mixing of radiation in high frequency waves up to infrared (IR) range [5, 6]. In 1978 Sanchez presented theoretical analysis with experimental verification for the metal-oxide-metal (MOM) antenna/diode that can be used for detected microwave and infrared radiation [7].
An interesting line of research focuses on MIM diodes for energy harvesting applications [8, 9]. The large band width and ultrafast response make MIM devices well suited to this field, but the efficiency must be higher to compete against other energy harvesting devices, such as silicon solar cells. The unique carrier and photon confinement properties of nanowire-based rectennas are the main reason for our interest in studying MIM nanowire systems. We wanted to see whether the confinement of both electrons and photons could show a pathway to a new design principle for such devices.

Surface Plasmon Resonance (SPR) provides a new concept to explore additional design rules for making photodetectors with higher responsivity and solar cells with greater energy harvesting efficiency [10]. In MIM structures plasmonic enhancement of the electromagnetic field has a strong effect on the tunneling current, even though it has a smaller effect on the responsivity. For a gap that is only a few nanometers in width, the local field enhancement in the nanometer gap between the two metals can be perhaps three to five orders of magnitude. However, SPR is a resonance with a limited band width. On the other hand, the electrostatic charge build-up near the metal surface leads to a much broader band width enhancement of the local field and could be used as an additional mechanism to improve MIM diode action. The field enhancement in the insulating gap region of several orders of magnitude can make MIM devices more suited to photodetection. The SPR and electrostatic field enhancement concepts will be discussed again in Chapter 4.

1.2 MIM Tunneling Devices

MIM devices based on nanorods are proposed and studied in this thesis. An illustration of the devices is shown in Figure 1. The nanorods are composed
of two different metals with a thin insulator material of only a few nanometers thickness separating the two metals. The lateral quantum confinement of the electrons alters the electronic density of states. The effect of the shape dependence of the metals concentrates the electromagnetic field in the insulating gap which enhances the field’s effect on the electron tunneling. Order of magnitude enhancement of the electromagnetic field will lead to substantial changes in the tunneling current.

Figure 1.1 A conceptual illustration of the MIM tunneling structures. On the left we have a forest of nanowires that fill a region of space. On the right we show the MIM structure with a thin insulator sandwiched between two metal nanorods. There are two different metals on each side, which give the MIM a diode tunneling current characteristic.

1.3 Thesis Outline

In this thesis we explore applications of MIM diodes to design broad band and ultrafast photodetectors that integrate the quantum and photonic aspects of MIM devices. We want to study the devices in a nanowire geometry, so we present for the first time the dark current density versus applied voltage with lateral quantum confinement effects. Also, we develop theoretical result of photon-assisted tunneling theory for illuminated dc and ac current calculation.
Finally, we calculate the responsivity for both the weak and strong applied radiation field.

This thesis is composed of five chapters. Next chapter is covers the quantum physics of MIM structures and shows their diode-like characteristics. We introduce electron tunneling current probability, which we calculate using two different methods: transfer matrix method (TMM) and shooting method. Both methods give identical results for the cases we study. We also compare our results to analytical approximations to validate the results further. However, we use TMM for calculating the tunneling current in Chapter III.

Chapter III summarizes the tunneling principles applied to measured dark (dc) currents and shows the asymmetry tunneling current properties in MIM diode under dark current conditions with externally applied voltages. The results of the dark currents for laterally quantum confined MIM quantum diodes will also presented.

Chapter IV shows the main results where we calculate the illuminated current for a photon-assisted tunneling model. The illuminated MIM diode current depends entirely on the dark tunneling current results in Chapter III. The current responsivity is calculated from the MIM diode’s illuminated I-V characteristics. The dc and ac current results are evaluated to determine the MIM responsivity. The surface plasmon resonance for a single ellipsoidal particle is solved and related to quantum confinement in the MIM quantum wires. We also discuss a simple case of two MIM elliptical nanowires and find the enhanced field in the gap due to electrostatic charges building up at the surfaces. Finally, Chapter V provides a summary of our findings and we point to future work that needs to be done.
CHAPTER II

QUANTUM WAVE PROPAGATION AND THE MIM TUNNELING DIODE

2.1 Introduction

In this Chapter the problem of a free electron wave driven by an applied voltage and traveling across a region with a barrier potential is solved. The current density is a combination of the electron tunneling probability current and the occupation densities of the energy levels on both sides of the barrier. Electron tunneling current probability is determined by quantum mechanics. The energy band diagram for an MIM diode is described in this section. In addition, we solve the theoretical expression for tunneling current probability obtained using two different methods which are the TMM and the shooting method. Those two methods give us an identical result, as expected. We also compare our results to an analytic approximation to further validate our numerical approach.
2.2 Electron Tunneling

In nanometer scale devices, the quantum tunneling phenomenon can be very important. In our devices quantum tunneling leads to an electron current flow between the two metals. Applying quantum mechanics the electron tunnels through the potential barriers is represented by a wave function. For a stationary state the wave function is expressed as:

\[ \Psi(\vec{r},t) = \psi(\vec{r},E)e^{-iEt/\hbar}, \]  

(2.1)

We can solve for the wave function by using Schrödinger’s equation, which has the form:

\[ H \psi = \hbar^2 \nabla^2 \psi + (V(z) + V_{\text{sidewalls}}(x,y))\psi. \]  

(2.2)

In Eq. (2.2), the potential is separated into two parts: one for the longitudinal potential across the interfaces of the MIM materials, \( V(z) \), Here the potential \( V \) is separated into two parts: one for the longitudinal potential across the interfaces of the MIM materials, which includes a static applied field and the second, is for lateral confinement geometries to create a nanoslab or nanowire. The Hamiltonian \( H_0 \) does not include the interaction of the MIM structure with the electromagnetic field that will be discussed later. Right now we only assume static field biases are included in Eq. (2.2).

There are many methods that could be applied to solve Schrödinger’s equation and we use two of them. The first one is the transfer matrix method (TMM) [11] of solving for plane waves in regions that have constant potentials. The second method can be called a shooting method [12] of directly solving Schrödinger’s equation by using a finite difference technique. Both of them
have to compare with WKB (Wentzel, Kramers, Brillouin) [13] approximation to the electron tunneling probability.

The operation diagram of active region for an MIM diode is presented in Figure 2.1. The MIM devices made from sandwiching an insulator between two different metals. The energy barrier shape is determined by the material properties, which are the work function of metals on both sides (\( \phi_1 \) and \( \phi_2 \)) and electron affinity of the insulators (\( \phi_i \)). The work functions are the energy difference between the electron’s kinetic energy and the Fermi energy which marks the filled electronic bands of the material. We take the Fermi energy as 10 eV, but its precise value is not important for calculating the tunneling current characteristics. The potential barrier energy for metal 1 is the work function (plus the Fermi energy) minus the electron affinity: \( \varphi_1 = \phi_1 - \phi_i \). Similarly in metal two the barrier height is given by: \( \varphi_2 = \phi_2 - \phi_i \) [14]. The metal work functions and dielectric electron affinities are found in the literature and results for selected materials are tabulated in Appendix A.
Figure 2.1 The ideal energy band for an asymmetric MIM tunneling diode. Two different metals (NbN, Nb) are separated by 2nm insulator (Nb$_2$O$_5$). The Fermi level of both metals is assumed as 10eV in this case.

If we applied a voltage across the diode, the potential energy is shifted by the addition of the field across the dielectric. Figure 2.1 is an illustration of the potential energy function for a MIM diode with the different metals used for the two electrodes of different applied voltage condition.
2.2 Energy band diagram of a MIM diode with different metal electrodes (Metal 1 and Metal 2). (a) Forward bias: electron tunneling from metal 1 to metal 2 is dominant, (b) Backward bias: A bias voltage applied in metal 1 result in electrons in metal 2 tunnels through the barrier into metal 1.

2.2.1 Transfer Matrix Method (TMM)

The TMM is easy to implement. For the moment the sidewalls are neglected. Since the potential depends only on the z-coordinate, so we can separate the transverse coordinates and assume they are plane waves using:

$$\psi(x, y, z) = \tilde{\psi}(z)e^{i(k_x x + k_y y)}.$$  \hspace{2cm} (2.3)

Infinite barriers for sidewalls will quantize \((k_x, k_y)\) and the solution for the tunneling problem will remain unchanged.

This reduces the Schrödinger’s equation (2.2) to a one-dimensional form

$$-\frac{\hbar^2}{2m} \frac{d^2 \tilde{\psi}(z)}{dz^2} = (E_z - V(z))\tilde{\psi}(z).$$  \hspace{2cm} (2.4)

The electronic states of energy \(E_z\) are produced by the solution of the one-dimensional Schrödinger equation using the wave function in Eq. (2.2) the total electron energy is given by:
Figure 2.2 is an illustration of a potential energy band for an MIM diode. In the barrier region the potential is not constant, but it can be approximated as piece-wise constant by dividing the region into sufficiently small slices called sub-regions.

\[ E = E_z + \frac{\hbar^2}{2m}(k_x^2 + k_y^2). \]  
(2.5)

Figure 2.3 An illustrative electronic potential (blue) with a barrier region that is characterized by a linear slope. The sub-regions of constant potential are indicated by boxes of small width and heights that are adjusted to the potential height in the region.

The energy band system of MIM diode we used in Figure 2.3 is Niobium Nitride (NbN) for the metal 1 and Niobium (Nb) for the metal 2 with a 2nm thickness Niobium oxide (\( \text{Nb}_2\text{O}_5 \)) sandwiched in between. The Fermi level of both metals in Figure 2.3 is assumed to be 10 eV. The work function parameters of metals and electron affinity parameters for insulators are found in Appendix A.

We sub-divide the barrier region into \( N \) slices the \( \alpha \text{th} \) sub-region is assumed to have a constant potential, \( V(z_\alpha) \). So the wave function in the \( \alpha \text{th} \)
sub-region can be written as a summation of forward and backward traveling plane waves:

\[ \psi_a(z) = A_a e^{ik_a(z-z_a)} + B_a e^{-ik_a(z-z_a)}, \quad z_a < z < z_{a+1}, \quad (2.6) \]

The longitudinal wave vector is

\[ k_a = \sqrt{\left(E_z - V(z_a)\right) \frac{2m}{\hbar^2}}. \quad (2.7) \]

The boundaries between each region are the set of values \( \{z_a, \alpha=1,2,...,N\} \). The boundary conditions are the continuity of the wave function and its derivative, which are explicitly written as:

\[ A_a e^{ik_a(z_{a+1}-z_a)} + B_a e^{-ik_a(z_{a+1}-z_a)} = A_{a+1} + B_{a+1}, \]

\[ k_a \left( A_a e^{ik_a(z_{a+1}-z_a)} - B_a e^{-ik_a(z_{a+1}-z_a)} \right) = k_{a+1} \left( A_{a+1} - B_{a+1} \right), \quad z = z_{a+1} \quad (2.8) \]

In matrix form the boundary conditions can be expressed as:

\[ M_{a} V_{a} = M_{a+1,0} V_{a+1}, \quad (2.9) \]

where

\[ V_{a} = \begin{pmatrix} A_a \\ B_a \end{pmatrix}, \quad M_{a} = \begin{pmatrix} e^{ik_a(z_{a+1}-z_a)} & e^{-ik_a(z_{a+1}-z_a)} \\ k_a e^{ik_a(z_{a+1}-z_a)} & -k_a e^{-ik_a(z_{a+1}-z_a)} \end{pmatrix}, \quad M_{a,0} = \begin{pmatrix} 1 & 1 \\ k_a & -k_a \end{pmatrix}. \quad (2.10) \]

The determinant of the matrices \( M_{a} \) and \( M_{a,0} \) is \(-2k_a\). The program for the solution is given below. The matrices in Eq. (2.9) are further evaluated using the relation:

\[ V_{a} = T_{a} V_{a+1} = M_{a}^{-1} M_{a+1,0} V_{a+1}, \quad (2.11) \]

The matrix \( T_{a} \) is given by:

\[ T_{a} = \begin{pmatrix} 0.5(k_a + k_{a+1})/k_a e^{-ik_a(z_{a+1}-z_a)} & 0.5(k_a - k_{a+1})/k_a e^{-ik_a(z_{a+1}-z_a)} \\ 0.5(k_a - k_{a+1})/k_a e^{ik_a(z_{a+1}-z_a)} & 0.5(k_a + k_{a+1})/k_a e^{ik_a(z_{a+1}-z_a)} \end{pmatrix}. \quad (2.12) \]

The transmission is determined by the relation:
\[ T = \left| \frac{A_N}{A_1} \right|^2. \]  

(2.13)

The transmission for the potential in Figure 2.3 is plotted in Figure 2.4 for a number of energies (9eV~12eV) on a log scale plot. We have 2nm thickness barrier (Niobium Oxide) and with a positive voltage applied (0.3V) on the metal 2 (Niobium).

![Figure 2.4 The tunneling probability (log base 10) as a function of energy \( E_z \) (from 9eV to 12eV) for the MIM structure shown in Figure (2.2-a).](image)

The transmission coefficient changes by nearly 10 orders of magnitude over the range of energies from 9 eV to 12 eV.

The wave function is plotted by plotting the points:

\[
\{ z_{\alpha+1}, \quad \tilde{\psi}_\alpha(z_{\alpha+1}) = A_\alpha e^{ik_d(z_{\alpha+1}-z_\alpha)} + B_\alpha e^{-ik_d(z_{\alpha+1}-z_\alpha)}, \quad \text{for} \quad \alpha = 1,2,...N-1. \}
\]

(2.14)

This is shown in Figure 2.5 below where we plot for an energy \( E_z = 12[eV] \).
Figure 2.5 The wave function magnitude plotted versus position for an energy of 12 [eV] with the same potential as in Figure (2.2-a).

2.2.2 Shooting Method

In this section, we will use the direct finite-difference, numerical solution of Schrödinger’s Equation to solving tunneling probability for any potential well. We still start with the time-independent Schrödinger Equation, Eq. (2.4). The shooting method is used to find a numerical solution of both the energy eigenvalues and the eigenfunctions for any specified potential well [12]. In this case we are only interested in evaluating the tunneling probability for a significant range of electron energies that depend on potential barrier of the MIM structures. Therefore, we limit our calculation of the tunneling probability to electron energies in the range from 9eV to12eV. Now our problem is to find a numerical solution for solving the differential Eq. (2.4) which is known as shooting method.

To solve Schrödinger’s equation numerically, we have to know each wave function at each point. With this aim, we have to expand the second-order
derivative in Schrödinger’s equation in the form of a backward finite difference.

Any function can be illustrated in Figure 2.6:

![Figure 2.6 An illustration of the first derivative of a function using finite differences.](image)

From Figure 2.6, the first derivative can be defined as two known points:

\[
\frac{df}{dz} = \frac{\Delta f}{\Delta z} = \frac{f(z) - f(z - \delta z)}{\delta z}.
\] (2.15)

Hence, the second derivative follows as:

\[
\frac{d^2 f}{dz^2} = \frac{df}{dz}\left|_z - \frac{df}{dz}\right|_{-\delta z}.
\] (2.16)

The second derivative can be used in the finite difference forms such as first derivative:

\[
\frac{d^2 f}{dz^2} \approx \frac{f(z) - 2f(z - \delta z) + f(z - 2\delta z)}{(\delta z)^2}.
\] (2.17)

Substituting Eq. (2.17) in the original Schrödinger equation (2.4) then we have:

\[
-\frac{\hbar^2}{2m} \frac{\psi(z) - 2\psi(z - \delta z) + \psi(z - 2\delta z)}{(\delta z)^2} = [E_z - V(z - \delta z)]\psi(z - \delta z),
\] (2.18)

\[
\therefore \psi(z - 2\delta z) = \left[\frac{2m}{\hbar^2} (\delta z)^2 (V(z - \delta z) - E_z) + 2\psi(z - \delta z) - \psi(z)\right].
\] (2.19)

Eq. (2.19) shows that if the wave function is known at the two points \((z - \delta z)\) and \(z\), then the value of wave function at third point \((z - 2\delta z)\) can
be calculated for any electron energy $E_z$. Therefore, using this new point $\psi(z-2\delta z)$, together with $\psi(z-\delta z)$ and by making the transformation $(z-2\delta z-\delta z)$, a fourth point $\psi(z-3\delta z)$ can be calculated, and so on. The shooting method expression for solving Schrödinger equation numerically is complete once the exact form of wave function and its derivative at the starting of two points is included. To determine the first two points, we can simply use boundary conditions for stationary states. The shooting method must be solved by starting at the output (after tunneling) end of the potential structure. In our case, we treat the problem after tunneling through the barrier as no reflection. In other words there is only an outgoing wave. Therefore, we can simply assume that the first value of wave function is given as:

$$\psi(z)=1,$$  

(2.20)

Then for second point we should have:

$$\psi(z-\delta z)=\psi(z)\exp(-ik\delta z).$$  

(2.21)

Now the third point is solved following by applying the shooting method expression in Eq. (2.19). Other points are solved by repeated application of Eq. (2.19). The complete wave function $\psi(z)$ can be deduced for all electron energies in the range considered $E$ (9eV~12eV) by using the shooting method with boundary conditions Eqs. (2.20-21) and applying the finite difference result in Eq. (2.19).

The tunneling probability of electron can be defined as the square of the ratio between the transmitted amplitude of the wave function within metal 2 to the incident amplitude of the wave function within metal 1, which is

$$T = \left|\frac{C}{A}\right|^2$$

(see Figure 2.7 for a definition of the amplitudes).
In Figure 2.7, A is the incident amplitude, B is reflected amplitude, C is transmitted amplitude and there is no reflected wave on the right barrier surface. Mathematically we may express the wave amplitudes by the following derivation.

The wave function decays exponentially into the end barriers. According to previous section, the wave function in the left region can be rewritten as a linear combination of travelling waves.

\[ \psi_l(z) = Ae^{ikz} + Be^{-ikz}. \] (2.22)

Similarly, for the right side, we have:

\[ \psi_r(z) = Ce^{ikz}. \] (2.23)

According to the “Connection rules” [12] at a potential step, we should have the wave function and its derivative at both \( z=0 \) and \( z=2 \text{nm} \) continuous and thus the amplitudes satisfy the following conditions (for real parameters):

\[ A^2 - B^2 = C^2. \] (2.24)
For simplicity, we assume that the amplitude of transmission has to be equal to 1 ($C=1$), so the tunneling probability is:

$$T = \left| \frac{C}{A} \right|^2 = \frac{1}{A^2}. \quad (2.25)$$

To determine the amplitudes $A$ from above equations, one finds the relation:

$$\psi_j(z) = Ae^{i k z} + Be^{-i k z}$$

$$= A(\cos k z + i \sin k z) + B(\cos k z - i \sin k z)$$

$$= (A + B) \cos k z + i(A - B) \sin k z$$

$$\left| \psi_j(z) \right|^2 = (A + B)^2 \cos^2 k z + (A - B)^2 \sin^2 k z \quad (2.26)$$

$$= (A^2 + B^2 + 2AB) \cos^2 k z + (A^2 + B^2 - 2AB) \sin^2 k z$$

$$= (A^2 + B^2) (\cos^2 k z + \sin^2 k z) + 2AB (\cos^2 k z - \sin^2 k z)$$

$$= A^2 + B^2 + 2AB \cos k z$$

Therefore, for the maximum and minimum values of above relation, we have:

$$\left| \psi_j(z) \right|_{\text{max}}^2 = (A + B)^2$$

$$\left| \psi_j(z) \right|_{\text{min}}^2 = (A - B)^2 \quad (2.27)$$

$$\left| \psi_j(z) \right|_{\text{max}}^2 + \left| \psi_j(z) \right|_{\text{min}}^2 = 2(A^2 + B^2).$$

Since we have $A^2 - B^2 = C^2 = 1$, we can obtain:

$$\left| \psi_j(z) \right|_{\text{max}}^2 + \left| \psi_j(z) \right|_{\text{min}}^2 = 2(2B^2 + 1) = 4B^2 + 2,$$

$$\Rightarrow B^2 = \frac{\left| \psi_j(z) \right|_{\text{max}}^2 + \left| \psi_j(z) \right|_{\text{min}}^2 - 2}{4}. \quad (2.28)$$

Therefore, the tunneling probability can be calculated by:

$$T = \frac{1}{A^2} = \frac{1}{B^2 + 1} = \frac{4}{\left( \left| \psi_j(z) \right|_{\text{max}}^2 + \left| \psi_j(z) \right|_{\text{min}}^2 + 2 \right) \psi_j(z)^2 + 1}. \quad (2.29)$$

Obviously, the tunneling probability expression through the barriers can be calculated from the wave function expression in shooting method Eq. (2.19).
We plotted electron tunneling probability over a span of energies $E_z$ (from 9eV to 12eV) in Figure 2.8. The minimum potential for each metal in the absence of an applied field is 10 eV. The barrier height is 10.3 eV for the case plotted here.

![Figure 2.8 The tunneling probability as a function of energy for the energy diagram of MIM diode as same as Figure 2.3 with 0.3V applied voltage. The solution is plotted for both TMM (blue) and shooting method (red). The WKB approximation [13] is shown for comparison (green).](image)

The Figure 2.8 gives us an identical result for both TMM and shooting methods, as expected. The analytic WKB approximation [13] gives a good approximation well below the barrier height, but takes on a higher tunneling probability current value compared with TMM and shooting method, as the top of the barrier is approached. The WKB result is monotonic and takes the value of unity for energies larger than the barrier height. The WKB approximation has a smooth curve since it neglects the reflection and interference of the waves within barrier region.

The shape of the tunneling probability current is determined by the applied voltage across the MIM diode. The applied voltage changes the slope of the potential in the insulating region which directly corresponds to a change of
the applied electric field. We plotted the tunneling probability as a function of applied voltage and z-directed electron energy in Figure 2.9.

![Figure 2.9](image)

**Figure 2.9** The tunneling probability as a function of z-directed electron energy and applied voltage ($V_{\text{bias}}$) for the energy diagram of MIM diode as same as Figure 2.3. The simulation result obtained by TMM.

Note that the curves are all similar in shape, but there is a noticeable shift of the transmission maximums. In general for the applied bias voltage the tunneling probability current is increased. When the bias voltage is applied in the opposite direction a similar tunneling current is calculated, but the shifts are different. This will manifest itself as an asymmetry between the forward- and backward-biased MIM structures which gives it a diode action.
2.3 Chapter Summary

Quantum tunneling through a potential barrier has been described by quantum mechanics in this chapter and applied to the MIM structures of interest. Two simulation methods were used for calculating tunneling probability: TMM and shooting method. The results were compared with the analytical WKB method, which does not include electron reflection and interference effects. WKB is accurate well below the potential barrier where interference effects are negligible. We chose to use more accurate methods to describe the tunneling current. All of three methods were written in Matlab simulation software. The parameters we chose for MIM structures were taken from accepted values in the literature [15]. Grover’s paper studied the NbN/Nb$_2$O$_5$/Nb structure for the MIM. His gap parameter was 2 nm. The comparison between our result and Grover’s paper agreed very well and his results are reproduced in Figure 2.10. Figure 2.10a is the figure taken from Grover’s paper and on the right are our results reproduced from both TMM and the Shooting methods.
Figure 2.10 Comparison of tunneling probability between Grover's paper and our result.
(a) Grover’s paper (b) our result for the NbN/Nb$_2$O$_5$/Nb structure with a 2 nm insulator gap.

In Chapter 3, we discuss dc or unilluminated or dark tunneling current density for materials with plasmonic metals included as one of the metal layers. We also examine sidewall lateral confinement of the electrons and the effect of the walls on the dc current density. The dc tunneling current as a function of applied voltage and barrier thickness is plotted for several material combinations with different work functions and electron affinities.
CHAPTER III

TUNNELING CURRENT WITH SIDEWALL CONFINEMENT IN THE ABSENCE OF ILLUMINATION

3.1 Introduction

To understand the dark tunneling current of MIM diode is very important to characterize the electronic properties of the optical device and determine the photo response to illumination. In this chapter the tunneling current is derived for lateral confinement of the electrons in a nanowire (1D) or nanoslab (2D) geometry. Our terminology is as follows: the nanowire is a device with electron confinement in both lateral dimensions, and the nanoslab is a device with electron confinement for one lateral dimension. Our motivation for this is to understand the effect that small lateral dimensions would have on the tunneling current by electron confinement and quantization of the energy in the confinement directions. The electron current density in a quantum system is defined as:

\[ J_{QM} = \frac{e}{2m_e} \left[ \psi^* \frac{\hbar}{i} \nabla \psi - \psi^* \frac{\hbar}{i} \nabla \psi^* \right], \]

(3.1)

where \( J_{QM} \) is tunneling current, \( e \) is electron charge, \( m_e \) is electron mass, \( \psi^* \) is complex conjugate of wave function \( \psi \).

The sign of the charge is not important for this calculation. This is the not the measured current density. The current must be averaged over all possible wave
functions and weighted by the occupation probabilities. The current density consists of the contributions of electron longitudinal momentums, which are decomposed into plane waves:

\[ \psi = \psi(x, y, k_z)e^{ik_zz} \]  \hspace{1cm} (3.2)

The momentum \( k_z \) is related to the electron’s longitudinal kinetic energy. The lateral coordinates are not yet treated. The wave function is a superposition of all the possible longitudinal wave vectors weighted by amplitudes that are solution of Schrödinger’s equation.

### 3.2 Current Density 3D

We first consider the usual case that an electron traveling in a no sidewall confinement quantum system. 3D represents three degrees of freedom of electron motion. The dimensional relations for all three models (1D, 2D and 3D) are shown as outline in Table (3.1) \[12\]. As lateral confinement is introduced the degrees of freedom are reduced by the same number.

<table>
<thead>
<tr>
<th>System</th>
<th>( D_c )</th>
<th>( D_f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>2D (nanoslab)</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>1D (nanowire)</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 3.1 Expression of three different models (3D, 2D, 1D). \( D_f \) is the number of degrees of freedom, \( D_c \) is the number of direction confinement in the electron motion.

According to Eq. (3.1) and (3.2), the quantum mechanical current density in the longitudinal direction is:

\[ J_{\text{QM}}^{\text{out}} = \frac{e\hbar k_z}{m} |\psi|^2, \]  \hspace{1cm} (3.3)

The velocity of the particle in longitudinal direction is defined as:

\[ v_z = \frac{\hbar k_z}{m}, \]  \hspace{1cm} (3.4)
Obviously, the velocities in the transverse directions are similarly defined. The wave function after the barrier (i.e. in the metal) is expressed as a plane wave decomposition:

\[ \psi_{\text{after}}(\vec{r}) = \psi_{\text{after}}(\vec{k}) e^{\vec{k} \cdot \vec{r}}, \]  

(3.5)

Where \( \psi_{\text{after}}(\vec{k}) \) represent the wave function after the barrier.

The tunneling probability is related to the initial wave function by the relationship shown above:

\[ \psi_{\text{after}}(\vec{k}) = \sqrt{T_E(\vec{k})}. \]  

(3.6)

The current density is averaged over all wave vectors and weighted by the tunneling probability of finding an electron with the total energy \( E \). The occupation probability for an electron with energy \( E \) in Metal 1 is given by the Fermi-Dirac distribution function defined as (shown in Figure 3.1):

\[ f_1(E) = \frac{1}{e^{(E-E_f)/k_BT} + 1}, \]  

(3.7)

where \( E_f \) is the Fermi energy, \( T \) the lattice temperature and \( k_B \) is Boltzmann’s constant. An example of the MIM potential with Fermi energy 10 eV is shown in Figure 3.1. The Fermi Dirac distribution functions indicate the occupation probabilities of particular energy states. On the left hand side of Figure 3.1 the electron occupation is lowered due to the applied bias potential and on the right hand side the occupation probability remains the same.
Figure 3.1: Biased MIM junction with Fermi level and occupation probabilities indicated.

The metal on the left side is biased by an applied dc potential.

The average electron current density from metal 1 to metal 2 is expressed as

$$J^{3D}(1 \rightarrow 2) = 2e\int_0^\infty dk_z v_z T_E(E) \int f_1(E)(1 - f_2(E))dk_xdk_y. \quad (3.8)$$

The first integral is the integration over the longitudinal wave vector and it is weighted by the quantum tunneling current calculated in Chapter 2. The second integral appearing in Eq. (3-8) is the occupation probability that the state in Metal 1 is occupied and the same state in Metal 2 is not occupied. The occupation probability for the states is given by the expression:

$$f_1(E) = f(E + eV_{bias}) = \frac{1}{e^{(E + eV_{bias} - E_F)/k_BT} + 1}. \quad (3.9)$$

The average current density in the reverse direction is expressed as:

$$J^{3D}(2 \rightarrow 1) = 2e\int_0^\infty dk_z v_z T_E(E) \int f_2(E)(1 - f_1(E))dk_xdk_y. \quad (3.10)$$

The current density can be simplified to:
\[ J^{3D} = 2e\frac{m^3}{\hbar^3} \int_0^\infty dv_x v_x T(E_x) \int_0^\infty (f(E) - f(E + eV_d)) dv_y dv_y. \]  

(3.11)

This result is exactly the result found in literature [15]. Since our desired tunneling current expression is three dimensional quantum system, so the integration of expression (3.11) can be performed in polar coordinates by using following definition.

\[ dv_x dv_y = d\theta v_r dv_r = \frac{1}{m} d\theta dE_r, \quad \text{and} \quad v_z dv_z = \frac{1}{m} dE_z. \]  

(3.12)

The lateral and longitudinal electron energy is written by the summation of total electron energy:

\[ E = E_r + E_z. \]  

(3.13)

For constant values of \( E_z \) the lateral energy differential can be written as: \( dE_r = dE \). The current density in 3D is transformed to a simplified form:

\[ J^{3D} = 4\pi e\frac{m}{\hbar^3} \int_0^\infty dE_r T(E_r) \int_0^\infty (f(E) - f(E + eV_d)) dE. \]  

(3.14)

This expression is integrated using numerical techniques. It is straightforward to carry out the integrations.

### 3.3 Current Density 2D

The nanoslab has two degrees of freedom of electron motion so called 2D quantum system. Confine the x lateral dimension of the metal to a width \( d_x \). The energy is quantized due to this restriction. We posit that the corresponding 2D current density is

\[ J^{2D} = 2e\frac{m^2}{\hbar^2} \int_0^\infty dv_x v_x T^{1 \to 2}_E(E_x) \frac{1}{d_x} \sum_{n_y=1}^\infty \int (f(E) - f(E + eV_d)) dv_y. \]  

(3.15)

The total energy of the electron in the slab is:
\[ E = E_z + \frac{\hbar^2}{8m} \left( \frac{n_x}{d_x} \right)^2 + \frac{mv_y^2}{2}. \]  

(3.16)

The expression for \( J^{2D} \) is chosen because it yields the 3D result in the limit \( d_x \) goes to infinity. To show this result note that the differential of the wave vector \( x \)-component is

\[ \Delta k_x = \frac{\pi}{d_x}, \]  

(3.17)

and the velocity differential is

\[ \Delta v_x = \frac{h}{2\pi m} \Delta k_x. \]  

(3.18)

Extending the sum to include negative and positive momenta and making the above transformation to velocity space we have the sum replaced by an integral

\[ \frac{1}{d_x} \sum_{n_x=1}^{\infty} \rightarrow \frac{m}{h} \int_{-\infty}^{\infty} dv_x. \]  

(3.19)

Our evaluation shows that Eq. (3.15) for \( J^{2D} \) is nearly equal to \( J^{3D} \) for lateral confinement of the electron down to 10 nm.

3.4 Current Density 1D

Deriving the expression for the 1D current density is straight forward and can be done by extending the analysis presented in the previous section. The 1D current density is

\[ J^{1D} = 2e \frac{m}{\hbar} \int_{0}^{\infty} dv_x v_x T^{1 \rightarrow 2}_E (E_x) \frac{1}{d_x d_y} \sum_{n_x=1}^{\infty} \left( f(E) - f(E + eV_{z0}) \right). \]  

(3.20)

The total energy for this case is:

\[ E = E_z + \frac{\hbar^2}{8m} \left( \frac{n_x}{d_x} \right)^2 + \frac{\hbar^2}{8m} \left( \frac{n_y}{d_y} \right)^2. \]  

(3.21)
These can be applied to determine the current density in a similar fashion to the 3D case.

### 3.5 Simulation Results For Lateral Confinement

The current density calculations in 3D have been compared with results in the literature [15]. The 2D and 1D results are constructed to reduce to the 3D result in the limit of large dimensions. In Figure 3-2 (a, b, c and d) below four cases are exhibited. The current densities are plotted on a logarithmic (base 10) scale. The current density is lower for the confined electron cases. The 1D shows a trend toward lower current density than the 2D case. This establishes a consistent result for the confined electron geometry. For \( d_x = d_y = 100\,\text{nm} \) the current densities for the 2D and 1D geometries are within 2% and 4%, resp. of the 3D case.
Figure 3.2: Applied voltage as a function of current density for the case of MIM diode in Figure 2.3 design with gap=2nm. The lateral confinement parameters are: (a) $d_x = d_y = 100\,\text{nm}$, (b) $d_x = d_y = 50\,\text{nm}$, (c) $d_x = d_y = 25\,\text{nm}$, (d) $d_x = d_y = 10\,\text{nm}$.

3.6 Unilluminated Current Density Results For The MIM Structure

We explore several material combinations to calculate the unilluminated current flow for MIM diode in this section. The designs of two metals are chosen based on one having a pronounced surface plasmon resonance (SPR) properties and the difference of their work functions being within 1 eV of one another. The value is somewhat arbitrary, but is only meant as a rule of thumb for our studies. The insulator (or gap material) is chosen from a selection of metal oxides; the electron affinity is another important quantity for choosing the right oxide. A plasmonic metal (Au, Ag, Cu, Al) was chosen as one of the metal
elements to promote a strong field in the gap region between the two metals. Based on our numerical findings we look at the compatibility between the work functions and the electron affinity in determining which metals and insulators will be good candidates for MIM photodetectors. When the work functions are different by more than 1 eV and/or the electron affinity creates a barrier that is more than 1 eV the tunneling current is severely suppressed by many orders of magnitude.

In the previous section, we observed that the voltage bias applied across the gap plays an important role in determining the tunneling current. Another important factor is the thickness of gap of MIM diode. In a thicker electrode, the electron current density is suppressed and the photon field will be reduced because the charges are separated by a larger distance. So the insulation gap is typically thinner than 5 nm for quantum device operation. We change the thicknesses of the gap and voltage bias to explore how the tunneling current is affected by these two parameters.

We chose good plasmonic materials such as silver (Ag), gold (Au), copper (Cu), aluminum (Al) for one of metal elements of MIM diode in following dark current calculations. For instance, the calculated dark current curve for the Ag/TiO$_2$/Ti MIM diode is plotted the on log scale for forward and backward current flow in Figure 3.3. The current density is plotted in semilog plot, so that, for instance, a 10 on the vertical axis corresponds to a current density of $10^{10}$ A/cm$^2$. The thickness of gap is sampled by 23 points from 0.4 nm to 5 nm. And the applied voltage is sampled by 201 points from negative 5 V to positive 5 V. The current density is asymmetric due to the asymmetry in the MIM potential. Several examples are illustrated in this section and the rest
are relegated to an Appendix B. For zero applied voltage the current is zero and the lower bound on the vertical axis was set to 0.

Figure 3.3: The calculated tunneling current curve Vs. applied voltage and different gap thickness for Ag/TiO$_2$/Ti MIM diode. The tunneling current curve calculated by the TMM and plotted by surface function in Matlab.

Figure 3.4 through Figure 3.6, we plotted three more illustrative examples of the dark tunneling current versus identical variables. The for MIM diode cases chosen were Al/Nb$_2$O$_5$/Nb, Cu/Nb$_2$O$_5$/Nb, Au/Nb$_2$O$_5$/Nb. The parameters for the materials for the current calculations are shown in Appendix A. We do not use combination of silver and niobium, since silver and aluminum have very similar work function and that would lead to nearly identical results, as far as the quantum tunneling part of the calculations are concerned. It is worth noting that all these cases have nearly the same range of values for the dark current density.
Figure 3.4: The calculated tunneling current curve vs. applied voltage and different gap thickness for Al/Nb$_2$O$_5$/Nb MIM diode.

Figure 3.5: The calculated tunneling current curve vs. applied voltage and different gap thickness for Cu/Nb$_2$O$_5$/Nb MIM diode.
Figure 3.6: The calculated tunneling current curve vs. applied voltage and different gap thickness for Au/Nb$_2$O$_5$/Nb MIM diode.

The trends in all the dark current figures are the same (Figure 3.3 - 6). For a fixed applied voltage, the dark tunneling current decreases with increasing gap thickness; in other words it is more difficult for the electron to tunnel through a thicker barrier. Also for a fixed gap thickness, a higher dark tunneling current obtained by increasing the applied voltage. It is not apparent in these figures, but the dominant current (forward or backward) for a given magnitude of bias may not be the same for all bias voltages. The two can cross one another at a given voltage which will affect the asymmetry in the net rectified diode current.

In Figure 3.4 and 3.5, the dark tunneling current results show a modest asymmetry (1 order of magnitude difference) of forward and backward current flow at the largest applied bias voltages. But in Figure 3.6 we have a tremendous forward-to-backward current ratio. Since the asymmetry of two
opposite motion is dominated by differences between two work function of metals. The MIM diode $\text{Au/Nb}_2\text{O}_5/\text{Nb}$ which has large asymmetry is not a good choice for responsivity calculation. The responsivity saturates for large asymmetry. The evidence for this will be discussed in next chapter. For more MIM diode simulation results with different combinations of materials the reader is referred to APPENDIX B.
CHAPTER IV
ILLUMINATED MIM CHARACTERISTICS

4.1 Introduction

The previous chapter determined the dc tunneling current applying quantum tunneling calculations applying statistical occupation properties of the electronic states. The current flow was a direct result of a bias voltage applied across an insulator between the two metals and the fact that the metals has different work functions different led to an asymmetry in the forward- and backward-biased MIM structure leading to diode action.

In this chapter we incorporate the effects of the electromagnetic field to find the MIM diode action. The MIM response time is ultrafast which means that the carriers respond in time faster than the period of oscillation of the electromagnetic field. The relevant theory for photoelectrons was presented by Tien and Gordon [16] and applied to MIM structures with superconducting metals (sometimes referred to as SIS structures). An applied microwave field elicits an I-V response curve. The theory has been applied in a number of cases to other systems including normal metals and especially we are interested in the systems with two different normal metals [16, 17].

In their theory an effective ac voltage that represents the strength of the electromagnetic field in the insulator region between the two metals. The dc current density is the only quantity required to calculate the ac response and the responsivity of the MIM structures due to the electromagnetic field.
4.2 Weak Radiation Field

The Hamiltonian for the electromagnetic field that affects the tunneling across the barrier is given by

\[ H(t) = H_0 + V_\omega \cos(\omega t). \]  \hspace{1cm} (4.1)

The last term on the right hand side is the ac voltage, \( V_\omega \), across insulator gap of the MIM structure. The time-dependent contribution to the Hamiltonian is modeled as a voltage across the MIM structure. The potential \( V_\omega \) is related to the strength of the electric field. The field in the gap can increase the coupling which is accomplished by incorporating plasmonic effects into the MIM design. When the electric field parallel to the current flow direction is denoted as \( E_\omega \), the voltage is given by

\[ V_\omega = E_\omega d, \]  \hspace{1cm} (4.2)

where \( d \) is the thickness of the insulating gap. For this Hamiltonian the wave function becomes

\[ \Psi(\vec{r}, t) = \psi(\vec{r}) e^{-i[H_0 + \frac{1}{\hbar} \int_0^t V_\omega \cos(\omega t) \, dt]}/(2 \hbar). \]  \hspace{1cm} (4.3)

The integral over the cosine function yields the exact result

\[ e^{-i\int_0^t V_\omega \cos(\omega t) \, dt/\hbar} = e^{-i(V_\omega/\hbar) \sin(\omega t)} = \sum_{n=-\infty}^{\infty} J_n(\alpha) e^{-i\omega n}, \]  \hspace{1cm} (4.4)

where the alpha parameter is defined as: \( \alpha = eV_\omega/\hbar \omega = eV_\omega/E_{ph} \) and \( J_n(\alpha) \) is the \( n^{th} \) order Bessel function. \( E_{ph} \) is photon energy of electromagnetic field.

The illuminated MIM structure wave function is expressed as:

\[ \Psi(\vec{r}, t) = \sum_{n=-\infty}^{\infty} J_n(\alpha) e^{-iE_\omega/\hbar} e^{-i\omega n} \psi(\vec{r}). \]  \hspace{1cm} (4.5)
After the interaction with the electromagnetic field the total energy of the electron, \( E + n\hbar \omega \) is increased or decreased depending on the sign of \( n \) by interaction with the electromagnetic field. The transmitted portion of the wave function for a plane wave after passing through the barrier is now modified by the photons’ energy and is expressed as:

\[
\psi_{\text{after}}(\vec{r}) = \psi_{\text{after}}(\vec{k}) e^{iE \tau} = \sqrt{T_E(\vec{k})} e^{iE \tau}.
\]  

(4.6)

The current density is recalculated using this wave function as the starting expression for the quantum mechanical tunneling current:

\[
J_{\text{QM}}(E) = \frac{e}{2m_e} \left[ \psi^* \frac{\hbar}{i} \nabla \psi - \psi \frac{\hbar}{i} \nabla \psi^* \right] = \frac{e}{2m_e} |\Psi(\vec{r}, t)|^2
\]

\[
= \frac{e}{2m_e} \sum_{n=-\infty}^{\infty} \sum_{n'=\infty}^{\infty} \sqrt{T_E(\vec{k})} T_{E'}(\vec{k}) e^{-\frac{i(n-n')\hbar \omega + E \hbar}{\hbar}} J_n(\alpha) J_{n'}(\alpha).
\]

(4.7)

The current flows along the z axis, so only a scalar quantity needs to be considered in the following development [14, 17]. The average dc tunneling current is determined by the case \( n' = n \) and averaging over the occupation probabilities of the states. The dc current flow from metal 1 to metal 2 is obtained from the quantum mechanical result by multiplying by the occupation probability of the initial state, \( f_1(E) \), which is the same as the occupation probability in the dark current calculation. However, the probability that the final state is unoccupied is changed by the photon energy. The shift depends on the number of photons and is given by:

\[
1 - f_2(E) = 1 - f(E + n\hbar \omega + eV_D) = 1 - \frac{1}{e^{(E + n\hbar \omega + eV_D - E_F)/k_B T} + 1}.
\]

(4.8)

In other words it is as though the applied potential is shifted by the number of photon quanta assisting in the electron tunneling.
\[
J_{dc}^{(1 \rightarrow 2)} = \sum_{n=-\infty}^{\infty} J_n^2(\alpha) 2e \frac{m^3}{\hbar^3} \int_0^{\infty} dv_x v_z T_{E_n}^{E_z, V_{D_n} + n\hbar \omega} \int \left[ f(E) (1 - f(E + eV_{D_n} + n\hbar \omega)) \right] dv_x dv_y,
\]

(4.9)

and the average dc current from metal 2 to 1 is calculated in the same fashion:

\[
J_{dc}^{(2 \rightarrow 1)} = \sum_{n=-\infty}^{\infty} J_n^2(\alpha) 2e \frac{m^3}{\hbar^3} \int_0^{\infty} dv_x v_z T_{E_n}^{E_z, V_{D_n} + n\hbar \omega} \int \left[ f(E + eV_{D_n} + n\hbar \omega) \right] dv_x dv_y.
\]

(4.10)

The net average dc current assumed the transmission amplitude is the difference of the two expressions Eq. (4.9) and (4.10):

\[
J_{dc} = \sum_{n=-\infty}^{\infty} J_n^2(\alpha) 2e \frac{m^3}{\hbar^3} \int_0^{\infty} dv_x v_z \left( T_{E_n}^{E_z, V_{D_n} + n\hbar \omega} \right) \int \left[ f(E) - f(E + eV_{D_n} + n\hbar \omega) \right] dv_x dv_y
\]

(4.11)

Eq. (4.11) is the photon assisted tunneling current density or dc current and it depends only on the dark current density already calculated in Chapter 3.

The effect of illumination on the tunneling process is illustrated in Figure 4.1 below where effectively the photon changes the bias by a multi-photon process. The number, \( n \), can be either positive or negative. When it is negative the effective Fermi energy can be larger than for the unbiased metal which will block the current from passing through the barrier because the electron states are occupied. At optical frequencies the photon assisted bias can be quite large for very few photon excitations. We will keep the net photon assisted bias to 5eV or less. That limits the wavelengths we can study and we arbitrarily chose the wavelength of 1 micron as our shortest value.
Figure 4.1: Illustration of the photon assisted tunneling process. The interaction of the electromagnetic field raises the energy of the electron to help it transition across the barrier. At single photon energies approaching the visible or near IR regime or for multi-photon cases at longer wavelengths (i.e. n>1 in this case) the electron’s energy can be larger than the barrier height.

The illuminated dc current depends only on the photon frequency via the shift of the applied potential. The effect of adding an electromagnetic field alters the rectified current in the MIM device and even in the case without an applied voltage \( V_{bias} = 0 \) a dc current flows. For small \( \alpha \) parameter or small incoming signal, the Bessel functions are expanded in lowest-order in the parameter. The leading terms of Eq. (4.11) are \( n = 0 \) and \( \pm 1 \) terms. Therefore, the illuminated dc current expression (4.11) for small incoming field can be reduced as:

\[
J^{dc}_{V_{bias}}(V_{bias}) = J_1^2(\alpha)J^{3D}(V_{bias} + \frac{\hbar \omega}{e})
+ J_{-1}^2(\alpha)J^{3D}(V_{bias} - \frac{\hbar \omega}{e}) + J_0^2(\alpha)J^{3D}(V_{bias}).
\]
The calculated illuminated dc current curve for MIM diode Ag/TiO$_2$/Ti in Figure 3.3 is plotted on log scale below. For constant of alpha parameter, the illuminated dc current only depends on the photon frequency via the shift of the applied potential. The illuminated dc curves are plotted for 4 different values of alpha parameters in Figure 4.2. The $\alpha = 0$, curve is the dark current we found in Chapter 3, as expected from the above expressions. As the alpha parameter increases, corresponding to an increasing the electromagnetic field energy incident on the MIM diode, the illuminated dc current increases and the minimum shifts to the negatively bias potential region. We only use small alpha in Figure 4.2 for the weak incoming field.

![Illuminated dc current vs. applied voltage for MIM diode Ag/TiO$_2$/Ti under small incoming field. The thickness is fixed at 2nm as an example and the photon energy is 1.4 eV. The red curve shows when alpha is equal to zero corresponding to dark current in Chapter 3.](image)

Using Eq. (4.12), the change of dc current due to the electromagnetic field is written as:
\[ \Delta J^{dc}(V_{bias}) = \frac{\alpha^2}{4} \left[ J^{3D}(V_{bias} + \frac{\hbar \omega}{e}) - 2J^{3D}(V_{bias}) + J^{3D}(V_{bias} - \frac{\hbar \omega}{e}) \right]. \tag{4.13} \]

The quantum mechanical ac current has all the harmonic components of the applied field \((n' = n - 1)\). The final expression is expressed as [18].

\[ J^{\omega} = \sum_{n=-\infty}^{\infty} J_n(\alpha)(J_{n+1}(\alpha) + J_{n-1}(\alpha))J^{3D}(V_D + n\hbar \omega / e). \tag{4.14} \]

Similarly, expanding Bessel function in lowest-order, we have:

\[ J^{\omega} = \frac{\alpha}{2} \left[ J^{3D}(V_{bias} + \hbar \omega / e) - J^{3D}(V_{bias} - \hbar \omega / e) \right]. \tag{4.15} \]

The results for the ac and change of dc current for a weak incoming electromagnetic field are evaluated to determine the MIM responsivity. The weak-field, MIM diode responsivity expression is given by [18, 19]:

\[ R = \frac{\Delta J^{dc}}{J^{\omega}} = \frac{2e}{\alpha \hbar \omega} \left[ \frac{J^{3D}(V_{bias} + \hbar \omega / e) - 2J^{3D}(V_{bias}) + J^{3D}(V_{bias} - \hbar \omega / e)}{J^{3D}(V_{bias} + \hbar \omega / e) - J^{3D}(V_{bias} - \hbar \omega / e)} \right]. \tag{4.16} \]

Without applied voltage and with applied voltage, the calculated responsivity as a function of gap and wavelength \((\lambda)\) for several MIM diodes are shown in following Figures. It is interesting that the theory calculates the current density for the illuminated MIM diode using only the dark current results. This simplifies the calculation of the illuminated current because we can calculate the dark current once and us the data as a look-up table for exploring the effect of various parameter values on the responsivity of the MIM used as a photodiode. We used the data of dark current \(J^{3D}\) from Chapter 3 for MIM diode in Figure 3.3 through Figure 3.6. For weak electromagnetic field, we use small alpha parameter which is equal to 0.05.
Figure 4.3: Responsivity vs. wavelength and gap for MIM diode Ag/TiO$_2$/Ti under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.

Figure 4.4: Responsivity vs. wavelength and gap for MIM diode Al/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.1V bias applied.

Figure 4.5: Responsivity vs. wavelength and gap for MIM diode Cu/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.
Figure 4.6: Responsivity vs. wavelength and gap for MIM diode Au/Nb$_2$O$_5$/Nb under small incoming field $\alpha = 0.05$. Right: Zero bias applied. Left: 0.3V bias applied.

In Figures 4.3-6 the MIM diode responsivity is plotted for two cases: zero applied bias and a non-zero applied bias. In all cases the responsivity increases as the insulator gap increased from 0.4nm. The responsivity is tiny when the gap parameter is small. However, the dependence on the gap parameter is not monotonic for larger gap parameter. This is more clearly seen in the zero bias cases. The responsivity can even decrease when the thickness of gap increases from about 4.6nm up to 5nm, as seen in Figures 4.3-5. The highest responsivity is often located for a gap parameter around 4.6nm. Another common trend is that increase of the responsivity at longer wavelengths with an eventual plateau as the photon energy becomes vanishingly small.

The responsivity is greatly modified by the bias, as shown in Figures 4.3-6. The curves become higher and smoother as the bias voltage is increased. The reason for the increase can be understood by considering Eq. (4.13, 15, 16). For zero bias the dc current vanishes for the term with no photon contribution and the two currents on either side of the zero bias are opposite in sign. This makes the change of the dc current the smaller and the ac current the larger; their ratio, i.e. the responsivity, is therefore suppressed.
To explore the response further consider the MIM diode case, Ag/TiO$_2$/Ti, as an illustrative example. The responsivity versus wavelength for MIM diode Ag/TiO$_2$/Ti with a fixed gap is plotted for five different biases in following Figures. All of five curves are compared with quantum efficiency limit $e / E_{ph}$ (shown in dot line). Simulations based on the responsivity versus gap parameter in Figure 4.3 helped guide our selection for value of gap. The thickness of gap for MIM diode Ag/TiO$_2$/Ti is 4nm with a weak applied electromagnetic field ($\alpha = 0.05$) in Figure 4.7 through Figure 4.11. The alpha parameter is not important here because it cancels out in the final expression.

Figure 4.7: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}$=0V. Quantum efficiency limit (dot).
Figure 4.8: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$(4nm)/Ti under small incoming field, with V$_{bias}$=0.1V. Quantum efficiency limit (dot).

Figure 4.9: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$(4nm)/Ti under small incoming field, with V$_{bias}$=0.2V. Quantum efficiency limit (dot).
Figure 4.10: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}=0.4$V. Quantum efficiency limit (dot).

Figure 4.11: Responsivity vs. log scale plot of wavelength for MIM diode Ag/TiO$_2$ (4nm)/Ti under small incoming field, with $V_{bias}=0.5$V. Quantum efficiency limit (dot).
At zero bias the quantum limit lies well above the responsivity curves for all wavelengths shown. The shortest wavelength we consider is $\lambda = 1$ micron and our longest wavelength is 25 microns. As previously mentioned increasing the wavelength raises the responsivity plateaus to a higher value. Increasing the dc bias voltage, $V_{bias}$, corresponds to probing a higher asymmetry along dc current curve. The results for adding or subtracting a photon have a higher change of the dc current and a smaller ac current, which drives up the responsivity. The responsivity results calculated for small bias do not show too much difference in the plateau (long wavelength) result (Figure 4.8 and Figure 4.9). At shorter wavelengths (or high photon energy), the responsivity approaches the quantum efficiency limit of $e/E_{ph}$ for modest bias voltages. However, for larger bias the longer wavelength responsivity can be improved over the entire range. Changing from 0.2 V to 0.4 V applied bias raises the responsivity plateau by a factor of 2. Increasing the applied bias voltage further has little effect on the plateau value.

### 4.3 Responsivity’s Radiation Field Strength Dependence

The responsivity for a range of electromagnetic field strengths is evaluated using the expression on the first line of Eq. (4.16) with the complete results in Eq. (4.13) and (4.14). All higher-order processes of Bessel function $n = 2, 3, 4, \ldots$ contributing to the dc current could not be neglected when the electromagnetic voltage is strong. In Figure 4.12 through Figure 4.15 the responsivity vs. lambda and alpha (i.e. strong electromagnetic field strength) is plotted for several MIM diode combinations. In these figures we use zero bias.
and the best gap parameter chosen for highest responsivity found in Figure 4.3 through Figure 4.6.

**Figure 4.12:** Responsivity vs. wavelength and alpha for MIM diode Ag/TiO\textsubscript{2} (4.6nm)/Ti under strong incoming field, with $V_{\text{bias}}=0V$.

**Figure 4.13:** Responsivity vs. wavelength and alpha for MIM diode Al/Nb\textsubscript{2}O\textsubscript{5} (4.6nm)/Nb under strong incoming field, with $V_{\text{bias}}=0V$. 
Figure 4.14: Responsivity vs. wavelength and alpha for MIM diode Cu/Nb$_2$O$_5$/Nb under strong incoming field, with $V_{bias}=0$V.

Figure 4.15: Responsivity vs. wavelength and alpha for MIM diode Au/Nb$_2$O$_5$/Nb under strong incoming field, with $V_{bias}=0$V.
At a large alpha parameter, the responsivity is not changed significantly compared to responsivity at a small alpha. In fact somewhat surprisingly the responsivity is reduced as alpha increases.

In the following section we will estimate the alpha parameter under different circumstances. The strength of the electromagnetic field in the gap regions is an important parameter that will ultimately determine the efficiency of the energy harvesting and the responsivity of MIM photodetector devices. The optical voltage is concentrated in the gap between the two metals and therefore can be quite large due to the nanometer size gap and the surface plasmon resonance effects.

### 4.4 Concentrated Solar Irradiance

Up to this point we have used the electromagnetic voltage appearing in the alpha parameter as an unknown variable. Now let’s consider what is the strength of the field for solar optical fields? The average irradiance from the sun on the earth is about $125\text{W/m}^2$. First, let us consider a solar concentrator that focuses light with an aperture radius of 10 cm to a spot size of 100 microns. The irradiance at the focus is: $1.25 \times 10^8 \text{W/m}^2$. The corresponding electric field is:

\[
E_\omega = \sqrt{2I/e_0c} = 3.069 \times 10^5 \text{V/m}. \tag{4.17}
\]

The voltage across the MIM junction for an insulator of thickness 2 nm is $V_\omega = 0.6138 \text{mV}$ which is a very small voltage, but not negligible. In comparison with the photon energy per electron charge at a wavelength of 1 micron the result is:

\[
E_{\text{ph}} = \hbar \omega / e = 1.24 \text{V}. \tag{4.18}
\]
As a result the alpha parameter in the Tien and Gordon [15, 16] theory is small, which is:

\[ \alpha = \frac{V_{\alpha}}{E_{ph}} = 4.94 \times 10^{-4}. \]  \hspace{1cm} (4.19)

Therefore, the Bessel functions appearing in the expression for the current will be correspondingly tiny. For this case, we have:

\[ J_1(\alpha)^2 = 6.1 \times 10^{-8}. \]  \hspace{1cm} (4.20)

4.5 Plasmonic Enhancement

Plasmonic enhancement of the electromagnetic field increases the coupling constant. In a gap that is only a few nanometers in width, the field enhancement can be orders of magnitude. The open question now is: how strong can the field become? The field enhancement in the insulating gap region of three orders of magnitude could be useful for efficient detection and energy harvesting.

4.6 Electric Field Enhancement

Surface plasmon resonance for a single ellipsoidal particle is an analytically solved problem. We use the results for plasmonic material silver here. The absorption spectra for different particle geometries (the major and minor axes ratio is changed) are shown below for the field along two different principal axes. In the spherical case the resonance frequencies are degenerate and they separate further as the axes are changed.
Figure 4.16 (a) Absorption as a function of wavelength (350nm–800nm) for different particle shape from spherical to aspect ratio 10:1. (b) Local electrical field distribution around a prolate spheroidal shaped particle at the wavelength of the surface plasmon resonance (x,z) plane.

In Figure 4.16a, the ratio of minor to major axes $r$ controls the shape of metallic spheroid. The green curve shows the electric field parallel to major axis, and the blue curve shows the electric field perpendicular to major axis. We use 8 values of $r$ to compute the curves ($r=0.99, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3$).
The arrows show the progression in r values from 0.3 to 0.99 for each resonance. The stronger resonance is due to the field along the z-axis. The two resonances overlap in the limit of a sphere (r=1). One case of the field squared relative to the applied field is shown in Figure 4.16b. The field is enhanced about 10x near the end of the prolate spheroid. We can exactly to see the strong field confinement at the tip of the nanorod based on surface plasmon resonance (SPR) theory. The field close to the surface is enhanced by about 1 order of magnitude, but the surface plasmon resonance is relatively narrow which means that the field is enhanced only for a relatively narrow band of wavelengths.

However, SPR is not the only mechanism for increasing the field in the gap between two spheroids. Electrostatic charges at the tips of the spheroids will also create enhanced fields. The electrostatic mechanism is illustrated in Figures 4.17. The applied field is nominally taken as 1 V/m. In Figure 4.17a the field is strongly confined to the gap region between the two nanowires. A close up of the gap in Figure 4.17b shows that the field is concentrated to a narrow region and it is increased by about 70 time over the value of the applied field.

![Figure 4.17: Field intensity in the vicinity of two elliptical cross-section nanowires with major and minor axes 50nm and 10 nm respectively. The gap is 1.9 nm. (a) the two elliptic cross sections of the nanowires with field strength indicated in color. (b) a close up of the gap region with field magnitude shown on the bar. Courtesy of Domenico deCeglia.](image)
The map of the field enhancement in the gap versus wavelength and gap size is shown in Figure 4.18. The field is strongest for the smallest gaps with an enhancement of three orders of magnitude. The value drops rapidly for gap sizes in the 2-3 nm range the enhancement rages from 30 to 100 times the applied field.

Figure 4.18: Plot of the field intensity versus wavelength for the maximum field as a function of wavelength. Courtesy of Domenico deCeglia.

The enhancement for the above two cases is somewhat modest given the alpha parameter values will still be small. However, for two prolate spheroids brought close together the field enhancement in the gap region will be much larger. To explore the field enhancement more results will have to be obtained. That is not the main purpose of this thesis and is left for future work.

4.7 Chapter Summary

In this chapter, we report our illuminated current calculations for several MIM structures. The MIM structure is treated as a photodetector whose responsivity is calculated as a function of wavelength and gap for small alpha parameter. We also examine the responsivity as a function of wavelength and alpha for strong incoming field, but it has little effect on the result up to a value
of unity. We also estimated the strength of the electromagnetic field for a hypothetical case of concentrated solar irradiance. The alpha parameters remain small for most scenarios we examined. For plasmonic and electrostatic enhancement cases alphas can be increased by orders of magnitude over a broad band of wavelengths. All our calculations still indicate a relatively small value for the alpha parameter even with the enhancement mechanisms.
CHAPTER V
CONCLUSION AND FUTURE WORK

The applicability of MIM diodes for broad band and ultrafast response time of photodetectors was explored during this research. We studied responsivity for MIM diodes made using different combinations of metals. The calculations of the dark current were performed using quantum tunneling currents weighted by equilibrium electron occupation probabilities. The magnitude of the dark current is strongly determined by applied bias voltage and the gap parameter of the MIM diode. The dark current is all that is required to determine the magnitude of the illuminated current.

We have analyzed the dark current characteristics of MIM diodes as a function of applied voltage and insulator gap for several material combinations and configurations. We wanted to find out whether we could design a more efficient MIM device, by using good plasmonic materials such as silver (Ag), gold (Au), copper (Cu), aluminum (Al) for one of metal elements of MIM diode. And all these cases have nearly the same range of values for the dark current density. However, the dark current density such as MIM diode of the Au/Nb$_2$O$_5$/Nb is more asymmetric to forward- and backward applied bias voltages. While the responsivity is not strongly affected by the alpha parameter, the dc current depends on the square of the alpha parameter. Therefore a local field that is 10x higher will produce a change of the dc current that is 100x
higher.

Also we examined sidewall lateral confinement of the electrons and the effect of the sidewalls on the dark current density. Even for large lateral confinement parameters, the current densities for the 2D and 1D geometries are reduced within 2% and 4% of the 3D case. So in all our responsivity calculations we used the 3D model for simplicity.

The illuminated current density calculations include the effects of the electromagnetic field strength on MIM structures. The responsivity of the MIM structures due to the electromagnetic field consists of a ratio of change in the dc current density and the ac current density. We calculated the MIM diode’s responsivity for weak electromagnetic fields to examine several variables: the gap, applied bias voltage and wavelength dependence. The responsivity increases as the insulator gap increased from 0.4nm, but saturates at large gap thickness (about 4.6nm) for zero bias. However, even with a small bias, the location of highest responsivity often changed a lot. Therefore, the responsivity can be large with thinner insulating gaps separating the metals with a relatively small applied bias voltage.

To illustrate the dependence of the responsivity on applied voltage we calculated its wavelength dependence for one MIM diode case, namely Ag/TiO$_2$/Ti. We used five different biases voltages. For all five biases, the responsivity increased the plateaus to a fixed value by increasing the wavelength. For higher photon energies (or short wavelengths), the responsivity approaches the quantum limit of $e/E_{ph}$ when a bias is applied. Therefore, we predict that the MIM diode will show much greater efficiency over a very broad range of wavelengths. The responsivity results for strong applied field (large
alpha parameter) did not show an improvement in the responsivity over that of the weak electromagnetic field results.

The future work should revisit the enhancement of the alpha parameter due to a MIM device made with both lateral dimensions confined. The calculations of the field enhancement for a elliptically shaped nanowire shown in Chapter 4 indicted a strong field enhancement over a very wide band of wavelengths, but that calculation needs to be extended to nanoparticles that are small in all three dimensions. This should put a realistic number on the magnitude of the local field enhancement.

Future work should also explore the application of MIM diodes to energy harvesting applications by calculating the efficiency of converting the solar spectrum into useful current. The requirements for energy harvesting need to be examined in a realistic device configuration with many nanorods soaking up energy and for light with random polarizations. There are clearly many issues to resolve before this problem can be adequately handled within the context of an MIM device.
BIBLIOGRAPHY


APPENDIX A

MATERIAL PARAMETERS

<table>
<thead>
<tr>
<th>Metal</th>
<th>Work Function (eV)</th>
<th>Insulator</th>
<th>Electron Affinity (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ag (Silver)</td>
<td>4.26</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al (Aluminum)</td>
<td>4.28</td>
<td>Al₂O₃</td>
<td>1.78</td>
</tr>
<tr>
<td>Au (Gold)</td>
<td>5.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cu (Copper)</td>
<td>4.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ti</td>
<td>4.33</td>
<td>TiO₂</td>
<td>3.9</td>
</tr>
<tr>
<td>W (tungsten)</td>
<td>4.55</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nb (Niobium)</td>
<td>3.99</td>
<td>Nb₂O₅</td>
<td>4.23</td>
</tr>
<tr>
<td>Pt (Platinum)</td>
<td>5.65</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sn (Tin)</td>
<td>4.38</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ta (Tantalum)</td>
<td>4.25</td>
<td>Ta₂O₅</td>
<td>3.83</td>
</tr>
<tr>
<td>NbN (Niobium Nitride)</td>
<td>4.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cr (Chromium)</td>
<td>4.5</td>
<td>Cr₂O₃</td>
<td>3.76</td>
</tr>
</tbody>
</table>

Table A.1 Material property values for metals and insulators [8, 15].
APPENDIX B

SIMULATION RESULTS

The unilluminated tunneling current as a function of applied voltage and barrier thickness is plotted for several MIM combinations in this section. The two metals are chosen based on their surface plasmon resonance properties and the difference of their work functions. Figure B.1a through B.5a plot the dark tunneling current for the following MIM cases: Ag/Cr$_2$O$_3$/Cr, Cu/Ta$_2$O$_5$/Ta, Al/Ta$_2$O$_5$/Ta, Au/Nb$_2$O$_5$/NbN and Cu/TiO$_2$/Ti. Figure B.1b through B.5b plot the responsivity vs. gap and wavelength for same diodes with a non-zero applied bias. For the selection of gold MIM diode, we only choose niobium nitride as a combination due to very high work function of gold, NbN has a large enough work function to enable tunneling currents that will produce a large enough responsivity. In all cases the barrier thickness is sampled by 23 points from 0.4nm to 5nm, the applied voltage is sampled by 201 points from -5V to 5V. In all the cases below the tunnel currents can be on the order of $10^{10}$ A/cm$^2$ at the highest applied voltages.
Figure B.1: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Ag/Cr\(_2\)O\(_3\)/Cr MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Ag/Cr\(_2\)O\(_3\)/Cr with 0.3V bias applied under small incoming field \(\alpha = 0.05\).
Figure B.2: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Cu/Ta$_2$O$_5$/Ta MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Cu/Ta$_2$O$_5$/Ta with 0.3V bias applied under small incoming field $\alpha = 0.05$. 
Figure B.3: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Al/Ta$_2$O$_5$/Ta MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Al/Ta$_2$O$_5$/Ta with 0.3V bias applied under small incoming field $\alpha = 0.05$. 
Figure B.4: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Au/Nb$_2$O$_5$/NbN MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Au/Nb$_2$O$_5$/NbN with 0.3V bias applied under small incoming field $\alpha = 0.05$. 
Figure B.5: (a) The calculated tunneling current curve Vs. applied voltage and different gap thickness for Cu/TiO$_2$/Ti MIM diode. (b) Responsivity vs. wavelength and gap for MIM diode Cu/TiO$_2$/Ti with 0.3V bias applied under small incoming field $\alpha = 0.05$. 

\[ \log_{10}(J_{3D} [\text{A/cm}^2]) \]

\[ \text{Responsivity [A/W]} \]
C.1 Dark_tunneling_current3D2D1D.m

clear all;
clc;
%close all;
tic;

% Quantum tunneling probability
Conv=1.6e-19; % energy conversion (J/eV)
c=3e8;% speed of light (m/s)
hbar=1.055e-34 ; % Planck's constant/2pi (Js)
me=0.511*1e6*Conv/c^2; % mass of the electron (Kg)
Constant=2*me/hbar^2; % convenient constant definition
%
% MIM geometry
L=2e-9; % junction thickness (m)
d_x=100e-9; % Nanoslab thickness
d_y=d_x; % nanowire thickness
%
% data for wave function calculations
Np=100; % number of discretization points in each segment
z1=linspace(-L/2,-L/Np,Np);
z3=linspace(L+L/2/Np,3*L/2,Np);
z2=linspace(0,L,Np); % discretization of the longitudinal axis
z=[z1,z2,z3];
Vd = linspace(.01,0.3,41); % applied voltage (eV)
for mm = 1:length(Vd);
    Ntot=length(z); % number of points along the z-axis
    Vin=0*Vd(mm)*Conv; % Potential at input
    Vout=-Vd(mm)*Conv;%11.*Conv; % Potential at output
    V0=(10.47+0*Vd(mm))*Conv;%11.74*Conv; % Left-side Barrier Potential (eV)
    V1=(10.1-Vd(mm))*Conv;%12.36*Conv; % Right-side Barrier Potential (eV)
    DV=(V1-V0)/L; % Film potential gradient (eV/m)
    VV1=Vin*ones(1,Np);
    VV2=V0+DV*z2; % Potential profile in z
    VV3=Vout*ones(1,Np);
    V=[VV1,VV2,VV3];
% figure(1); % plot of the potential
% plot(z,V./Conv);
% xlabel('z (nm)');
% ylabel('V(z) (eV)');
Ne=400; % number of energy points
% the transmission depends on the longitudinal energy of the electron
E=linspace(9,12,Ne)*Conv; % energy spectrum for transmission calculations
dE=E(2)-E(1);  % energy differential
k=zeros(1,Ntot);
Ex1=zeros(1,Ntot);
Ex2=zeros(1,Ntot);

% Solve Scroedinger's equation
%T=zeros(400,Ne);

for jj=1:Ne;

% Output wavefunction at z=L;
    Vect=[1,0]';
    A=zeros(1,Ntot);
    B=zeros(1,Ntot);
    A(Ntot)=Vect(1);
    B(Ntot)=Vect(2);
    k(Ntot)=sqrt((E(jj)-V(Ntot))*Constant);%

    longitudinal wave vector
    Dz=z(Ntot)-z(Ntot-1);
    Ex1(Ntot)=1;%exp(1i*k(Ntot)*Dz);
    Ex2(Ntot)=1;%exp(-1i*k(Ntot)*Dz);
    M0=[1,1; k(Ntot),-k(Ntot)];% Matrix representing the boundary conditions for right region

    for ii=Ntot-1:-1:1;
        k(ii)=sqrt((E(jj)-V(ii))*Constant);%
    longitudinal wave vector
Dz=(z(ii+1)-z(ii));
Ex11=exp(1i*k(ii)*Dz);
Ex21=exp(-1i*k(ii)*Dz);

% M=[Ex11,Ex21; k(ii)*Ex11,-k(ii)*Ex21];% Matrix representing the boundary conditions for left region
% Minv=[.5*Ex21,.5*Ex21/k(ii); 0.5*Ex11,
-0.5*Ex11/k(ii)]; % Inverse matrix of M
% Vect=Minv*M0*Vect;

Sk=k(ii)+k(ii+1);
Dk=k(ii+1)-k(ii);
M11=0.5*Sk/k(ii)*Ex21;
M22=0.5*Sk/k(ii)*Ex11;
M12=-0.5*Dk/k(ii)*Ex21;
M21=-0.5*Dk/k(ii)*Ex11;
MM=[M11,M12,M21,M22];
Vect=MM*Vect;
Ex1(ii)=Ex11;
Ex2(ii)=Ex21;

% M0=[1,1; k(ii),-k(ii)];% Next Boundary condition matrix formed
    A(ii)=Vect(1);
    B(ii)=Vect(2);
end;
B=B/A(1); % normalization
A=A/A(1); % normalization
\[ T(m,m,j) = \text{abs}(k(N_{tot})/k(1)) \times \text{abs}(A(N_{tot}))^2; \]

end;

end;

\% \text{[X Y]=meshgrid(E/Conv,Vd)};
\% \text{figure(1)};
\% \text{waterfall(X,Y,T)}

\% \% WKB approximation
\% \text{zt1=0;zt2=L;}
\% \text{for iw=1:Ne;}
\% \% if E(iw)>min(V0,V1) & E(iw)<max(V0,V1);
\% \text{zt2=L*((min(V0,V1)-E(iw))/abs(V0-V1));}
\% \text{Area(iw)=0.667*sqrt(2*me/hbar^2)*sqrt(V0-E(iw)-(V0-V1)*zt2/L)^3-sqrt(V0-E(iw))^3)/DV;}  
\% \% elseif E(iw)>max(V0,V1);
\% \text{Area(iw)=0.;}
\% \% else
\%
\% \text{Area(iw)=0.667*sqrt(2*me/hbar^2)*sqrt(V0-E(iw)-(V0-V1)*zt2/L)^3-sqrt(V0-E(iw))^3)/DV;}  
\% \end
\% \text{TWKB(iw)=exp(-2*Area(iw));}
\% end
\%
% figure(2); % plot of the TMM transmission and WKB transmission
% semilogy(E/Conv,T,E/Conv,TWKB);
% xlabel('Energy (eV)');
% ylabel('log(T)');

% current density with applied voltage equal
linspace(0,0.3V,20)
%
% 3D calculation
%
% h = 6.626*10^(-34); % Planck's constant (Js)
KT = 0.026*Conv;
Ef = 10.*Conv; % Fermi energy
for nnn=1:1:length(Vd);
    for nn = 1:1:length(E);
        Ex = linspace(E(nn),12*Conv,1500);
        dEx=(max(Ex)-E(nn))/length(Ex);
        % for n = 1:1:length(Ex) % limit of integral for the difference of fermi distribution function
        f1 = 1./(exp((Ex-Ef)./KT)+1); % Fermi distribution function for metal 1
        f2 = 1./(exp((Ex-Ef+Vd(nnn).*Conv)./KT)+1); % Fermi distribution function for metal 2
        f3 = (f1-f2); % Difference between two fermi function
after applied bias voltage

% end;

Intel(nn) = sum(f3)*dEx; % sum of 400 points for calculate the integral of fermi function(f2-f1) of limit(1,13)

Inte2(nnn,nn) = Intel(nn)*T(nnn,nn)*dE;

end;

J3D(nnn) =

(4*pi*me*Conv/(h^3))*sum(Inte2(nnn,:))*1e-4;

end

% figure(3);
% plot(Vd,J3D)
% xlabel('Applied Voltage V_d [V]');
% ylabel('Current Density J^{3D} [A/cm^2]');
% clear Ex;
%
% quantum confined case: nanoslab
% 2D calculation
%
for nnn=1:1:length(Vd);
    for nn = 1:length(E);

nmax=fix(sqrt((12*Conv-E(nn))*Constant*d_x^2/pi^2));

f3=zeros(1,1000);

Intel(nn)=0;

for np=1:nmax;% only one sign is considered for
momenta. Multiply by (2x) in the final result

\[ En = E(nn) + \pi^2/\text{Constant}/d_x^2*np^2; \]
\[ vymax = \sqrt{2/me*(12.1*\text{Conv}-En)}; \]
\[ vy = \text{linspace}(0, vymax, \text{length}(f3)); \] % Only positive values are considered here. Multiply by (2x) in final result
\[ dvy = (vymax)/(\text{length}(vy)-1); \]
\[ Etot = En + me/2*vy.^2; \]
\[ f1 = 1./\exp((Etot-Ef)/\text{KT})+1; \] % Fermi distribution function for metal 1
\[ f2 = 1./\exp((Etot-Ef+Vd(nnn).*\text{Conv})/\text{KT})+1); \] % Fermi distribution function for metal 2
\[ f3 = (f1-f2)*dvy; \] % Difference between two Fermi function after applied bias voltage
\[ \text{Intel}(nn) = \text{Intel}(nn) + 2*\text{sum}(f3); \] % sum of 400 points for calculate the integral of fermi function (f2-f1) of limit(1,13)
end;
\[ \text{Inte2}(nnn,nn) = \text{Intel}(nn)*T(nnn,nn)*dE; \]
end;
\[ J2D(nnn) = (2*me*\text{Conv}/(h^2)/d_x)*\text{sum}(\text{Inte2}(nnn,:))*1e-4; \]
end
% quantum confined case: nanowire
% 1D calculation
% for nnn=1:length(Vd);
    for nn = 1:length(E);

    nmax=fix(sqrt((12*Conv-E(nn))*Constant*d_x^2/pi^2));
    f3=zeros(1,1000);
    Intel(nn)=0;
    for np=1:nmax;% only one sign is considered for momenta. Multiply by (2x) in the final result
        En=E(nn)+pi^2/Constant/d_x^2*np^2;
        nymax=round(sqrt((12.5*Conv-En)*Constant*d_y^2/pi^2))+1;
        ny=linspace(1,nymax+1,nymax);
        Ey=pi^2/Constant/d_y^2*ny.^2; % Only positive values are considered here. Multiply by (2x) in final result
        Etot=En+Ey;
        f1 = 1./(exp((Etot-Ef)./KT)+1); % Fermi distribution function for metal 1
        f2 = 1./(exp((Etot-Ef+Vd(nnn).*Conv)./KT)+1); % Fermi distribution function for metal 2
        f3 = (f1-f2); % Difference between two Fermi function after applied bias voltage
        Intel(nn) =Intel(nn)+ sum(f3); % sum of 400
points for calculate the integral of fermi function (f2-f1) of limit (1,13)

end;

    Inte2(nnn,nn) = Inte1(nn)*T(nnn,nn)*dE;

end;

    J1D(nnn) =

(2*Conv/(h)/d_x/d_y)*sum(Inte2(nnn,:))*1e-4;

end

figure(2);
plot(Vd,log10(J3D),Vd,log10(J2D),'r',Vd,log10(J1D),'g ')
xlabel('Applied Voltage V_d [V]');
ylabel('Current Density J^{1D, 2D,3D} [ A/cm^2]');
toc;
clc;
close all;
x1=[-10:20./64.:-10+63.*20/64];
z=3.5;
w0=3;
nref=1;

C.2 Shootingmethod.m

clear all;
clc;
% close all;
Eout=9:0.01:12;
Eg=0;
Eg3=0.3;
v1=Eg*ones(1,100);
%v2=Eg2*ones(1,v22);
v2=linspace(10.47,9.8,200);
v3=-Eg3*ones(1,100);
v=[v1 v2 v3];
h=6.626*10^(-34)/(2*pi); %J*s
m0=9.10938188e-31; %kg
m=m0; %kg
ev=1.602*10^(-19); %J
%z=linspace(-300-v22/2,300+v22/2,600+v22);
ddz=1e-11;
for r=1:length(Eout)
%kesai=zeros(700,1000);
kesai(1,r)=1;
k=((Eout(r)+0.3)*ev*2*m/(h^2))^(1/2);
i=(-1)^(1/2);
kesai(2,r)=exp(-i*k*ddz);
z=2;
dz=1;
while z<400

kesai(z+dz,r)=((2*m/(h^2))*ddz^2*(v(z)-Eout(r)).*ev+2).*kesai(z,r)-kesai(z-dz,r);


\[ z = z + dz; \]

end

end

\[ a = (\max(\text{abs}(\text{kesai}(301:400, :)).^2) + \min(\text{abs}(\text{kesai}(301:400, :)).^2) - 2)/4; \]

\[ T = 1/(a+1); \]

figure (1);

plot(Eout, T, 'r')

C.3 Responsivity_alpha_gap.m

clear all;
clc;
%close all;
tic;

% Quantum tunneling probabaility
Conv=1.6e-19; % energy conversion (J/eV)
c=3e8; % speed of light (m/s)
hbar=1.055e-34; % Planck's constant/2pi (Js)
me=0.511*1e6*Conv/c^2; % mass of the electron (Kg)
Constant=2*me/hbar^2; % convenient constant definition
%
% photon detection
%
lambda=linspace(1e-6, 10.e-6, 10); % wavelength in m
Mode=1;
if Mode==1;
NMax=1; % Mode 1

savefile='MIMAgNbN2Nb.dat'; % filename to save dark
current data
else NMax=length(lambda); % Mode 2
end;

for il=1:NMax;

omega=2*pi*c./lambda(il); % angular frequency of the
photon
E_photon=hbar.*omega; % Photon energy (J)

Mode=1; % dc current only no photon field
if Mode==1;
    Vd=linspace(-5,5,201)*Conv;% (J)
else
    Mode=2; % ac contributions due to photon field
    V_bias=0.0*Conv; % J Bias Voltage
    n_Bessel=4;

    Vd=linspace(-n_Bessel*E_photon,n_Bessel*E_photon,2*n_Bessel+1);
    Vd=Vd+V_bias;
end;

% 3D current density

J3D = Current3D(Vd);
% 2D current density

% [J2Df J2Db] = Current2D(Vd, Tf, Tb)

% 1D current density

% [J1Df J1Db] = Current1D(Vd, Tf, Tb)

if Mode==1;
    save(savefile, 'Vd', 'J3D', '-ASCII')
    set(h3,'DefaultFigureColor','w')
    figure1=figure('Color',[1 1 1]);
    h3=plot(Vd/Conv,log10(abs(J3D)));
    set(h3,'linewidth',[2.0]);
    set(gca,'Fontsize',[14]);
    %get(gcf,'default');
    set(gca,'DefaultFigureColor','w');
    axis([Vd(1)/Conv Vd(length(Vd))/Conv 5
    ceil(log10(max(abs(J3D))))]);
    xlabel('Applied Voltage V_d [V]');
    ylabel('log_{10}(Current Density) [A/cm^2]');
    figure1=figure('Color',[1 1 1]);
    h4=plot(Vd/Conv,J3D);
    set(h4,'linewidth',[2.0])
    set(gca,'Fontsize',[14])
axis([Vd(1)/Conv Vd(length(Vd))/Conv
-10^ceil(log10(max(abs(J3D))))
10^ceil(log10(max(abs(J3D)))) ])
xlabel('Applied Voltage V_d [V]');
ylabel('Current Density [A/cm^2]');
grid on;

else
    alpha=linspace(.0001,5,50); % photon field strength parameter

% Responsivity calculation

% strong field limit

DeltaJDC2=((besselj(0,alpha)).^2-1)*J3D(n_Bessel+1); % n=0
Jomega2=besselj(0,alpha).*(besselj(1,alpha)+besselj(-1,alpha)).*J3D(n_Bessel+1); % n=0
    for ia=1:n_Bessel;
        DeltaJDC2=DeltaJDC2+besselj(ia,alpha).^2*J3D(ia+n_Bessel+1); % n positive
    end
    DeltaJDC2=DeltaJDC2+besselj(ia,alpha).^2*J3D(n_Bessel+1-ia); % n negative

end
Jomega2=Jomega2+besselj(ia,alpha).*(besselj(ia-1,alpha)+besselj(ia+1,alpha)).*J3D(n_Bessel+1+ia); % n positive

Jomega2=Jomega2+besselj(-ia,alpha).*(besselj(-ia+1,alpha)+besselj(-ia-1,alpha)).*J3D(n_Bessel+1-ia);  % n negative
end;
R2(il,:)=DeltaJDC2./(alpha./2)./Jomega2./(E_photon/Conv);
end;
end;
if Mode==2;
    figure(5);
    [XX YY]=meshgrid(alpha,lambda*1e6);
    waterfall(XX,YY,R2)
    %plot(alpha, abs(R1),alpha, abs(R2))
    ylabel(’\lambda (\mu m)’);
    xlabel(’\alpha’);
    zlabel(’Responsivity [A/W]’);
end;
Conv/E_photon
toc;
C.4 Responsivity_quan_limit.m

%%
clear all;
clc;
%close all;
tic;

% Quantum tunneling probability
Conv=1.6e-19; % energy conversion (J/eV)
c=3e8;% speed of light (m/s)
hbar=1.055e-34 ; % Planck's constant/2pi (Js)
me=0.511*1e6*Conv/c^2; % mass of the electron (Kg)
Constant=2*me/hbar^2; % convenient constant definition
%
% photon detection
%
%lambda=linspace(1e-6,25e-6,NMax); % wavelength in m

%load 'MIMAgnbN2Nb.dat'; % This filename corresponds to
the data being evaluated
load 'AgTiO2Ti_J3D.mat'
% Vd1=MIMAgnbN2Nb(1,:);
% J3D1=MIMAgnbN2Nb(2,:);

gap=4e-9;
NMax=101;
lambda=linspace(1e-6,25e-6,NMax);
\alpha=0.05;
Vd1=Vd;

%figure;waterfall(J3D);

for il=1:NMax;
    \text{E\_photon}(il) = 2\pi\hbar c/\lambda(il)/\text{Conv}; \text{ eV}
    %for ig=1:length(gap);

    J3D1 = J3D(:,18);

    \% dc current only no photon field
    \text{V\_bias} = 0.5; \% Bias Voltage
    Vdp = \text{E\_photon}(il) + \text{V\_bias};
    J3Dp = spline(Vd1,J3D1,Vdp*Conv);
    Vdm = -\text{E\_photon}(il) + \text{V\_bias};
    J3Dm = spline(Vd1,J3D1,Vdm*Conv);
    Vd0 = \text{V\_bias};
    J3D0 = spline(Vd1,J3D1,Vd0*Conv);
    JDC = J3Dp + J3Dm - 2*J3D0;

    % Responsivity calculation

    % Weak field limit
    \text{DeltaJDC1}(il) = \alpha^2/4*(JDC);
    \text{Jomegal}(il) = \alpha/2*(J3Dp-J3Dm);
    R1(il) = DeltaJDC1(il)/Jomegal(il)/(\alpha/2*E\_photon(il)
end;

figure;
semilogx(lambda*1e6,abs(R1));
xlabel('log ($\lambda (\mu m)$');
ylabel('Responsivity [A/W]');

%[X2 Y2]=meshgrid(gap*1e9,lambda*1e6);

figure;surf(X2,Y2,abs(R1));
xlabel('gap [nm]');
ylabel('Wavelength [um]');
zlabel('Responsivity [A/W]');
toc;