A Quantum Simulation Study of III-V Esaki Diodes and 2D Tunneling Field-Effect Transistors

Patsy Cadareanu
pxc7985@rit.edu

Follow this and additional works at: https://scholarworks.rit.edu/theses

Recommended Citation

This Thesis is brought to you for free and open access by the Thesis/Dissertation Collections at RIT Scholar Works. It has been accepted for inclusion in Theses by an authorized administrator of RIT Scholar Works. For more information, please contact ritdswork@rit.edu.
A Quantum Simulation Study of III-V Esaki Diodes and 2D Tunneling Field-Effect Transistors

Patsy Cadareanu
A Quantum Simulation Study of III-V Esaki Diodes and 2D Tunneling Field-Effect Transistors

Patsy Cadareanu
July 19, 2018

A Thesis Submitted
in Partial Fulfillment
of the Requirements for the Degree of
Master of Science
in
Microelectronic Engineering

R·I·T
Kate Gleason
College of Engineering

Department of Electrical and Microelectronic Engineering
A Quantum Simulation Study of III-V Esaki Diodes and 2D Tunneling Field-Effect Transistors

Patsy Cadareanu

Committee Approval:

Dr. Sean L. Rommel Advisor
Gleason Professor, Electrical and Microelectronic Engineering

Dr. James E. Moon
Professor, Electrical and Microelectronic Engineering

Dr. Santosh K. Kurinec
Professor, Electrical and Microelectronic Engineering

Dr. Robert Pearson
Associate Professor, Electrical and Microelectronic Engineering
Program Director, Microelectronic Engineering

Dr. Sohail A. Dianat
Department Head of Electrical and Microelectronic Engineering
Acknowledgments

This thesis is the culmination of my 7th and final year at the Rochester Institute of Technology spent in pursuit of my bachelor's and master's degrees in Microelectronic Engineering, none of which would have been possible without the unfa
tering support of many. Here's a few of them:

Dr. Sean Rommel, my advisor, introduced me to the idea of 2D semiconductors and, with greater consequence, to the importance of doing research grounded in theoretical knowledge. I am extremely thankful for his guidance and especially his patience.

Dr. Robert Pearson has supported me in the Microelectronic Engineering program since I joined in 2011. Considering how “green” I was when I started out, without his constant pushes I would have never made it through.

Drs. Santosh Kurinec and James Moon are two of my inspirations for pursuing a doctorate. I hope to one day be as passionate for semiconductors as they are.

Udita Kapoor, my partner on this project, is a true joy to work and talk with and you should read her thesis if you're going to go through the trouble of reading this one.

The Materials Design team, specifically Ray Shan and Volker Eyert and Purdue University’s Gerhard Klimeck, Yuanchen Chu, and Tillman Kubis provided invaluable assistance with producing and interpreting simulations.

My parents have given me continuous support even in preparing this document (dad walked my dog while I reread incomprehensible papers and mom made my most tedious LaTeX tables), and I wouldn’t have made it this far without them.

And last but never least, my speed-dial: CLF, MB, KTN, and CJR.
Abstract

Tunnel field-effect transistors (TFETs) have long been considered as a replacement technology for metal-oxide-semiconductor field-effect transistors (MOSFETs) in low-power digital applications due to their low OFF-current ($I_{OFF}$) and small subthreshold swing ($SS$). These benefits are somewhat neutralized by the low ON-current ($I_{ON}$) exhibited by TFETs fabricated with large bandgap ($E_g$) semiconductors such as silicon. To offset this drawback, different material systems can be used, with material optimization required for the channel material, the gate stack, and their corresponding geometries. This study considers the novel idea of using 2-dimensional (2D) semiconductors for the channel material in TFETs, and the potential effects of such a channel on the physics of the resulting device. After this theoretical discussion of TFETs, the simulation requirements of such a device are introduced as well as the two quantum simulation systems of choice, Vienna Ab initio Simulation Package (VASP 5.4) as offered by Materials Design and NanoHUB's NEMO5. Topics examined with simulation theory in mind include the density functional theorem (DFT) and convergence criteria. Previously fabricated Esaki diodes from Pawlik et al. are simulated using NEMO5 and the necessity of bowing application to the tight-binding parameters is shown. Tables clarifying the tight-binding parameters of InGaAs from the NEMO5 all.mat file and their associated bowing parameters are included. The simulations performed with the bowing parameters included are shown to match the experimental data almost exactly. Initial VASP 5.4 simulations for GaAs and InAs are shown and the practicality of DFT using the generalized gradient approximation (GGA), HSE06 with GGA, and Hartree-Fock methods is discussed; HSE06 with GGA is shown to produce simulations closest to reality, though there is a significant computation time trade-off. A designed experiment varying the lattice constants of MoS$_2$ and WTe$_2$ is performed and included as an example of the simulation system's capabilities. A plot of VASP 5.4 and NEMO5 MoS$_2$ bandstructure results is also included.
## Contents

Signature Sheet  i

Abstract  iii

Table of Contents  iv

List of Figures  vii

List of Tables  xi

List of Symbols  xii

1 Introduction and Motivations  1

2 Diode and Tunnel FET Theory  8
   2.1 Esaki Diode Introduction  8
   2.2 Subthreshold Swing Analysis for TFETs  9
   2.3 2D Semiconductors and their applications in conventional FETs and TFETs  17
   2.4 The Effects of Channel Geometry on TMD TFETs  27
   2.5 TMD Coupling in TFETs  31

3 Quantum Simulation Theory  33
   3.1 The Necessity of Quantum Simulations  33
   3.2 Choosing a Quantum Simulation Package  35
      3.2.1 The Vienna Ab initio Software Package  35
      3.2.2 NanoHUB’s NEMO  35
   3.3 Quantum Simulation Theory  36
      3.3.1 The Single-Body Problem  36
      3.3.2 Orbitals  37
      3.3.3 Density Functional Theorem  38
      3.3.4 Jacob’s Ladder  41
   3.4 Convergence  42
      3.4.1 Jacobian Iterative Method  44
## 4 NEMO5 Simulation Results: An InGaAs Bowing parameter study

4.1 Introduction to Esaki diode data to be simulated .......................... 48  
4.2 First NEMO5 Attempts at Benchmarking Homojunctions .................. 51  
4.3 Proposed Solution: Change the $E_g$ Calculation .......................... 55  
4.4 Proposed Solution: Consider the NEMO5 Tight-binding Parameters .... 57  
4.5 The Rosetta Stone of NEMO5 Tight-binding Parameters for InGaAs ... 58  
4.6 Bowing results ............................................................................ 61  
4.7 Second NEMO5 Attempts at Benchmarking Homojunctions .............. 66

## 5 VASP Benchmarking Results

5.1 Lattice Constant Variations ......................................................... 70  
5.2 The Effects of Varying the Functional: Part 1 ............................... 71  
5.2.1 GaAs VASP Simulation Results ............................................. 72  
5.2.2 InAs VASP Simulation Results ............................................. 75  
5.2.3 Reflections on Varying the Functional .................................... 77  
5.3 The Effects of Varying the Functional: Part 2 ............................... 77  
5.4 Some Effects of Changing the Lattice Constant ............................ 78

## 6 Conclusions

6.1 Summary of Work ................................................................. 82  
6.2 Future Work ............................................................................ 83

## Bibliography

A Hohenburg-Kohn Theorem Proof [1] ........................................... 89

B Brief Guide to Using MedeA 2.22.2 for VASP 5.4 Simulations .......... 90  
B.1 Part 1: MedeA Set-Up ............................................................. 90  
B.2 Part 2: Cell Set-Up ................................................................. 91  
B.3 Part 3: Structural Optimization using VASP 5.4 .......................... 92  
B.4 Part 4: Viewing and Controlling the Job requested ..................... 94  
B.5 Part 5: Band Structure and Density of States using VASP 5.4 ...... 95  
B.6 Part 6: Analysis ....................................................................... 96

## C NEMO5 Sample Device Simulation Files

C.1 Typical Material and Structure definition .................................... 97  
C.2 Domain definition ..................................................................... 98  
C.3 Contact definitions ................................................................... 98
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>C.4 Mesh Domain definition</td>
<td>98</td>
</tr>
<tr>
<td>C.5 Region definition</td>
<td>99</td>
</tr>
<tr>
<td>C.6 QTBM Solver definition</td>
<td>100</td>
</tr>
</tbody>
</table>
1.1 (a) The DG $n$-type TFET structure shown with carriers as arrows. (b) Transmission electron microscopy (TEM) micrograph of a fabricated TFET device. (c) Homojunction vs. heterojunction TFET carrier tunneling.\textsuperscript{1}[2] .......................................................... 4

2.1 (a) I-V characteristic, and schematic band diagram for (b) reverse bias, (c) equilibrium, (d) peak tunneling current, (e) minimum direct tunneling current, and (f) diffusion current for a generic ETD. \textsuperscript{3} ... 9

2.2 (Top) The structure of a DG n-TFET device. (b) The band diagram of this device.\textsuperscript{2}[4] ................................................................. 10

2.3 Simulated results of $SS$, $SS_T$, and $SS_{FD}$ as affected by change in the width of the tunnel window $\Delta E$.\textsuperscript{3}[4] .................................................. 13

2.4 $I_{BTBT}$ in terms of $I_{ON}$ (referred to as $I_{onset}$ in the graphs) and $I_{OFF}$ for homojunction and heterojunction TFETs as functions of $N_A, \lambda, E_g$, and $m_T$.\textsuperscript{4}[4] ............................................................... 15

2.5 $SS$ and $SSTT_\theta$ as functions of $N_A, \lambda, E_g$, and $m_T$.\textsuperscript{5}[4] .............. 16

2.6 (a) and (b) demonstrate the advantages of using 2D materials over bulk materials, (c) the degradation of carrier mobility with smaller layer thicknesses, and (d) schematic of a DG 2D FET. IEEE \textcopyright2015,\textsuperscript{6}[5] 18

2.7 (a) $E_C$ of a n-MOSFET in the channel region (that is, from source to drain) with \textit{Büttiker} probes inserted at every mesh point along the channel. (b) A single \textit{Büttiker} probe. (c) The simulation design. IEEE \textcopyright2015.\textsuperscript{7}[5] .................................................. 20

2.8 Monolayer TMD TFET structure. IEEE \textcopyright2015.\textsuperscript{8}[6] .......................... 22

2.9 Mobility and effective mass data for various 2D semiconductors. The green block corresponds to the ranges required for HP operation; the orange block corresponds to the ranges required for LSTP operation. IEEE \textcopyright2015.\textsuperscript{9}[5] .............................. 24

2.10 $I_{ON}$, seen as a color contour, is plotted as a function of effective mass along the $x$- and $z$- planes for HP (right) and LSTP (left) applications at the 5.9 nm node. The dashed blue lines correspond to isotropic materials. IEEE \textcopyright2015.\textsuperscript{10}[5] .................. 25


<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.11</td>
<td>The transfer characteristics of various simulated TMD TFETs by Ilatikhameneh et al. IEEE ©2015.11[6]</td>
</tr>
<tr>
<td>2.12</td>
<td>(a) The TFET structure used for simulations, and (b) the simulated energy band diagram of this device. IEEE © 2015.12[7]</td>
</tr>
<tr>
<td>2.13</td>
<td>Synopsis TCAD transfer characteristics of (a) drain doping, and (b) fin thickness dependence, with the device parameters as follows: gate length $L_G = 20$ nm, thickness of the InN layer $t_{InN} = 1.7$ nm, thickness of the GaN layers $t_{p-GaN} = t_{n-GaN} = 25$ nm, equivalent oxide thickness $EOT = 0.43$ nm, and $V_{DS} = 0.5V$. IEEE © 2015.13[7]</td>
</tr>
<tr>
<td>2.14</td>
<td>(a) The DG monolayer TMD TFET device structure, (b) the atomistic structure of the TMD monolayer along the ZD direction, and (c) the atomistic structure of the TMD monolayer along the AD direction. IEEE © 2016.14[8]</td>
</tr>
<tr>
<td>2.15</td>
<td>The simulated MoTe2 TFET transfer characteristics for different channel lengths in the (a) AD, and (b) ZD directions. IEEE © 2016.15[8]</td>
</tr>
<tr>
<td>2.16</td>
<td>Band alignment of various monolayer TMD materials. The grey columns correspond to the conduction band minimum and valence band maximum and the green columns are the corrected band edges. The Fermi level of each material is the blue line, and the vacuum level is set at 0 eV.16[9]</td>
</tr>
<tr>
<td>3.1</td>
<td>(a) Device geometry of the simulated TFET design. (b) Band profile plotted along dashed line in (a). IEEE ©2015.17[10]</td>
</tr>
<tr>
<td>3.2</td>
<td>Comparisons of dynamic nonlocal band-to-band (DNL) and non-equilibrium Green's function (NEGF) simulation results. Note that the straight-lines correspond to the DNL simulations and the lines with the bullets correspond to the NEGF simulations. IEEE ©2015.18[10]</td>
</tr>
<tr>
<td>3.3</td>
<td>NEMO5 Simulation flow.</td>
</tr>
<tr>
<td>3.4</td>
<td>The spherical coordinates of a hydrogen atom.</td>
</tr>
<tr>
<td>3.5</td>
<td>Electron configuration in each orbital. [11, 12]</td>
</tr>
<tr>
<td>3.6</td>
<td>Jacob’s Ladder via Perdew and Schmidt’s metaphor.19[13]</td>
</tr>
<tr>
<td>4.1</td>
<td>InGaAs device structure with doping. [14]</td>
</tr>
<tr>
<td>4.2</td>
<td>InGaAs devices experimental data. [14]</td>
</tr>
<tr>
<td>4.3</td>
<td>GaAs device structure with doping. [14]</td>
</tr>
<tr>
<td>4.4</td>
<td>GaAs device structure with doping. [14]</td>
</tr>
<tr>
<td>4.5</td>
<td>InAs device structure with doping. [14]</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

4.6 InAs device structure with doping. [14] .......................... 51
4.7 NEMO5 simulations for the InGaAs-on-InP structure. [14] .......... 52
4.8 NEMO5 simulations for the GaAs structure. [14] .................... 53
4.9 NEMO5 simulations for the InAs structure. [14] ..................... 54
4.10 NEMO5 simulations of E-k for GaAs and InGaAs. ................. 55
4.11 Electron band gap of \( In_x Ga_{1-x}As \) at room temperature as a function
   of the In concentration \( x \). Note that the paper had it wrong; the
   bottom axis should be the Ga concentration. This was corrected in
   this thesis. The solid line corresponds to the Ioffe data, the dotted line
   is the data with added bowing effects, and the dashed line is the data
   with no bowing effects. IEEE © 2009. 20 [15, 16] .......................... 57
4.12 NEMO5 bandstructure results for In=0.05 GaAs=0.95 composition
   with and without bowing effects included. .......................... 62
4.13 NEMO5 bandstructure results for In=0.50 GaAs=0.50 composition
   with and without bowing effects included. .......................... 63
4.14 NEMO5 bandstructure results for In=0.53 GaAs=0.47 composition
   with bowing effects included. \( E_g = 0.7662 \text{ eV} \). .................. 64
4.15 NEMO5 bandstructure results for In=0.95 GaAs=0.05 composition
   with and without bowing effects included. .......................... 64
4.16 Electron band gap of \( In_x Ga_{1-x}As \) at room temperature as a function
   of the In concentration \( x \) as plotted after applying the bowing effects
   and comparing to the Ioffe and Luisier data. [15, 16] ............... 65
4.17 InGaAs device structure with doping. [14] .......................... 66
4.18 InGaAs devices simulated with the new all.mat file and plotted against
   real data from Pawlik et al.. [14] .......................... 67
4.19 InGaAs device structure with doping. [14] .......................... 68
4.20 InGaAs devices with varying intrinsic (referred to as "i") region thick-
   nesses plotted against experimental data from Pawlik et al.. [14] ... 69

5.1 VASP simulations of GaAs lattice constant variation screen. .......... 71
5.2 VASP simulations of InAs lattice constant variation screen. .......... 71
5.3 VASP simulation of GaAs using DFT with GGA-PBE with spin-orbit. 73
5.4 VASP simulation of GaAs DFT as an artifact of the HSE06 simulation.
   Again with spin-orbit included. ........................................... 73
5.5 VASP simulation of GaAs DFT as an artifact of the Hartree-Fock
   simulation. Again with spin-orbit included. .......................... 74
LIST OF FIGURES

5.6 VASP simulation of GaAs using HSE06 with spin-orbit. .................. 74
5.7 VASP simulation of GaAs using Hartree-Fock with spin-orbit. ........ 75
5.8 VASP simulation of InAs using DFT with spin-orbit coupling included. 76
5.9 VASP simulation of InAs using HSE06 with spin-orbit. .............. 76
5.10 VASP simulation of InAs using Hartree-Fock with spin-orbit. ........ 77
5.11 VASP DFT with GGA simulation of MoS\(_2\) band diagrams varying with lattice constant. The top (solid black) line corresponds to the original lattice constant. ......................................................... 79
5.12 VASP DFT GGA simulation data of the MoS\(_2\) and WTe\(_2\) lattice constant variation designed experiment explained above. vdW corresponds to a setting in the simulation where van der Waals forces are applied. 80
5.13 VASP 5.4 van der Waals DFT GGA simulation data of MoS\(_2\) plotted against NEMO5 MoS\(_2\) simulations. Spin-orbit is applied during both simulations. .......................... 81

B.1 Materials Design folder as seen running Windows 10 Pro. ............... 90
B.2 InfoMaticA Search menu as seen after selecting InAs for this example. 91
B.3 (a) The InAs molecule chosen as seen without bonds applied. (b) The InAs molecule chosen as seen with bonds applied. ................. 92
B.4 General setup for Structural Optimization of the chosen InAs molecule. 93
B.5 The pre-run menu. .......................................................... 94
B.6 The Materials Design JobServer menu. ................................. 94
B.7 Sample set-up of band structure and density of states run for the InAs model chosen. .......................................................... 95
## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Data corresponding to the TMD TFET simulations seen in Fig.2.11. Note that effective mass/$m_0$ is referred to as the reduced effective mass, $m^*_e$. IEEE © 2015. 21[6]</td>
<td>26</td>
</tr>
<tr>
<td>2.2</td>
<td>TMD TFET simulations by Fei et al. $m_e/m_0$ is the reduced electron effective mass, and $m_h/m_0$ is the reduced hole effective mass. IEEE © 2016.22[8]</td>
<td>26</td>
</tr>
<tr>
<td>4.1</td>
<td>Device doping and output current density peak summary for InP/InGaAs structure. [14]</td>
<td>52</td>
</tr>
<tr>
<td>4.2</td>
<td>Device doping and output current density peak summary for GaAs structure. [14]</td>
<td>53</td>
</tr>
<tr>
<td>4.3</td>
<td>Device doping and output current density peak summary for InAs structure. [14]</td>
<td>54</td>
</tr>
<tr>
<td>4.4</td>
<td>Bowing effects for the anion (As) band energies.</td>
<td>59</td>
</tr>
<tr>
<td>4.5</td>
<td>Bowing effects for the cation (In or Ga) band energies.</td>
<td>59</td>
</tr>
<tr>
<td>4.6</td>
<td>Bowing effects for the $s$–$to$–$s$-orbital interactions.</td>
<td>60</td>
</tr>
<tr>
<td>4.7</td>
<td>Bowing effects for the $s$–$to$–$p$ and $s$–$to$–$d$ orbital interactions.</td>
<td>60</td>
</tr>
<tr>
<td>4.8</td>
<td>Bowing effects for the $p$–$to$–$p$ and $p$–$to$–$d$ orbital interactions.</td>
<td>61</td>
</tr>
<tr>
<td>4.9</td>
<td>Bowing effects for the $d$–$to$–$d$ orbital interactions.</td>
<td>61</td>
</tr>
<tr>
<td>4.10</td>
<td>Device doping and output current density peak summary for InGaAs structure as simulated with the new all.mat file. [14]</td>
<td>67</td>
</tr>
<tr>
<td>5.1</td>
<td>Materials simulated in VASP using HSE06 with GGA and DFT with GGA with spin orbit turned on. Note that the PWC is the plane-wave cutoff which refers to the distance the energy is simulated away from atom. The farther or larger this is, the more likely the simulation will converge to reality due to an increase in resolution, but also the longer the computation time. Note that the k-point spacing was 0.5/Å in a $\Gamma$-centered Monkhorst-Pack mesh, resulting in a 4x4x4 grid.</td>
<td>78</td>
</tr>
</tbody>
</table>
## List of Symbols

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
<th>Units/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C'_D )</td>
<td>Depletion region capacitance per unit area</td>
<td>( \text{F/cm}^2 )</td>
</tr>
<tr>
<td>( C'_{ox} )</td>
<td>Oxide capacitance per unit area</td>
<td>( \text{F/cm}^2 )</td>
</tr>
<tr>
<td>( \mathcal{E} )</td>
<td>Electric field</td>
<td>( \text{V/cm} )</td>
</tr>
<tr>
<td>( E_c )</td>
<td>Energy at the conduction band edge</td>
<td>( \text{eV} )</td>
</tr>
<tr>
<td>( E_F )</td>
<td>Fermi level</td>
<td>( \text{eV} )</td>
</tr>
<tr>
<td>( E_g )</td>
<td>Band gap energy</td>
<td>( \text{eV} )</td>
</tr>
<tr>
<td>( E_v )</td>
<td>Energy at the valence band edge</td>
<td>( \text{eV} )</td>
</tr>
<tr>
<td>( E_{x,y} )</td>
<td>Electric field normal and parallel to the gate</td>
<td>( \text{V/cm} )</td>
</tr>
<tr>
<td>( \hbar )</td>
<td>Reduced Planck constant</td>
<td>( 6.582 \times 10^{-16} \text{eV}\cdot\text{s} )</td>
</tr>
<tr>
<td>( I_D )</td>
<td>Drain current</td>
<td>( \text{A} )</td>
</tr>
<tr>
<td>( J_t )</td>
<td>Band to band tunneling current density</td>
<td>( \text{A/cm}^2 )</td>
</tr>
<tr>
<td>( k )</td>
<td>Boltzmann’s constant</td>
<td>( 8.617 \times 10^{-5} \text{eV/K} )</td>
</tr>
<tr>
<td>( m^* )</td>
<td>Carrier effective mass</td>
<td>( \text{kg} )</td>
</tr>
<tr>
<td>( N_A )</td>
<td>Acceptor concentration</td>
<td>( \text{cm}^{-3} )</td>
</tr>
<tr>
<td>( N_c )</td>
<td>Effective density of states in the conduction band</td>
<td>( \text{cm}^{-3} )</td>
</tr>
<tr>
<td>( n_i )</td>
<td>Intrinsic carrier concentration</td>
<td>( \text{cm}^{-3} )</td>
</tr>
<tr>
<td>( q )</td>
<td>Elementary charge</td>
<td>( 1.602 \times 10^{-19} \text{C} )</td>
</tr>
<tr>
<td>( SS )</td>
<td>Subthreshold swing</td>
<td>( \text{mV/dec} )</td>
</tr>
<tr>
<td>( T )</td>
<td>Temperature</td>
<td>( \text{K} )</td>
</tr>
<tr>
<td>( V_{th} )</td>
<td>Threshold voltage</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( V_{DS} )</td>
<td>Drain–Source voltage</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( V_{eff} )</td>
<td>Effective reverse bias voltage</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( V_{FB} )</td>
<td>Flatband voltage</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( V_G )</td>
<td>Gate voltage</td>
<td>( \text{V} )</td>
</tr>
<tr>
<td>( \epsilon_s )</td>
<td>Permitivity of a semiconductor</td>
<td>( \text{F/cm} )</td>
</tr>
<tr>
<td>( \mu_n, \mu_p )</td>
<td>Mobility of electrons and holes respectively</td>
<td>( \text{cm/V}\cdot\text{s} )</td>
</tr>
<tr>
<td>( \Psi_{sa} )</td>
<td>Surface potential</td>
<td>( \text{V} )</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction and Motivations

The intention of research is to further the respective field’s knowledge in a specific domain, but as it is easier to continue along the path of previous research than it is to take up something entirely new, sometimes these spheres of expertise become either irrelevant or so specific they lose meaning for anyone in the field. To avoid this, the research proposed in this study is new and unfamiliar at the Rochester Institute of Technology. To advance in a new field requires previous knowledge to build on. This means that while the primary interest of this research is in developing two-dimensional (2D) tunneling field-effect transistors (TFETs) through a quantum simulation study, simpler devices with real data available for comparison such as III-V Esaki diodes previously fabricated and tested by Dr. Sean Rommel’s research group in the past must first be simulated. Once these simulations are performed and their results are determined to match reality, 2D TFETs can then be similarly simulated and these simulations can be considered valuable. This way, an understanding of future research is intricately tied to the research of the past.

Academia is a potent breeding ground for ideas to feed industrial progress, especially in the semiconductor industry. As such, looking at the ideas currently being funded by industry giants is one of the best ways to determine where to focus future research and this was done prior to this study. The Center for Low Energy Systems Technology (LEAST) established in 2013 and led by Notre Dame University is
composed of 12 university microelectronics research centers and funded by the Semi-
conductor Research Corporation (SRC) and the Defense Advanced Research Projects
Agency (DARPA). Each of these 12 centers receives approximately $6 million annu-
ally for their research. The research of interest at these centers is the development of
more energy-efficient integrated circuits with a focus on ultra-low voltage and steep
transistors. There is no mention on the LEAST website of III-V material devices, so
even though there’s an industrial market for III-V’s, there is not a lot of research poten-
tial there because funding for such devices has been withdrawn. From this observed
shift in research areas in the industry towards non-III-V and non-CMOS devices, 2D
tunnel FETs are considered.

One of the main problems with transistor scaling and increased chip density is
that it leads to increased power density on the chip. This requires that the supply
voltage \( V_{DD} \) be decreased to reduce power consumption which in turn results in an
exponential increase in the leakage current. In metal-oxide-semiconductor field-effect
transistors (MOSFETs) only the carriers with enough energy to exceed the source-
channel potential barrier, and thus enter the channel from the source, will contribute
to the ON-current \( I_{ON} \) of the device. [2] The subthreshold swing \( SS \) parameter
refers to the gate-to-source voltage needed to change the drain current by one order
of magnitude [4]. Eq. 1.1 can be used to calculate the ideal \( SS \). [17, 18]

\[
SS(T) = \frac{kT}{q} \ln(10) \tag{1.1}
\]

For the non-ideal \( SS \), there is a dimensionless prefactor \( n \) which accounts for
non-idealities, so that the equation is:

\[
SS(T) = \frac{kTn}{q} \ln(10) \tag{1.2}
\]
where the non-ideality factor is defined as:

\[ n = 1 + \frac{\gamma}{2\sqrt{\Psi_{sa}}} \]  

(1.3)

\( \Psi_{sa} \) refers to the surface potential and \( \gamma \) is the body-effect coefficient.

A small \( SS \) value corresponds to a faster switching speed and allows operation at lower supply voltages, and is thus desired [8]. The minimum subthreshold swing (\( SS_{\text{min}} \)) in a MOSFET is limited to approximately 60 mV/decade at room temperature (300 K) because the carriers follow the Fermi-Dirac (FD) distribution and their energy is bounded by the fixed slope \( kT \) where \( k \) is the Boltzmann constant and \( T \) is the temperature [2].

Tunnel field-effect transistors (TFETs) differ from MOSFETs in that their \( I_{ON} \) is facilitated through a process called band-to-band tunneling (BTBT) at the source-channel potential barrier. In BTBT a considerable number of carriers with energy lower than the potential barrier will make it into the channel region because BTBT enables carriers to go through the potential barrier instead of limiting transport into the channel to only those that are energetic enough to get over the barrier. This results in the possibility of lowered \( SS \) values in TFETs; demonstrations have been shown with \( SS_{\text{min}} \) values as low as 21 mV/decade for a vertical III-V silicon (Si) nanowire with bias voltage (\( V_{DS} \)) of 0.1 V and 1 V. [2] A derivation of the \( SS_{\text{min}} \) as shown by Wei et al. as relevant for TFETs is provided in this study. Note that because the BTBT probability is often much smaller than 1, \( I_{ON} \) for TFETs is usually smaller than for MOSFETs, and special considerations must be taken to change this [8].

Owing to its tunneling-based current generation scheme, the structure of a TFET is different than that of a MOSFET. Fig. 1.1 (a) and (b), taken from Datta et al., show a typical double-gated (DG) \( n \)-type TFET structure with asymmetrical
source and drain doping and an intrinsic region. [2] Note that TFET structures do not require two gates, and this device in particular is designed with two gates for increased gate control.

For the transport cases shown in Fig. 1.1(c) to occur, a gate bias \( V_G \) is applied to either the top or bottom gate of the TFET which will cause the conduction band \( E_C \) of the intrinsic layer to lower. With enough voltage on the gate the \( E_C \) of the intrinsic layer can lower below the valence band \( E_V \) of the source, thus creating a window for the electrons to go from the source into the intrinsic region and then into the drain. As \( V_G \) is decreased, the bands will go back to their regular configurations and the tunneling window will close. Fig. 1.1(c) also shows that heterojunction TFETs can allow for increased \( I_{ON} \) when compared to homojunction TFETs by decreasing the

\[ I_{DS} \sim T_{WKB} \sim \alpha \exp \left( -\beta E_{eff}^{1.5} \right) \]

Figure 1.1: (a) The DG n-type TFET structure shown with carriers as arrows. (b) Transmission electron microscopy (TEM) micrograph of a fabricated TFET device. (c) Homojunction vs. heterojunction TFET carrier tunneling.\(^1\)[2]

\(^1\)Reprinted from Tunnel FET technology: A reliability perspective, vol. 54, no. 5, S Datta and H Lie and V Narayanan, pages 861-874, Copyright (2014), with permission from Elsevier.
tunnel barrier \(E_{\text{eff}}\) [2].

The operation of TFETs is limited by two parameters: the SS and the ON-OFF current ratio, sometimes referred to as the onset strength, both of which will be discussed in detail [8, 9]. Optimal SS and onset strength can be achieved through the selection of channel material, TFET gate stack, and the corresponding geometries [7]. The channel material and geometry in particular will be explored in depth.

Interfacial defects can increase SS considerably, thus negatively impacting device performance and overcoming the primary benefit of TFET devices. This SS degradation can be alleviated through the exploitation of dangling bond-free surfaces provided by two-dimensional (2D) materials. Transition metal dichalcogenides (TMDs) are particularly promising 2D materials due to their tunable bandgap \(E_g\) size, ability to adjust the Fermi level through doping, and receptivity to layer stacking. [9] The latter of these benefits will be considered.

Though the interest is clearly in fabricating TMD TFET devices, it would be irresponsible to start by jumping headfirst into making such devices due to the prohibitive cost of fabrication and materials. Instead, the research in this study is focused on determining the best quantum simulation packages and obtaining an understanding of how to use these systems most effectively.

First, the necessity of quantum simulations is deliberated. Quantum simulations software packages such as the Vienna Ab initio Simulation package are generally significantly more expensive than their TCAD counterparts. The Rochester Institute of Technology owns a license to the TCAD system Silvaco Athena and Atlas at the time of this research and corresponding publication, so this software package would have been the optimal choice to use. However, it is determined that TCAD simulations are not thorough enough to adequately capture tunneling effects and the negative differential resistance which is the defining characteristic of the Esaki diode and TFET, and this is discussed in detail.
The goal of quantum simulations are $E - k$ plots and $I - V$ characteristics that are similar to real data. Thus, the code must converge onto a single value. Each iteration in a quantum simulation is composed of a guess, followed by a calculation of the error (that is, the difference between two iterations), followed by an iteration corrected using the error, etc., until the error is small enough, as set by the user. At this point convergence is said to occur.

Once the two quantum simulation systems of choice are identified, previous Esaki diode data is simulated in Purdue’s NEMO5 package to determine how well the simulations corresponds to reality. The simulation model used originally is the virtual crystal approximation (VCA); this corresponds to the tight-binding parameters used. VCA assumes that the tight-binding parameters will vary linearly with the composition so that the two molecules of interest (in the case of this study, InAs and GaAs) both contribute equally in the final composition, but this is not the case. Instead, a correction factor called a **bowing parameter** must be applied. This bowing parameter is the empirical offset between the two molecules. Bowing parameters as described in Luisier *et al.* are considered [15]. An overview of the NEMO5 tight-binding parameters and what they correspond to in reality is included in this thesis. The Esaki diode simulations are run using the regular VCA model and the model adjusted with the bowing parameters, and comparisons of the results are made. VASP 5.4 and NEMO5 results for MoS$_2$ bandstructure simulations are plotted together in this thesis, and this is the first step to calculating a set of bowing parameters for this material system.

The density functional theory (DFT) is one solution to solving many-body Schrödinger equations, and this is the fastest VASP 5.4 simulation method to run for bandstructure simulations. A comparison of this and two other available simulation methods (DFT with GGA-PBE, HSE06 with GGA-PBE, and Hartree-Fock) is included in this study. The simulation speed and accuracy are both considered. Lattice constant
variation effects in VASP 5.4 are also considered for both standard III-V and MoS$_2$
and WTe$_2$ systems, as this sort of change corresponds to added strain or monolayer
directions, such as armchair or zigzag directions.
Chapter 2

Diode and Tunnel FET Theory

2.1 Esaki Diode Introduction

Tunnel diodes were first discovered in 1957 by Leo Esaki when he noticed the distinctive N-shaped transfer characteristic now called negative differential resistance (NDR) that has come to define them. They are also called Esaki diodes for this historical reason. [19, 20]

Tunneling occurs when a particle such as an electron actually penetrates the potential barrier if it is thin enough compared to the electron's Bloch wavelength. Seabaugh and Lake refer to tunneling as a ghostlike passage which is a good way to think of it. [20]

Tunnel diodes in particular are heavily doped on both $p$- and $n$-sides. They exhibit both normal minority-carrier-based diffusion current and majority-carrier-based tunneling current (the latter for low voltage conditions). Fig. 2.1 from Pawlik's doctoral thesis shows the transfer characteristics and band diagrams for the different types of bias in a typical tunnel diode. [3]
2.2 Subthreshold Swing Analysis for TFETs

Wei’s group investigated the SS of TFETs by deriving a comprehensive analytical model based on electrostatic and material effects. An analysis of their findings is used to provide more understanding of TFET requirements from an operation stand-point. The device and corresponding energy band diagram assumed in their derivation is seen in Fig. 2.2. Relevant parameters in this figure as well as in the derivations to come include: $f_s(E)$, the FD distribution of electrons in the source region; $f_d(E)$, the FD distribution of electrons in the drain region; $W_T$, the minimum tunnel width; $E_{cc}$, the minima of the conduction band in the channel region; $E_{vs}$, the maxima of the valence band in the channel region; $E_{vj}$, the maxima of the valence band at the source-to-channel junction; $E_g$, the band gap; $E_{fs}$, the source Fermi level; $E_{fd}$, the drain Fermi level; and $\Delta E$, the allowed tunnel window contributing to tunneling transport. [4]
The source-to-channel tunneling current \( I_{ds} \) Wei et al. employed is derived from making assumptions based on this device with respect to Eq. 2.1, the current for one conduction mode in TFETs within the Landauer's formalism. [4]

\[
I_{ds} = \frac{2q}{h} \int_{E_{cc}}^{E_{vs}} T(E)[f_s(E) - f_d(E)]dE \tag{2.1}
\]

where \( q \) is the electron charge, \( h \) is Planck's constant, \( T(E) \) is the BTBT probability, and \( f_{s/d}(E) \) is the source-to-drain FD distribution. These assumptions include: (1) the BTBT probability remains constant across the relevant tunnel window, which is valid for a small (within a few kT) tunnel window, and (2) the FD distribution of electrons in the drain region is small enough to ignore when compared to the FD distribution of electrons in the source region, and (3) the Fermi function integral is

---

\[1\] Reprinted from (C. Wei, D. Sarkar, Y. Khatami, K. Jiahao, and K. Banerjee, Subthresholdswing physics of tunnel field-effect transistors, AIP Advances, vol. 4, no. 6, June 2014) with the permission of AIP Publishing.
collected into a term $F_{Integral}$. The simplified tunneling current equation is then:

$$I_{ds} = \frac{2q}{h} T(\Delta E) F_{Integral}$$

(2.2)

where

$$F_{Integral} = kT \ln \frac{1 + \exp \left( \frac{E_{fs} - E_{vs} + \Delta E}{kT} \right)}{1 + \exp \left( \frac{E_{fs} - E_{vs}}{kT} \right)}.$$  

(2.3)

The BTBT probability is found by solving the 2D Poisson equation for channel potential. This is done by simplifying the Poisson equation into a 1D form through a parabolic approximation, then using an analytic model cited by Zhang et al. that defines the electrostatic potential profile around the tunnel junction in double-gated (DG) TFETs. This is used to find the valence band maxima at the source-to-channel junction, $E_{vj}$:

$$E_{vj} = \sqrt{(E_{vs} - E_{fs} + \delta E)^2 + \gamma^2 + 2\gamma(\Delta E_{sc} + E_{vs} - E_{fs}) - (\Delta E_{sc} + E_{vs} - E_{fs} + \gamma)}$$

(2.4)

where

$$\Delta E_{sc} = E_g + \delta E + \Delta E$$

(2.5)

$$\delta E = (E_{cc} - E_{vs}) \bigg|_{V_{gs}=0}$$

(2.6)

$$\gamma = \frac{q^2 N_{A,eff} \lambda^2}{\epsilon_{ch}}$$

(2.7)

$$N_{A,eff} = N_A - \frac{\epsilon_{ox} (\Delta E_{sc} + E_{vs} - E_{fs})}{\pi q^2 T_{ox} T_{ch}}$$

(2.8)

$$\lambda = \sqrt{\frac{\epsilon_{ch} T_{ox} T_{ch}}{2 \epsilon_{ox}}}$$

(2.9)

where $N_A$ is the source doping, $\epsilon_{ox}$ is the permittivity of the gate dielectric material, $T_{ch}$ is the corresponding thickness of the gate dielectric material, $\epsilon_{ch}$ is the permittivity of the channel material, and $T_{ch}$ is the corresponding thickness of the channel.
Using Eqs. (2.4 - 2.9), the minimum tunnel width is defined as follows:

\[
W_T = L_1 + L_2 - \lambda \cosh^{-1}\left( \frac{\Delta E + \delta E - E_{fs} + E_{v,WT}}{E_{vs} - E_{fs} + \delta E} \right) - \sqrt{\frac{2\epsilon_{ch}(E_{vs} - E_{v,WT} - E_g)}{q^2 N_{A,eff}}} \tag{2.10}
\]

where \( L_1 \) and \( L_2 \) are the depletion widths:

\[
L_1 = \sqrt{\frac{2\epsilon_{ch}(E_{vs} - E_{vj})}{q^2 N_{A,eff}}} \tag{2.11}
\]

\[
L_2 = \lambda \cosh^{-1}\left( \frac{\Delta E_{sc} + E_{vs} - E_{fs} - (E_{us} - E_{vj})}{E_{vs} - E_{fs} + \delta E} \right) \tag{2.12}
\]

and

\[
E_{v,WT} = \sqrt{(E_{vs} - E_{fs} + \delta E)^2 + \gamma^2 + 2\gamma(\Delta E + \delta E + E_{vs} - E_{fs}) - (\Delta E + \delta E + E_{vs} - E_{fs} + \gamma)} \tag{2.13}
\]

Finally, the BTBT probability is found using the Wentzel-Kramers-Brillouin (WKB) approximation and the two-band dispersion relation as established by Kane in his famous 1961 paper. [21, 4]

\[
T(\Delta E) = \exp\left( -\frac{\pi \sqrt{2m_T \Delta E^3/2}}{4q \left( \frac{k}{2\pi} \right)^4} \right) \tag{2.14}
\]

where \( m_T \) is the tunnel effective mass, and the junction electric field is given by \( \bar{F} = \frac{E_g}{W_T} \). As will be noted later in this thesis, full band structure consists of many bands. In certain circumstances, Kane's 2-band model is adequate. Also, Kane assumes a parabolic dispersion which is not always correct.

Equations (2.2 and 2.14) can be combined to define an equation for \( SS \), which in turn can be broken down into its contributions from the tunneling probability, \( SS_T \),
and from the FD distribution, $SS_{FD}$:

$$SS = \left( \frac{d \log_{10}(I_{ds})}{d(\Delta E/q)} \right)^{-1} = \frac{SS_T SS_{FD}}{SS_T + SS_{FD}} \quad (2.15)$$

where

$$SS_T = \left( \frac{d \log_{10}(T(\Delta E))}{d(\Delta E/q)} \right)^{-1} = \frac{2\sqrt{2}ln(10)h/(2\pi)}{-q\pi \sqrt{m_T E_g dW_T} \Delta E} \quad (2.16)$$

$$SS_{FD} = \left( \frac{d \log_{10}(FIntegral)}{d(\Delta E/q)} \right)^{-1} = \frac{\ln(10)kT}{q} \left( 1 + \exp \left( \frac{E_{vs} - E_{fs} - \Delta E}{kT} \right) \right) \ln \left( \frac{1 + \exp \left( \frac{E_{fs} - E_{vs} + \Delta E}{kT} \right)}{1 + \exp \left( \frac{E_{fs} - E_{vs}}{kT} \right)} \right) \quad (2.17)$$

Simulations using the preceding equations performed at room temperature for a DG Si TFET with $m_T = 0.65m_0$, $N_A = 3E20 \text{ cm}^{-3}$, $T_{ox} = 1 \text{ nm}$, $T_{ch} = 10 \text{ nm}$, and $E_g = 1.12 \text{ eV}$ resulted in Fig. 2.3. [4]

![Figure 2.3: Simulated results of $SS$, $SS_T$, and $SS_{FD}$ as affected by change in the width of the tunnel window $\Delta E$.][1]

The $\Delta E$ axis of Fig. 2.3 is broken up into three regions corresponding to the

\[1\] Reprinted from (C. Wei, D. Sarkar, Y. Khatami, K. Jiahao, and K. Banerjee, Subthresholdswing physics of tunnel field-effect transistors, AIP Advances, vol. 4, no. 6, June 2014), with the permission of AIP Publishing.

[2][13]
significant changes in $SS_{FD}$. In region I, $SS_{FD}$ simplifies to [4]

$$SS_{FD,RegionI} = \frac{ln(10)kT}{q}(1 - exp\left(\frac{-\Delta E}{kT}\right))$$ (2.18)

From this equation, as well as Fig. 2.3, it is observed that $SS_{FD}$ exponentially approaches zero as the tunneling window decreases in size. According to Wei et al. this phenomenon is due to the FD distribution being truncated by the bandgap of the source region. It is this region of operation, referred to as the onset stage, that Wei et al. are most interested in because, as a result of the FD truncation phenomenon, the onset stage will result in the $SS_{min}$ for the system. To further highlight this focus, recall that the first assumption made when deriving Eq. (2.2) is true for small $\Delta E$ only; thus, the resultant equations, including those for the various $SS$ values, are only accurate for region I. Note that these equations, while not numerically accurate for $\Delta E > 2kT$, still provide approximate qualitative models for $SS$ in regions II and III. [4]

It would follow from Eq. (2.15) and Eq. (2.18), as well as Fig. 2.3 that the $SS$ at the onset stage would result in a near-zero $SS$, but this is not the case. The reason for this is that the OFF-current, ($I_{OFF}$) will dominate the low BTBT current, $I_{BTBT}$. An equation for OFF-current is as follows: [4]

$$I_{OFF} = \frac{2q}{\hbar} \int_{E_{cs}}^{+\infty} f_s(E)dE = \frac{2qkT}{\hbar} exp\left(\frac{E_g + E_{vs} - E_{fs}}{-kT}\right)$$ (2.19)

This equation for $I_{OFF}$ does not include tunnel and gate leakage effects which would result from factors such as interface states near the tunneling junction. The effects of such interface states are a huge issue in TFETs, and this is discussed in depth in later sections, but it is beyond the scope of Wei’s group’s research on SS physics in Si and III-V TFETs. [4]

The hurdle posed by the OFF-current can be overcome and $SS$ can be brought
down if the BTBT current in the onset stage, $I_{ON}$, is larger than $I_{OFF}$. The ratio between $I_{ON}$ and $I_{OFF}$ is called the onset strength of the device. Note that the minimum $SS$, $SS_{min}$, occurs when the BTBT current is equal to the OFF-current; that is,

$$SS_{min} = SS\bigg|_{I_{OFF}=I_{BTBT}}$$  \hspace{1cm} (2.20)

To determine the optimal material and electrostatic parameter values for establishing a large onset strength, four main TFET parameters: source doping level ($N_A$), natural length ($\lambda$), bandgap ($E_g$), and tunnel effective mass ($m_T$) are changed and their effects on $I_{ON}$ and $I_{OFF}$ are simulated. Fig. 2.4 illustrates these findings. [4]

![Figure 2.4: $I_{BTBT}$ in terms of $I_{ON}$ (referred to as $I_{onset}$ in the graphs) and $I_{OFF}$ for homojunction and heterojunction TFETs as functions of $N_A$, $\lambda$, $E_g$, and $m_T$.][4]

From Fig. 2.4 it can be seen that small $\lambda$ and $m_T$ are always desired and there is a simulated optimal $N_A$ value of approximately $3E20$ $cm^{-3}$ that corresponds to maximized $I_{ON}$; for the latter, it is interesting to note that both lowering and increasing the doping past this optimal value will correspond to lowered onset strength. Also, for

---

the case of heterojunction TFETs, small $E_g$ is desired, while the relationship between bandgap and onset strength in homojunctions is not clear-cut. [4]

The final element of the total $SS$ left to consider in pursuit of $SS_{\text{min}}$ are the effects on $SS$ of the tunneling probability, $SS_T$. Fig. 2.5 presents the effects of the four critical TFET parameters previously examined in terms of onset strength (that is: of $N_A$, $\lambda$, $E_g$, and $m_T$) on $SS_{\text{min}}$ and $SS_T$ evaluated at $\Delta E = 2kT$. [4]

The results of Fig. 2.5 at first seem contrary to logic: $SS_{T@2kT}$ increases with increased $N_A$, and decreased $\lambda$, $E_g$, and $m_T$, even though tunneling efficiency is known to increase with these same changes in critical parameters. The reason for this is that the increased $N_A$, and/ or decreased $\lambda$ correspond to a decrease in the depletion widths $L_1$ and/ or $L_2$, as seen in equations (2.11) and (2.12), respectively. These changes in turn correspond to a decrease in the minimum tunnel width $W_T$. TFETs with small tunnel widths are affected more strongly by junction electrostatic effects, and so the rate of change of $W_T$ with respect to $\Delta E$, $\frac{dW_T}{d\Delta E}$, will decrease accordingly.

---

for devices with increased $N_A$ and/or decreased $\lambda$. The effect this decrease in $\frac{dW_T}{d\Delta E}$, as well as the decrease in either or both other two parameters $E_g$ and $m_T$, have on $SS_T$ is clear from Eq. (2.16) where these terms are in the denominator and thus correspond to an increase in $SS_T$ per their decrease. Wei et al. notes that this degradation in total $SS$ through the effects of intrinsic properties on $SS_T$ is often wrongly overlooked in the TFET community. [4]

Solutions to the problem of having both high $I_{ON}$ and small $SS$ suggested by Wei et al. include the use of heterojunction materials to boost tunneling, as well as using 2D semiconductors for the channel materials [4]. 2D semiconductors will be considered next.

2.3 2D Semiconductors and their applications in conventional FETs and TFETs

Atomic scale thickness is a huge benefit of using 2D semiconductors as channel materials in ever-shrinking FETs. Conventional bulk semiconductors such as Si can also be deposited at atomic thicknesses, but 2D semiconductors have multiple advantages over these bulk materials including dangling bond-free surfaces and fixed thicknesses which can be reproduced consistently for the chosen number of layers, resulting in minimal bandgap variation and carrier scattering. This is seen in Fig. 2.6 (a) and (b). [5]
The atomic thicknesses capability of the 2D channel devices results in devices with superior electrostatics when compared to bulk channel devices; the fewer the number of layers, the better the electrostatics [5]. This is in part because the 2D materials provide increased gate control over the channel, resulting in higher electric fields at the junction [6]. Eq. (2.21) from Ilatikhameneh et al. can be used to explain this concept; note that the parameters for this equation are defined as part of the Wei et al. SS derivation [6].

$$\lambda = \sqrt{\frac{\epsilon_{ch}}{2\epsilon_{ox}}(1 + \frac{\epsilon_{ox}I_{ch}}{4\epsilon_{ch}T_{ox}})T_{ch}T_{ox}}$$

(2.21)

Scrutiny of Eq. (2.21) shows that the reduction of the channel thickness will also result in a reduction of the device $\lambda$, and this is known to result in higher electric...
fields. The BTBT probability is exponentially dependent on the electric field, so atomically thin devices also result in better tunneling, which means higher $I_{ON}$. [6]

Another benefit to 2D materials is that thinning 2D materials will increase the bandgap significantly less than thinning a 3D material due to the weaker bonds between the layers of 2D materials. This is useful because increasing the bandgap corresponds to a shortening of the tunneling window which means that the $I_{ON}$ will also be diminished. Besides this, monolayer 2D materials are known to have small dielectric constants which also corresponds to increased $I_{ON}$. [6]

While carrier mobility decreases with decreasing layer thickness for all materials, it is a slower decrease for molybdenum disulfide (MoS$_2$) than for Si, which results in MoS$_2$ having a higher mobility than Si at the monolayer (1L) level. One demonstrated hero device, as shown by Liu et al., achieved a MoS$_2$ 1L mobility of 44 cm$^2$/V · s, significantly higher than the usual 13 cm$^2$/V · s for the same material. This can be seen in Fig. 2.6 (c). For comparison, consider that a 5 nm x 5 nm Si nanowire, given that a Si unit cell is known to be 0.545 nm, is about 9-10 monolayers in height. [5]

According to Wei et al. most theoretical simulations of 2D semiconductor-on-insulator (SOI) or DG FETs use inappropriate ballistic transport or poor back scattering simulations instead of dissipative transport theory, as is required for accurate predictions at and below the sub-10 nm node. Ballistic transport has been shown to overestimate drain current for 8 nm channel lengths. [5]

A balance must be struck between the scattering events considered during simulation and those ignored so that the simulations will be accurate but also computationally feasible. The approach taken by Wei et al. is summarized succinctly in Fig. 2.7. [5]
CHAPTER 2. DIODE AND TUNNEL FET THEORY

Figure 2.7: (a) $E_C$ of a n-MOSFET in the channel region (that is, from source to drain) with Büttiker probes inserted at every mesh point along the channel. (b) A single Büttiker probe. (c) The simulation design. IEEE ©2015.6[5]

For their simulations, Wei et al. use an approach adapted from Venugopal et al. [22] and Anantram et al. [23] use of Büttiker probes [24]; these are shown in Fig. 2.7 (a) and (b). The probes are inserted at each mesh point along the channel; each probe will take as its inputs the momentum and energy of the carriers at its location in the mesh, and its outputs will be the momentum and energy as changed by the predicted scattering events of the carriers at the probe's location. It is important to note that the probe will only affect the momentum and energy of the carriers at the

---

given point in the channel, and not the quantity of carriers passing through. The function of the probe is as follows: [5, 22, 23, 24]

1. Take as inputs the momentum and energy of the carriers;

2. Solve Poisson equation for the relevant electrostatics;

3. Solve the effective mass transport equation with a nonequilibrium Green's function (NEGF) for charge distribution and transmission;

4. Adjust the Fermi levels so that the net current at each probe is maintained to be zero;

5. Solve NEGF again, this time for carrier density and density of states (DOS);

6. Determine the appropriate scattering strength \( U_p \) from the carrier density and DOS;

7. Finally, output the momentum and energy of the carriers as affected by the calculated scattering strength.

In comparison, Ilatikhameneh et al.'s simulations are based on tight-binding (TB) with a Poisson-quantum transmitting boundary method (QTBM) methodology. This is equivalent to a more efficient form of solving the NEGF without scattering and is performed by the NEMO5 simulation tool available through the NanoHub at Purdue University. Because such simulations do not consider the scattering they can be done computationally faster than those performed by Wei et al. but are also less accurate. The monolayer TMD TFET simulated by Ilatikhameneh et al. is seen in Fig. 2.8 and has the following parameters: channel length= 15 nm, source/drain length = 10 nm, \( T_{ox} = 0.43 \) nm, and \( N_A/N_D = 1x10^{20} \ cm^{-3} \). [6]
Short-channel effects caused by lateral electric fields (that is, strong electric fields caused by the source/drain depletion regions being too close together) diminish control of the gate and are a widespread problem in short-channel bulk semiconductor FETs. These short-channel effects do not occur to the same degree in FETs with 1L to three-layer (3L) 2D semiconductor channels because such channels are too thin to maintain the significant lateral electric field strength. Instead, most of the lateral electric fields in FETs with 1L to 3L 2D semiconductor channels occur in the gate dielectric and through the spacers. Low-$k$ dielectric materials are effective in muzzling the lateral electric fields, but high-$k$ materials provide better gate control; thus, a compromise is reached in device design by selecting gate materials with high-$k$ and spacer materials with low-$k$. [5]

1L to 3L SOI and DG FETs with MoS$_2$ channel simulations consistently surpassed the $SS$ and $I_{ON}$ values simulated for Si ultrathin-body DG FETs. The DG 2D-channel devices outperformed the SOI 2D-channel devices for 2L and 3L due to the effects of the added lateral electric field through the 50 nm bottom gate dielectric of the latter device; for this reason, the DG 2D-channel device is considered superior to the SOI 2D-channel device. [5]

Low-standby-power (LSTP) applications require high threshold voltage ($V_{th}$), which corresponds to lowered $I_{ON}$. In contrast, high performance (HP) applications

---

require high $I_{ON}$, which corresponds to lowered $V_{th}$, and high-standby-power consumption. LSTP is a direct function of $SS$, and HP is instead a function of device parameters such as carrier mobility and DOS. Simulations by Wei et al. show better performance for MoS$_2$ FETs than for Si FETs for both HP and LSTP; the best device for HP is 2L, and the best device for LSTP is 1L. Devices with channels thicker than 3L will have significantly degraded electrostatics, outweighing the benefits of the higher DOS and increased carrier mobility provided by the increased layer thicknesses; thus, such channels should not be used for sub-10 nm nodes. According to the simulations, the LSTP requirement cannot be met with a MoS$_2$ channel device beyond the 7 nm node. [5]

High carrier mobility and relatively low effective mass $m_0$ are desired for all applications; while high mobility is always desired, care must be taken to ensure that the latter is not excessively small as this can result in increased source-to-drain tunneling leakage. Fig. 2.9 includes available data on material mobility and corresponding effective mass of 2D TMD semiconductors based on experiments and calculations performed by various groups as presented by Wei et al. [5]
From Fig. 2.9, WSe$_2$ is clearly the better material in terms of both effective mass and mobility. In fact, WSe$_2$ is capable of meeting all requirements down to the 5.9 nm node without any advanced techniques such as strain engineering, which is required of materials such as MoS$_2$ beyond the 7 nm node. [5]

Workable solutions for the sub-5 nm nodes include the use of anisotropic 2D materials and TFETs. An anisotropic material has different effective masses along the $x$- and $z$- planes; it has been found that a large effective mass in the transport or $z$-plane $m_z$ can increase the density of states and boost $I_{ON}$. As seen in Fig. 2.10, this results in useable materials for HP applications beyond the 5 nm node, but is not useful for LSTP applications. [5]

---

Figure 2.10: $I_{ON}$, seen as a color contour, is plotted as a function of effective mass along the $x$- and $z$- planes for HP (right) and LSTP (left) applications at the 5.9 nm node. The dashed blue lines correspond to isotropic materials. IEEE ©2015.

Ilatikhameneh et al. simulated multiple TMD TFETs with fixed $I_{OFF}= 1$ nA/µm at $V_G= 0$ V. The results are seen in Fig. 2.11.

Figure 2.11: The transfer characteristics of various simulated TMD TFETs by Ilatikhameneh et al. IEEE ©2015.

Fig. 2.11 shows that optimal TMD gate material is WTe$_2$, both in terms of SS and $I_{ON}$. This is due to factors such as its small bandgap and effective mass. These and other material parameters as well as the simulated results are seen in Table 2.1.

Table 2.1: Data corresponding to the TMD TFET simulations seen in Fig.2.11. Note that effective mass/$m_0$ is referred to as the reduced effective mass, $m^*_r$. IEEE © 2015.

<table>
<thead>
<tr>
<th>Material</th>
<th>$I_{ON}$ ($\mu$A/$\mu$m)</th>
<th>$E_g$ (eV)</th>
<th>$m^*_r$ (a.u.)</th>
<th>$\lambda$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WTe$_2$</td>
<td>127</td>
<td>0.75</td>
<td>0.17</td>
<td>0.45</td>
</tr>
<tr>
<td>WSe$_2$</td>
<td>4.6</td>
<td>1.56</td>
<td>0.21</td>
<td>0.41</td>
</tr>
<tr>
<td>MoTe$_2$</td>
<td>2.3</td>
<td>1.08</td>
<td>0.32</td>
<td>0.5</td>
</tr>
<tr>
<td>MoS$_2$</td>
<td>0.3</td>
<td>1.68</td>
<td>0.29</td>
<td>0.38</td>
</tr>
</tbody>
</table>

From these results WTe$_2$ would seem the clear winner for use as a channel material with a simulated $I_{ON}$ almost 28 times as large as that of WSe$_2$ [6]. This conclusion sadly cannot be compared to Wei et al.'s findings because that group did not simulate WTe$_2$. They can, however, be compared to Fei et al.'s simulated results for 6 different TMD TFETs with channel lengths of 12 nm and $V_D = 0.5$ V [8]. These results are listed in Table 2.2.

Table 2.2: TMD TFET simulations by Fei et al. $m_e/m_0$ is the reduced electron effective mass, and $m_h/m_0$ is the reduced hole effective mass. IEEE © 2016.

<table>
<thead>
<tr>
<th>Material</th>
<th>$E_g$ (eV)</th>
<th>$m_e(m_0)$</th>
<th>$m_h(m_0)$</th>
<th>SS$_{min}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS$_2$</td>
<td>1.66</td>
<td>0.42</td>
<td>0.54</td>
<td>48.3</td>
</tr>
<tr>
<td>WS$_2$</td>
<td>1.81</td>
<td>0.30</td>
<td>0.39</td>
<td>56.1</td>
</tr>
<tr>
<td>MoSe$_2$</td>
<td>1.43</td>
<td>0.48</td>
<td>0.59</td>
<td>49.4</td>
</tr>
<tr>
<td>WSe$_2$</td>
<td>1.54</td>
<td>0.32</td>
<td>0.41</td>
<td>58.6</td>
</tr>
<tr>
<td>MoTe$_2$</td>
<td>1.07</td>
<td>0.39</td>
<td>0.54</td>
<td>58.6</td>
</tr>
<tr>
<td>WTe$_2$</td>
<td>1.07</td>
<td>0.25</td>
<td>0.34</td>
<td>71.2</td>
</tr>
</tbody>
</table>


Table 2.2 tells a different story in terms of the best TMD channel material because it lists the $SS_{min}$ values for each of the materials, and WTe$_2$ is the highest and worst of these. This is because smaller bandgap and effective mass, as is the case for the monolayer WTe$_2$, results in lower $I_{ON}$ but smaller onset strength and thus higher $SS_{min}$. According to this data, MoS$_2$ would be the best TMD material to use, though it has been shown that this is untrue from the Wei et al. paper. [8] The trade-off of $SS$ and onset strength must be considered when choosing the TMD channel material and makes the choice more difficult than at first expected. It should be noted that Seabaugh et al. mention that as of 2015 no fabricated TMD TFETs have shown sub-60 mV/decade $SS$.

For LSTP applications, TFETs with TMD channels are a viable solution due to the numerous established advantages of 2D semiconductors. These include restraint on tunneling leakage and therefore improvement of $SS$ due to the dangling bond-free surface of a 2D semiconductor, as well as increased gate control and increased $I_{ON}$ caused by having an ultrathin body. [5] Next, focus will shift on the effects of having an ultrathin body in TFETs, as seen through an analysis of channel geometry, namely in terms of fin thickness and channel length.

2.4 The Effects of Channel Geometry on TMD TFETs

Electric fields responsible for tunneling of up to approximately 20 MV/cm have been observed in DG $p$-gallium nitride/$intrinsic$-indium nitride/$n$-gallium nitride ($p$-GaN/InN/$n$-GaN) fin TFET tunnel junctions; this is five times higher than the maximum electric fields observed in IV and III-V tunnel junctions. The reason for this is that this stack uses the physics of the heterojunction to positively influence tunneling capabilities: specifically, InN has a bandgap of 0.7 eV which is narrow compared to

\footnote{Reprinted from (L. Fei, W. Jian, and G. Hong, Atomistic simulations of device physics in monolayer transition metal dichalcogenide tunneling transistors, IEEE Transactions on Electron Devices) with the permission of IEEE © 2016.}
the GaN bandgap of 3.2 eV. The narrow InN bandgap is responsible for increased inter-band tunneling and the wide GaN bandgap suppresses the OFF-current of the TFET device. Fig. 2.12 is the device and its corresponding band diagram. [7]

Figure 2.12: (a) The TFET structure used for simulations, and (b) the simulated energy band diagram of this device. IEEE © 2015.\textsuperscript{13}[7]

Dependences on the fin thickness $L_D$ and the drain (that is, the $n$-GaN layer) doping $N_D$ are observed from simulated transfer characteristics for a DG $p$-GaN/InN/$n$-GaN TFET device. The transfer characteristics, which can be seen in Fig. 2.13, correspond to the drain current per unit width $I_D/W$, a variable synonymous to the tunnel current, as a function of changing $V_{GS}$. [7]

Figure 2.13: Synopsis TCAD transfer characteristics of (a) drain doping, and (b) fin thickness dependence, with the device parameters as follows: gate length $L_G = 20$ nm, thickness of the InN layer $t_{InN} = 1.7$ nm, thickness of the GaN layers $t_{p-GaN} = t_{n-GaN} = 25$ nm, equivalent oxide thickness $EOT = 0.43$ nm, and $V_{DS} = 0.5$V. IEEE © 2015.\[7\]

Assuming a fixed drain doping $N_D$ of $1x10^{17}$ cm$^{-3}$, an optimum fin thickness $L_D$ is found to be between 10 to 20 nm; for $L_D < 10$ nm, the $I_D/W$ will start to decrease as the current cross section diminishes; similarly, for $L_D > 20$ nm, the $I_D/W$ will also decrease, though in this case as a result of lowered gate electrostatic control with increased $L_D$. Assuming a fixed fin thickness $L_D$ of 12 nm, increasing the drain doping $N_D > 1x10^{18}$ cm$^{-3}$ increases the density of carriers in the channel, thus reducing the number of free states available for tunneling to occur; this directly correlates to a decrease in tunnel current; contrarily, for changing $N_D < 1x10^{18}$ cm$^{-3}$, the tunnel current will remain unchanged.\[7\]

To supplement these findings, the behavior of a different device with changing channel length is explored in the Fei et al. paper. The device is a DG TFET with the monolayer MoTe$_2$ used as the gate material. Unlike the device explored in the

Seabaugh et al. paper, this DG device, seen in Fig. 2.14 along with the atomistic structures of the monolayer along the armchair (AD) and zigzag (ZD) directions, is not a fin TFET, and so instead of the fin-thickness $L_D$, the channel length $L_G$ is varied and observed. [8]

Figure 2.14: (a) The DG monolayer TMD TFET device structure, (b) the atomistic structure of the TMD monolayer along the ZD direction, and (c) the atomistic structure of the TMD monolayer along the AD direction. IEEE © 2016. [8]

Fei et al. notes that the performance of the TMD TFET is orientation dependent; for example, ZD can lead to higher $I_{ON}$, but no NDR, whereas AD has a very large NDR. These differences are, however, beyond the scope of this study. [8]

In the corresponding simulation which uses the TMD material MoTe$_2$, the channel length $L_G$ is varied from 5 nm to 20 nm in increments of 5 nm with the drain voltage $V_D = 0.5$ V. The general transfer characteristics of the device with different gate lengths are shown in Fig. 2.15. [8]

---

Figure 2.15: The simulated MoTe2 TFET transfer characteristics for different channel lengths in the (a) AD, and (b) ZD directions. IEEE © 2016. \[8\]

Two conclusions can be drawn from Fig. 2.15: larger $L_G$ corresponds to smaller OFF-current, and the $I_{ON}$ is not a function of channel length. \[8\] From these two papers, the impact of the channel geometry of different devices has been studied and determined to be a significant source of variation in terms of device behavior.

### 2.5 TMD Coupling in TFETs

Heterogeneous TFETs can be made by stacking p-n junctions of different TMD materials into what is known as couple configurations. To determine the most optimal such couples, Gong et al. characterizes the individual TMD materials based on band alignment. The results are seen in Fig. 2.16. \[9\]

According to Fig. 2.16, electrons at the $E_V$ of WTe$_2$ and MoTe$_2$ could easily tunnel into the $E_C$ of ZrS$_2$, ZrSe$_2$, HfS$_2$, and HfSe$_2$. Gong et al. suggests the following couplings: $n$-type source as WTe$_2$, WSe$_2$, MoTe$_2$, or MoSe$_2$ with $p$-type drain as ZrS$_2$, ZrSe$_2$, HfS$_2$, or HfSe$_2$. [9] This is an interesting and note-worthy application of TMDs in TFETs because it uses the TMD materials for what would typically be the source/drain regions. When the two energy bands meet and open a tunneling window, the channel is created out of these regions without the use of an intrinsic layer.

3.1 The Necessity of Quantum Simulations

Computer-aided design is the first step to reducing fabrication cost of new devices, but determining the required software to use can be a challenge. This is considered.

Tunneling is calculated based on the assumption of straight-line tunneling paths in the popular dynamic nonlocal band-to-band (DNL) simulation method, whereas in the non-equilibrium Green’s function (NEGF) method, the electrostatic potentials are obtained from self-consistent semiclassical Poisson calculations. Software packages such as Silvaco primarily use DNL-type simulations, whereas VASP and nanoHub’s NEMO are both quantum-based. Determining which type of simulation software to use when simulating the desired devices is the necessary first step to conducting novel research. The Rochester Institute of Technology’s Microelectronic Engineering department has a license for Silvaco’s Athena software at the time of this writing, so this was the evident choice before massive drawbacks were recognized. The largest of these is illustrated in the example by Jiang et al.; Fig. 3.2 compares simulation results from DNL and NEGF results in a AlGaSb/InAs TFET (see Fig. 3.1 for the simulated device geometry). The simulation results in this paper follow from experimental results by Zhou et al. The parameters being varied in the simulations are gate length ($L_g$) and undercut length ($L_{uc}$). [25]
CHAPTER 3. QUANTUM SIMULATION THEORY

Figure 3.1: (a) Device geometry of the simulated TFET design. (b) Band profile plotted along dashed line in (a). IEEE ©2015.\textsuperscript{1}[10]

Figure 3.2: Comparisons of dynamic nonlocal band-to-band (DNL) and non-equilibrium Green's function (NEGF) simulation results. Note that the straight-lines correspond to the DNL simulations and the lines with the bullets correspond to the NEGF simulations. IEEE ©2015.\textsuperscript{2}[10]

It is seen that the NEGF simulation results in a higher $SS$ than the DNL method. This observed difference is because the DNL model underestimates the contributions from the direct source–drain tunneling in the simulated geometries. NEGF simulations also take quantum-level scattering into consideration. Fig. 3.2 is an extreme

exaggeration of the required results because the experiment will look worse than the
TCAD simulation. Thus, the atomistic model produced via NEGF simulations is
required to show negative differential resistance (NDR) in the simulations. Determin-
ing NDR is pivotal to simulating both Esaki diodes and especially TFETs, so an
appropriate quantum simulator must be selected to continue with this research.

3.2 Choosing a Quantum Simulation Package

3.2.1 The Vienna Ab initio Software Package

The Vienna Ab initio Software Package (VASP) 5.4 is a simulation package capable
of computing an approximate solution to the many-body Schrödinger equation either
by solving the Kohn-Sham equations which will be discussed later in this chapter or by
other methods such as the Hartree-Fock solution. It has built-in Born-Oppenheimer
molecular dynamics, spin-orbit coupling, and strain application capabilities, among
many others. VASP is frequently used in the semiconductor industry for interface
studies and is one of few software packages capable of simulating non-standard in-
terfaces such as the 2D TMDs of interest in this study. The VASP 5.4 package was
commercially compiled for RIT by Materials Design, Inc. as a part of their MedeA
software. Appendix B in this document offers a simple tutorial for using MedeA
2.22.2 for a general VASP 5.4 simulation.

3.2.2 NanoHUB’s NEMO

NEMO5 is offered and supported by the NanoHUB at Purdue University. There
are approximately 500 NEMO5 users, some industrial and most academic. NEMO5
can solve band structure or energy-momentum \((E-k)\) problems directly through
user-selected solvers, the most common being the non-equilibrium Green's function
(NEGF). It is also capable of plotting I-V characteristics of devices built in the in-
put deck of the file. In contrast with VASP, which is an Ab initio package, NEMO uses empirical tight-binding which has been fit to VASP band structures. For further reading, consider Yaohua Tan’s thesis from Purdue University. In this thesis, a comparison is made as a sanity check. [26]

Fig. 3.3 shows the basic NEMO5 simulation flow.

As mentioned previously, simulations should have a fundamental basis on experimental results. The simulation results must be compared to real data to determine if they correspond to anything true. The best way to do this is to start with existing experimental data and try to recreate them using simulations. Such simulations follow in the next chapter.

3.3 Quantum Simulation Theory

3.3.1 The Single-Body Problem

The energy-momentum \((E - k)\) relationship of a crystalline solid is most often obtained by solving the Schrödinger equation for a one-electron problem. The Schrödinger equation defines the total energy of a system and is as follows:

\[
\hat{H}(x)\phi(x) = \frac{-\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).
\]  

(3.1)

A hydrogen atom is composed of a single electron and a proton. In spherical
coordinates, the Schrödinger equation for such a problem is shown in Eq. 3.2, with Fig. 3.4 explaining the spherical coordinates.

\[ \hat{H}(r, \theta, \phi) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi). \]  \hspace{1cm} (3.2)

Figure 3.4: The spherical coordinates of a hydrogen atom.

This single-electron problem can be solved explicitly. [27, 28, 29, 30]

3.3.2 Orbitals

The hydrogen atom wavefunctions, \( \psi(r, \theta, \phi) \), are the atomic orbitals. An atomic orbital is a function that describes one electron in an atom. It is important to understand the orientation and restrictions of each orbital when doing quantum simulations. Fig. 3.5 shows the \( s \), \( p \) and \( d \) orbitals and their various allowed states.
As shown by Vogl et al. and Jancu et al., quantum models including an excited $s$-like orbital, $s^*$, and excited $d$ orbitals improve the simulation model fits of $E - k$ and effective mass plots. [31, 32, 33] This makes the relevant states for the type of quantum simulations of interest $s$, $p$, and $d$. The $s$-sublevels have one orbital and can hold two electrons. The $s$-orbital only forms sigma bonds. The $p$-sublevels have three orbitals and can hold six electrons. The $p$-orbital forms both sigma and pi bonds. The $d$-sublevels have five orbitals and can hold ten electrons. The $d$-orbital forms sigma, pi, and delta bonds. [11, 12, 34]

3.3.3 Density Functional Theorem

In real world applications the systems of interest are extremely complicated; there is no such thing as a “single-body” problem such as the solution for the hydrogen atom expressed earlier outside an introductory course in quantum mechanics. The systems of interest, at least in the semiconductor industry, are “many-body” solids. The relevant interactions to consider when solving a many-body quantum system are
the following:

- The nuclei kinetic energy,
- The electron kinetic energy,
- The nuclei Coulombic interactions,
- The electron Coulombic interactions,
- And the nuclei-electron Coulombic interactions.

The solid’s behavior can be described by the wavefunction $\psi(r, \theta, \phi)$, which can in turn be found by solving the Schrödinger equation. But of course, a Schrödinger equation relating potentially millions of interactions as can be present at a transistor’s interface is not the sort of problem that can be solved explicitly. Instead, the problem must be significantly simplified by eliminating some of the interactions listed above. [35, 36]

One specific solution to dealing with many-body Schrödinger equations is using the density functional theory (DFT). This is based on multiple simplifications which will be covered in the following cursory overview. [35, 36]

The first of these simplifications is the Born-Oppenheimer approximation. This approximation states that the wavefunction depends primarily upon the nuclear part of the atomic system. The nuclear motion is significantly slower than the electron motion due to the former’s weight, and so it can be considered fixed. Therefore, only the position of the nuclei and not their velocity needs to be considered when performing calculations, reducing the required degrees of freedom drastically. [35, 36]

After the Born-Oppenheimer approximation is applied, the nuclei are now considered fixed in space, so they have no kinetic energy, and their Coulombic interaction with each other is a fixed value so it doesn’t affect the solution. The only term where the nuclei still have an effect is in the nuclei-electron Coulombic interactions, and
this term comes to define which type of problem is being solved because it determines what molecule is being considered. In DFT context, this is often called the external potential because the nuclei determine the Coulombic potential in which the electrons move, and this defines the problem being solved. In summary, the relevant interactions are now:

- The electron kinetic energy,
- The electron Coulombic interactions,
- And the nuclei-electron Coulombic interactions (also known as the external potential).

The second simplification required for DFT is the Hohenburg-Kohn theorem. Note that a proof of this theorem is included in Appendix A. This theorem states that the electron density, $\rho$, of any system determines every ground-state property of the system. That is, the total ground state energy of a many-electron system is a function of the density, so therefore, if the electron density function is known, so too is the total energy of the system. This means that using this electron density function, all other ground state properties can be calculated. A simpler way to think of this is the following: every external potential corresponds to one specific wavefunction which corresponds to one specific density function. Thus, the wavefunction can be taken out and the external potential can be connected directly to a specific density function, with no information loss. [35, 36, 37]

In DFT the many-body Schrödinger equation is transformed into single-particle Kohn-Sham equations, which are the types of equations that are solved through a software like VASP. [35, 36] The Kohn-Sham equations are seen in equations 3.3 and 3.4:

$$\hat{H}_{ks}(\hat{r}) = \frac{-1}{2} \Delta^2 + v_{ks}(\hat{r})$$  \hspace{1cm} (3.3)

$$v_{ks}(\hat{r}) = v_{ext}(\hat{r}) + v_{H}(\hat{r}) + v_{xc}(\hat{r})$$  \hspace{1cm} (3.4)
where $H_{ks}(\hat{r})$ is the effective Hamiltonian, $v_{ks}(\hat{r})$ is the effective Kohn-Sham potential, $v_{\text{ext}}(\hat{r})$ is the external potential, $v_{H}(\hat{r})$ is the Hartree potential, and $v_{xc}(\hat{r})$ is the exchange-correlational potential. \cite{35, 36, 37}

These equations operate by replacing the electrons in the crystal with non-interacting quasi-electrons. These new electrons are now only interacting with nuclei and not themselves. Next, an external field called the exchange-correlational field is applied to correct for the omitted interaction. The field is derived from the exchange-correlation potential, and if this functional is known the prediction that is made is without any accuracy loss. \cite{35, 36, 37}

The most important part of performing a DFT-type calculation is the choice of the exchange-correlation functional. There is no rule for finding the best functional and often the way to do this is to make an educated guess and go from there until the functional begins predicting experimental values as closely as possible. \cite{35, 36}

### 3.3.4 Jacob’s Ladder

Jacob’s ladder is an idea developed by Perdew and Schmidt which considers the efficiency and accuracy of using various methods for finding the external correlational functional. Fig. 3.6 shows a graphical representation of this idea. It shows the sacrifice in simulation simplicity that is often required to obtain accurate results.
The general idea of Jacob’s ladder is that things higher up the ladder are more effective so will converge faster, but each run will take longer. The discussion of convergence which follows in the next section should serve to clarify this idea.

The simulations performed in VASP that correspond to the rungs of this ladder include the DFT simulation using the generalized gradient approximation (GGA), the HSE06 simulation which is a hybrid-GGA, and the Hartree-Fock simulation which is not a DFT simulation at all.

### 3.4 Convergence

The goal of quantum simulations are $E - k$ plots and $I - V$ characteristics that match reality. To achieve this, the code must converge or focus onto a single value. The error is the difference between two iterations. Each iteration is composed of a guess, followed by a calculation of the error, followed by an iteration corrected using

---

3Reprinted from (John P. Perdew, Karla Schmidt, Jacob’s ladder of density functional approximations for the exchange-correlation energy, AIP Conference Proceedings, 2001) with the permission of AIP Publishing.
the error, etc., until the error falls within the convergence criteria (in other words, until the error is small enough). At this point convergence is said to occur. The convergence limit is set either by the user or the simulation software; the smaller the error is required to be, the longer the simulation will take. It is possible that if the convergence criterion is too small, the simulation may time out and never finish running, so it is important to consider the limits of the simulation software and servers when setting this criterion. In both VASP 5.4 and NEMO the starting convergence criterion is a standard $1 \times 10^{-5}$ (the units are determined by what the simulation is aimed at doing, but one example is eV).

In both VASP 5.4 and NEMO, the simulated devices are composed of matrix grids of points in the $x$, $y$, and $z$ directions. These matrices of differential equations are simplified into difference equations and can then be broken down into for loops integrated over $x$, $y$, and $z$. The results of these simulations are likewise put into matrices of energy vs. momentum and current density vs. location to be read out by the user. Note that all simulation methods use matrices, and the more elements in a matrix, the longer it will take to solve. The grid breakdown must be done as simply as possible while also minimizing the error. An example of such a process is seen in NEMO’s MetaPoissonQTBM5.py solver which has both fast and safe algorithms built into it for breaking down the device grids and performing the required calculations. The fast algorithm only checks against the most recent previously calculated term to determine the error, while the safe algorithm uses the Newton approach, which means it compares with both the most recent previously calculated term and the one before that and computes the average error. The determined error is then used to correct its next value and so on until convergence occurs. Thus, the safe algorithm, though requiring more computation per term in reality might converge faster because its error values are more significant.

NEMO uses the Jacobian iterative method as one of its solvers. A brief expla-
nation of this method is shown below to further understanding of convergence. This
explanation and method are taken from An Introduction to Numerical Linear Algebra
by Cullen [38].

3.4.1 Jacobian Iterative Method

Start with the linear system \( A X = B \) where the diagonal entries of \( A \neq 0 \). The
coefficient matrix \( A \) can then be broken up into three parts:

- A lower triangular matrix, \( L \),
- An upper triangular matrix, \( R \),
- And a nonsingular diagonal matrix, \( D \).

Then,

\[
A = D - L - R
\]  (3.5)

and

\[
(D - L - R)X = B,
\]  (3.6)

\[
DX = (L + R)X + B,
\]  (3.7)

so that

\[
X = D^{-1}(L + R)X + D^{-1}B.
\]  (3.8)

To find \( X \) at convergence, the iteration is

\[
X_k = D^{-1}(L + R)X_{k+1} + D^{-1}B.
\]  (3.9)

An example of this method in use follows:
CHAPTER 3. QUANTUM SIMULATION THEORY

\[
X = \begin{bmatrix}
4 & -1 & -1 & 0 \\
-1 & 4 & 0 & -1 \\
-1 & 0 & 4 & -1 \\
0 & -1 & -1 & 4
\end{bmatrix}
= \begin{bmatrix}
9 \\
12 \\
0 \\
-3
\end{bmatrix}
\]

where the true solution is known to be

\[
X = \begin{bmatrix}
3.5 \\
4 \\
1 \\
0.5
\end{bmatrix}
\]

Using the iterative method expressed above, the problem is solved for \( X \).

\[
A = \begin{bmatrix}
4 & -1 & -1 & 0 \\
-1 & 4 & 0 & -1 \\
-1 & 0 & 4 & -1 \\
0 & -1 & -1 & 4
\end{bmatrix}
= D - L - R
\]

Therefore,

\[
A = \begin{bmatrix}
4 & 0 & 0 & 0 \\
0 & 4 & 0 & 0 \\
0 & 0 & 4 & 0 \\
0 & 0 & 0 & 4
\end{bmatrix}
- \begin{bmatrix}
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 1 & 0
\end{bmatrix}
- \begin{bmatrix}
0 & 1 & 1 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]
The Jacobian iteration matrix, $J$, is then defined as:

$$J = D^{-1}(L + R) = \frac{1}{4} \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$ 

and

$$X = JX + D^{-1}B = JX + \frac{1}{4}B.$$  \hspace{1cm} (3.10)

Then,

$$X_{k+1} = JX_k + \frac{1}{4}B$$  \hspace{1cm} (3.11)

where $k$ is the iteration value, with $k = 0$ being the arbitrary first guess, say:

$$X_0 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$ 

Then

$$X_1 = JX_0 + \frac{1}{4}B = \begin{bmatrix} 2.75 \\ 3.50 \\ 0.50 \\ -0.25 \end{bmatrix},$$

$$X_2 = JX_1 + \frac{1}{4}B = \begin{bmatrix} 3.25 \\ 3.625 \\ 0.625 \\ 0.250 \end{bmatrix},$$
\[
X_3 = \begin{bmatrix} 3.3125 \\ 3.8750 \\ 0.8750 \\ 0.3125 \end{bmatrix}, \quad X_4 = \begin{bmatrix} 3.4375 \\ 3.9063 \\ 0.9063 \\ 0.4375 \end{bmatrix}, \quad X_5 = \begin{bmatrix} 3.4531 \\ 3.9688 \\ 0.9688 \\ 0.4531 \end{bmatrix}, \quad X_6 = \begin{bmatrix} 3.4844 \\ 3.9766 \\ 0.9766 \\ 0.4844 \end{bmatrix}, \quad \ldots \Rightarrow X = \begin{bmatrix} 3.5 \\ 4 \\ 1 \\ 0.5 \end{bmatrix}.
\]

Clearly, as seen above, this method will yield a convergent series after enough iterations. If \(A\) was a full matrix each iteration would require approximately \(n^2\) multiplications, so this method is more time-consuming than Gaussian elimination if more than \(n/3\) iterations are required. Iterative methods are useful in solving systems where \(A\) is large, sparse, and regularly structured. [38]
4.1 Introduction to Esaki diode data to be simulated

With the goal of benchmarking NEMO5 against previously fabricated homojunctions, multiple systems were considered from Pawlik’s research [3]. These included InAs, GaAs, and In$_{0.53}$Ga$_{0.47}$As Esaki diodes. Note that due to their small electron and hole effective masses, $p-i-n$ transistors made from InAs and GaAs materials are viable devices for generating large BTBT [15]. The initial designs introduced three regions: an intrinsic region sandwiched between a heavily-doped $p$-region and a heavily-doped $n$-region, with doping levels chosen to match the IEDM paper published by Pawlik and Rommel that were largely based on SIMS data [14].

The experimental data are seen in Fig. 4.1 - 4.6. The InGaAs devices are shown schematically in Fig. 4.1. Note that the 3 nm intrinsic region was included to ensure the $n+$ and $p+$ regions had minimal overlap due to diffusion or segregation during growth.

![Figure 4.1: InGaAs device structure with doping. [14]](image)
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

Figure 4.2: InGaAs devices experimental data. [14]

Fig. 4.3 illustrates the schematic diagram of the GaAs Esaki diodes. The accompanying experimental characteristics are shown in Fig. 4.4.

Figure 4.3: GaAs device structure with doping. [14]
Fig. 4.4: GaAs device structure with doping. [14]

Fig. 4.5: InAs device structure with doping. [14]

Fig. 4.5 illustrates the schematic diagram of the InAs Esaki diodes. The accompanying experimental characteristics are shown in Fig. 4.6.

<table>
<thead>
<tr>
<th>Thickness (nm)</th>
<th>Material</th>
<th>Type</th>
<th>Doping</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>InAs</td>
<td></td>
<td>$N_D^{++}$</td>
</tr>
<tr>
<td>3</td>
<td>InAs</td>
<td>$i$-layer</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>InAs</td>
<td></td>
<td>$N_A^{++}$</td>
</tr>
</tbody>
</table>

Figure 4.5: InAs device structure with doping. [14]
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

4.2 First NEMO5 Attempts at Benchmarking Homojunctions

The devices are designed as a "quasi-1D" structure in NEMO5 so as to cut down on simulation time. It is assumed that the structures are crystalline and repeat in the $x$- and $y$ directions. These initial designs introduced three regions ($p+$/intrinsic/$n+$), though the intrinsic region was treated as $p+$ in the case of the simulations. The doping levels were chosen to match the IEDM paper (see Fig. 4.1, 4.3, and 4.5) and were based on SIMS data. The homojunction device peak current densities were accurately predicted by David Pawlik via E.O. Kane's tunneling model. [3, 21]

Appendix C contains the NEMO5 structure files used to simulate the InGaAs-6 device. The NEMO5 simulation results are seen in Fig. 4.7 - 4.9 as well as the accompanying tables.
(a) Simulated vs. experimental transfer characteristics. Simulated data is the bulleted lines.

Figure 4.7: NEMO5 simulations for the InGaAs-on-InP structure.[14]

An initial NEMO simulation was performed using NEMO's virtual crystal approximation (VCA) method. VCA uses a straight Vegard's Law interpolation for all tight-binding parameters. Table 4.1 shows how severely the simulated current density is underestimated for the InGaAs devices. In the first two devices NDR is not even seen.

Table 4.1: Device doping and output current density peak summary for InP/InGaAs structure. [14]

<table>
<thead>
<tr>
<th>Device</th>
<th>$N_D \times 10^{19} \text{ cm}^{-3}$</th>
<th>$N_A \times 10^{19} \text{ cm}^{-3}$</th>
<th>Exp. $J_P / \text{cm}^2$</th>
<th>NEMO $J_P / \text{cm}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>InGaAs - 1</td>
<td>1.6</td>
<td>0.57</td>
<td>14 A</td>
<td>No NDR in NEMO</td>
</tr>
<tr>
<td>InGaAs - 2</td>
<td>3</td>
<td>1</td>
<td>360 A</td>
<td>No NDR in NEMO</td>
</tr>
<tr>
<td>InGaAs - 3</td>
<td>1.6</td>
<td>4.5</td>
<td>7 kA</td>
<td>0.997 kA</td>
</tr>
<tr>
<td>InGaAs - 4</td>
<td>3</td>
<td>5</td>
<td>56 kA</td>
<td>7 kA</td>
</tr>
<tr>
<td>InGaAs - 5</td>
<td>4.3</td>
<td>8</td>
<td>210 kA</td>
<td>41 kA</td>
</tr>
<tr>
<td>InGaAs - 6</td>
<td>7</td>
<td>9.6</td>
<td>975 kA</td>
<td>125 kA</td>
</tr>
</tbody>
</table>
(a) Simulated vs. experimental transfer characteristics. Simulated data is the bulleted lines.

Figure 4.8: NEMO5 simulations for the GaAs structure. [14]

As in the previous simulations, Table 4.2 shows how poorly the GaAs devices simulations fared when compared to the experimental data. NDR is again not even seen in the first two devices.

Table 4.2: Device doping and output current density peak summary for GaAs structure. [14]

<table>
<thead>
<tr>
<th>Device</th>
<th>$N_D \times 10^{19} \text{ cm}^{-3}$</th>
<th>$N_A \times 10^{19} \text{ cm}^{-3}$</th>
<th>Exp. $J_P / \text{cm}^2$</th>
<th>NEMO $J_P / \text{cm}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs – 1</td>
<td>3</td>
<td>0.5</td>
<td>11 $\mu$A</td>
<td>No NDR in NEMO</td>
</tr>
<tr>
<td>GaAs – 2</td>
<td>3</td>
<td>1</td>
<td>45 mA</td>
<td>No NDR in NEMO</td>
</tr>
<tr>
<td>GaAs – 3</td>
<td>3</td>
<td>5</td>
<td>55 A</td>
<td>68 A</td>
</tr>
</tbody>
</table>
(a) Simulated vs. experimental transfer characteristics. Simulated data is the bulleted lines.

**Figure 4.9:** NEMO5 simulations for the InAs structure. [14]

Table 4.3 shows that NEMO underestimated the current significantly. The predicted peak current is approximately 25% of the measured experimental peak current.

**Table 4.3:** Device doping and output current density peak summary for InAs structure. [14]

<table>
<thead>
<tr>
<th>Device</th>
<th>(N_D) x1E19 cm(^{-3})</th>
<th>(N_A) x1E19 cm(^{-3})</th>
<th>Exp. (J_P) /cm(^2)</th>
<th>NEMO (J_P) /cm(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>InAs – 1</td>
<td>0.3</td>
<td>1.8</td>
<td>2 kA</td>
<td>0.575 kA</td>
</tr>
<tr>
<td>InAs – 2</td>
<td>1</td>
<td>1.8</td>
<td>37.6 kA</td>
<td>11.5 kA</td>
</tr>
</tbody>
</table>

The results shown above might seem encouraging at a glance because the I-V characteristics follow generally similar trends to reality, but the severe current density underestimation is a problem. The devices with low levels of degenerate doping showed no NDR, likely due to being too narrow and the simulated contacts not being wide enough to cover them.

To determine the cause of the current density overestimation in the NEMO5 simulations, band diagrams for the materials were simulated to see how they matched published material data. Two of these are shown in Fig. 4.10.
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

Figure 4.10: NEMO5 simulations of E-k for GaAs and InGaAs.

The band gap for GaAs shown in Fig. 4.10a and for InAs (not shown) are reasonable calculations for bulk materials; these were performed using the VCA model in NEMO. The band gap for bulk In$_{0.53}$Ga$_{0.47}$As (this concentration is fixed), on the other hand, is shown to be 0.966 eV which is higher than the 0.74 eV expected from literature. [16] It was hypothesized that if the band gap for In$_{0.53}$Ga$_{0.47}$As could be brought closer to reality then the simulated current densities would be closer to reality.

A conference call with the NEMO5 team at Purdue University suggested a look at the material file and mentioned that the VCA model assumes an InGaAs concentration of In$_{0.53}$Ga$_{0.47}$As, might be the culprit.

4.3 Proposed Solution: Change the $E_g$ Calculation

The VCA model in the all.mat material file was considered the crux for solving the problem of the incorrect InGaAs $E_g$ value. The all.mat file contained the following
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

equation:

\[
E_g - \Gamma = 1.424 - 1.110*IN + 0.45*IN^2 + \frac{300 - Phys: Tkel}{300 - 77} \times (0.040*IN + 0.086*GA)
\]

(4.1)

where IN is the indium concentration and GA is the gallium concentration.

According to Bhattacharya, Eq. 4.1 assumes a strained GaAs substrate with a low indium concentration. This is known to not be the case, as seen from Fig. 4.7b which shows that the devices being simulated were grown on InP. Bhattacharya provides a different model to use that assumes a InP unstrained substrate for an In\textsubscript{0.53}Ga\textsubscript{0.47}As material. [39] This is Eq. 4.2 which follows:

\[
E_g = 0.75 - 1.05 \times IN + 0.45 \times IN^2
\]

(4.2)

Another similar model was found on the Ioffe website and follows as Eq. 4.3 [16]

\[
E_g = 0.36 + 0.63 \times IN + 0.43 \times IN^2
\]

(4.3)

The all.mat file was edited first with Eq. 4.2 and then Eq. 4.3 with no visible changes in the results seen in the simulated band gaps with either of the changes. On a whim, the \( E_g - \Gamma \) variable was changed to a ridiculous number that had no basis in reality, to see if this would have any effect and, again, no effect was observed. Thus, this attempt was determined to have been futile and a new approach was considered.
4.4 Proposed Solution: Consider the NEMO5 Tight-binding Parameters

VCA assumes that the parameters vary linearly with the composition. That is, VCA can be considered as a weighted average between the relevant (in this case, InAs and GaAs) molecules. Luisier et al. shows the necessity of using a correction factor referred to as a bowing parameter. The bowing parameter refers to the empirical offset determined from the linear interpolation used in the VCA. It is called a bowing factor because the parameters seem to bow with the composition, as seen in Fig. 4.11, depending on what it is. Fig. 4.11 shows Luisier et al.'s fix with the applied bowing parameters.

Figure 4.11: Electron band gap of $In_xGa_{1-x}As$ at room temperature as a function of the In concentration $x$. Note that the paper had it wrong; the bottom axis should be the Ga concentration. This was corrected in this thesis. The solid line corresponds to the Ioffe data, the dotted line is the data with added bowing effects, and the dashed line is the data with no bowing effects. IEEE © 2009.[15, 16]

The parameters found in Luisier et al. and Boykin et al. were applied to the

---

1Reprinted from (M. Luisier and G. Klimeck, Investigation of $In_xGa_{1-x}As$ ultra-thin-body tunneling fets using a full-band and atomistic approach, 2009 International Conference on Simulation of Semiconductor Processes and Devices) with the permission of IEEE © 2009.
all.mat file tight-binding parameters using the parameterization equation which follows:

\[ P_{InxGa(1-x)As} = x \cdot P_{InAs} + (1 - x) \cdot P_{GaAs} + x(1 - x) \cdot B_{InAs, GaAs} \]  \hspace{1cm} (4.4)

where \( P \) is the relevant parameter, \( x \) is the indium concentration, and \( B \) is the bowing parameter used.

A new InGaAs material file was created with the applied bowing parameters. This comprises the next section.

Luisier et al. also notes that in their NEMO simulations the band gap and effective masses of InAs and GaAs could not be reproduced without spin-orbit coupling being included in the calculations. If this effect was not included the band gap and effective mass were both predicted larger than reality which caused an underestimation of BTBT. The spin-orbit parameters were kept as they were previously and not edited with an added bowing effect in the simulations which follow. Based on the results which follow, this is assumed to have been a reasonable assumption. [15]

4.5 The Rosetta Stone of NEMO5 Tight-binding Parameters for InGaAs

The results of this examination of the application of the bowing parameter are listed in the tables which follow. The anion is defined as arsenic in both GaAs and InAs. Thus, because there is no change in the anion composition between the two when combined to create InGaAs, the bowing parameter for all of the energies in this first table, Table 4.4, is 0. \( E_{sa} \) refers to the energy of the anion’s s-orbital, \( E_{pa} \) to the energy of the anion’s p-orbital, etc. Recall from the discussion of orbitals that the \( s^* \)-orbital is an \( s \)-like orbital often used to increase simulation accuracy.
Table 4.4: Bowing effects for the anion (As) band energies.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>GaAs all.mat</th>
<th>Value</th>
<th>InAs all.mat</th>
<th>Value</th>
<th>Bowing</th>
<th>InGaAs all.mat</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{sa}$</td>
<td>$E_{s_As}$</td>
<td>-5.5004</td>
<td>$E_{s_As}$</td>
<td>-5.5004</td>
<td>0</td>
<td>$E_{s_As}$</td>
<td>-5.5004</td>
</tr>
<tr>
<td>$E_{pa}$</td>
<td>$E_{Px_As}$</td>
<td>4.151</td>
<td>$E_{Py_As}$</td>
<td>4.1511</td>
<td></td>
<td>$E_{Py_As}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_{Pz_As}$</td>
<td></td>
<td>$E_{Py_As}$</td>
<td></td>
<td></td>
<td>$E_{Pz_As}$</td>
<td></td>
</tr>
<tr>
<td>$E_{da}$</td>
<td>$E_{Dxy_As}$</td>
<td>4.151</td>
<td>$E_{Dxy_As}$</td>
<td>4.1511</td>
<td></td>
<td>$E_{Dxy_As}$</td>
<td>4.1511</td>
</tr>
<tr>
<td></td>
<td>$E_{Dyz_As}$</td>
<td></td>
<td>$E_{Dyz_As}$</td>
<td></td>
<td></td>
<td>$E_{Dyz_As}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_{Dz2_As}$</td>
<td></td>
<td>$E_{Dz2_As}$</td>
<td></td>
<td></td>
<td>$E_{Dz2_As}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_{Dx2_y2_As}$</td>
<td></td>
<td>$E_{Dx2_y2_As}$</td>
<td></td>
<td></td>
<td>$E_{Dx2_y2_As}$</td>
<td></td>
</tr>
<tr>
<td>$E_{ss_a}$</td>
<td>$E_{Star_As}$</td>
<td>19.7106</td>
<td>$E_{Star_As}$</td>
<td>19.7106</td>
<td></td>
<td>$E_{Star_As}$</td>
<td>19.7106</td>
</tr>
</tbody>
</table>

The cation is different for the two materials (either indium or gallium), so all these following tables show the bowing parameter changes to note.

Table 4.5: Bowing effects for the cation (In or Ga) band energies.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>GaAs all.mat</th>
<th>Value</th>
<th>InAs all.mat</th>
<th>Value</th>
<th>Bowing</th>
<th>InGaAs all.mat</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{sc}$</td>
<td>$E_{s_Ga}$</td>
<td>-0.2412</td>
<td>$E_{s_In}$</td>
<td>-0.5819</td>
<td>-0.204</td>
<td>$E_{s_GaIn}$</td>
<td>-0.4726</td>
</tr>
<tr>
<td>$E_{pc}$</td>
<td>$E_{Px_Ga}$</td>
<td>6.7078</td>
<td>$E_{Py_In}$</td>
<td>6.9716</td>
<td>0.2621</td>
<td>$E_{Py_GaIn}$</td>
<td>6.9129</td>
</tr>
<tr>
<td></td>
<td>$E_{Pz_Ga}$</td>
<td></td>
<td>$E_{Py_In}$</td>
<td></td>
<td></td>
<td>$E_{Pz_GaIn}$</td>
<td></td>
</tr>
<tr>
<td>$E_{dc}$</td>
<td>$E_{Dxy_Ga}$</td>
<td>12.7485</td>
<td>$E_{Dxy_In}$</td>
<td>13.3071</td>
<td>0.3427</td>
<td>$E_{Dxy_GaIn}$</td>
<td>13.1299</td>
</tr>
<tr>
<td></td>
<td>$E_{Dyz_Ga}$</td>
<td></td>
<td>$E_{Dyz_In}$</td>
<td></td>
<td></td>
<td>$E_{Dyz_GaIn}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_{Dz2_Ga}$</td>
<td></td>
<td>$E_{Dz2_In}$</td>
<td></td>
<td></td>
<td>$E_{Dz2_GaIn}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$E_{Dx2_y2_Ga}$</td>
<td></td>
<td>$E_{Dx2_y2_In}$</td>
<td></td>
<td></td>
<td>$E_{Dx2_y2_GaIn}$</td>
<td></td>
</tr>
<tr>
<td>$E_{ss_c}$</td>
<td>$E_{Star_Ga}$</td>
<td>22.6635</td>
<td>$E_{Star_In}$</td>
<td>19.9414</td>
<td>-1.4772</td>
<td>$E_{Star_GaIn}$</td>
<td>20.8528</td>
</tr>
</tbody>
</table>

Table 4.6 shows parameters applied to the $s - to - s$ orbital interactions. Recall that the $s$-orbital only forms sigma bonds.
### Table 4.6: Bowing effects for the $s \rightarrow s$-orbital interactions.

<table>
<thead>
<tr>
<th>Param</th>
<th>Name</th>
<th>Value</th>
<th>Name</th>
<th>Value</th>
<th>Bowing</th>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$ss\sigma$</td>
<td>$V_{SS\Sigma \text{As, Ga}}$</td>
<td>-1.6451</td>
<td>$V_{SS\Sigma \text{As, In}}$</td>
<td>-1.6944</td>
<td>-0.0262</td>
<td>$V_{SS\Sigma \text{As, GaIn}}$</td>
<td>1.6777</td>
</tr>
<tr>
<td>$s^<em>s^</em>\sigma$</td>
<td>$V_{S^*S\Sigma \text{As, Ga}}$</td>
<td>-3.6772</td>
<td>$V_{S^*S\Sigma \text{As, In}}$</td>
<td>-4.2105</td>
<td>-0.2850</td>
<td>$V_{S^*S\Sigma \text{As, GaIn}}$</td>
<td>-4.0308</td>
</tr>
<tr>
<td>$sa^*c\sigma$</td>
<td>$V_{S^*c\Sigma \text{As, Ga}}$</td>
<td>-2.2078</td>
<td>$V_{S^*c\Sigma \text{As, In}}$</td>
<td>-2.2467</td>
<td>-0.0545</td>
<td>$V_{S^*c\Sigma \text{As, GaIn}}$</td>
<td>-2.3374</td>
</tr>
<tr>
<td>$sa\sigma$</td>
<td>$V_{SS\Sigma \text{As, Ga}}$</td>
<td>-2.6649</td>
<td>$V_{SS\Sigma \text{As, In}}$</td>
<td>-2.5982</td>
<td>-0.0667</td>
<td>$V_{SS\Sigma \text{As, GaIn}}$</td>
<td>-0.1022</td>
</tr>
<tr>
<td>$sc\sigma$</td>
<td>$V_{SS\Sigma \text{As, Ga}}$</td>
<td>-2.9603</td>
<td>$V_{SS\Sigma \text{As, In}}$</td>
<td>-2.8094</td>
<td>0.1488</td>
<td>$V_{SS\Sigma \text{As, GaIn}}$</td>
<td>0.9373</td>
</tr>
<tr>
<td>$s^*c\sigma$</td>
<td>$V_{S^*c\Sigma \text{As, Ga}}$</td>
<td>-1.0276</td>
<td>$V_{S^*c\Sigma \text{As, In}}$</td>
<td>-0.9373</td>
<td>-0.0902</td>
<td>$V_{S^*c\Sigma \text{As, GaIn}}$</td>
<td>-0.0131</td>
</tr>
<tr>
<td>$sp\sigma$</td>
<td>$V_{SS\Sigma \text{As, Ga}}$</td>
<td>-2.5836</td>
<td>$V_{SS\Sigma \text{As, In}}$</td>
<td>-2.2684</td>
<td>0.3152</td>
<td>$V_{SS\Sigma \text{As, GaIn}}$</td>
<td>0.2380</td>
</tr>
<tr>
<td>$sp\sigma$</td>
<td>$V_{SS\Sigma \text{As, Ga}}$</td>
<td>-2.2306</td>
<td>$V_{SS\Sigma \text{As, In}}$</td>
<td>-2.2931</td>
<td>-0.0131</td>
<td>$V_{SS\Sigma \text{As, GaIn}}$</td>
<td>-0.2395</td>
</tr>
<tr>
<td>$s^*p\sigma$</td>
<td>$V_{S^*p\Sigma \text{As, Ga}}$</td>
<td>-0.6282</td>
<td>$V_{S^*p\Sigma \text{As, In}}$</td>
<td>-0.8994</td>
<td>0.2711</td>
<td>$V_{S^*p\Sigma \text{As, GaIn}}$</td>
<td>0.8395</td>
</tr>
<tr>
<td>$s^*c\sigma$</td>
<td>$V_{S^*c\Sigma \text{As, Ga}}$</td>
<td>-0.1332</td>
<td>$V_{S^*c\Sigma \text{As, In}}$</td>
<td>-0.48899</td>
<td>-0.3556</td>
<td>$V_{S^*c\Sigma \text{As, GaIn}}$</td>
<td>0.2332</td>
</tr>
</tbody>
</table>

Table 4.7 shows parameters applied to the $s \rightarrow p$ and $s \rightarrow d$ orbital interactions. Again, the $s$-orbital can only form sigma bonds. Also note that $s \rightarrow d$ and $p \rightarrow d$ are the same.

### Table 4.7: Bowing effects for the $s \rightarrow p$ and $s \rightarrow d$ orbital interactions.

<table>
<thead>
<tr>
<th>Param</th>
<th>Name</th>
<th>Value</th>
<th>Name</th>
<th>Value</th>
<th>Bowing</th>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$sp\sigma$</td>
<td>$V_{SP\Sigma \text{As, Ga}}$</td>
<td>2.6649</td>
<td>$V_{SP\Sigma \text{As, In}}$</td>
<td>2.5982</td>
<td>-0.0667</td>
<td>$V_{SP\Sigma \text{As, GaIn}}$</td>
<td>2.6130</td>
</tr>
<tr>
<td>$sp\sigma$</td>
<td>$V_{SP\Sigma \text{Ga, As}}$</td>
<td>2.9603</td>
<td>$V_{SP\Sigma \text{In, As}}$</td>
<td>2.8094</td>
<td>0.1488</td>
<td>$V_{SP\Sigma \text{GaIn, As}}$</td>
<td>2.8432</td>
</tr>
<tr>
<td>$s^*p\sigma$</td>
<td>$V_{S^*p\Sigma \text{Ga, As}}$</td>
<td>1.9765</td>
<td>$V_{S^*p\Sigma \text{In, As}}$</td>
<td>2.8094</td>
<td>-0.1488</td>
<td>$V_{S^*p\Sigma \text{GaIn, As}}$</td>
<td>2.0475</td>
</tr>
<tr>
<td>$s^*p\sigma$</td>
<td>$V_{S^*p\Sigma \text{Ga, As}}$</td>
<td>1.0276</td>
<td>$V_{S^*p\Sigma \text{In, As}}$</td>
<td>0.9373</td>
<td>-0.0902</td>
<td>$V_{S^*p\Sigma \text{GaIn, As}}$</td>
<td>0.9573</td>
</tr>
<tr>
<td>$dp\sigma$</td>
<td>$V_{DS\Sigma \text{As, Ga}}$</td>
<td>2.5836</td>
<td>$V_{DS\Sigma \text{As, In}}$</td>
<td>-2.2684</td>
<td>0.3152</td>
<td>$V_{DS\Sigma \text{As, GaIn}}$</td>
<td>-2.3380</td>
</tr>
<tr>
<td>$dp\sigma$</td>
<td>$V_{DS\Sigma \text{Ga, As}}$</td>
<td>2.2306</td>
<td>$V_{DS\Sigma \text{In, As}}$</td>
<td>-2.2931</td>
<td>-0.0131</td>
<td>$V_{DS\Sigma \text{GaIn, As}}$</td>
<td>-2.3093</td>
</tr>
<tr>
<td>$s^*dp\sigma$</td>
<td>$V_{S^*dp\Sigma \text{Ga, As}}$</td>
<td>-0.6282</td>
<td>$V_{S^*dp\Sigma \text{In, As}}$</td>
<td>-0.8994</td>
<td>0.2711</td>
<td>$V_{S^*dp\Sigma \text{GaIn, As}}$</td>
<td>0.8395</td>
</tr>
<tr>
<td>$s^*dp\sigma$</td>
<td>$V_{S^*dp\Sigma \text{Ga, As}}$</td>
<td>-0.1332</td>
<td>$V_{S^*dp\Sigma \text{In, As}}$</td>
<td>-0.48899</td>
<td>-0.3556</td>
<td>$V_{S^*dp\Sigma \text{GaIn, As}}$</td>
<td>0.2332</td>
</tr>
</tbody>
</table>

Table 4.8 shows parameters applied to the $p \rightarrow p$ and $p \rightarrow d$ orbital interactions. The $s \rightarrow p$ orbital interactions were shown in the previous tables. The $p$-orbital forms both sigma and pi bonds so both of these are listed.
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

Table 4.8: Bowing effects for the \( p \rightarrow t \rightarrow p \) and \( p \rightarrow t \rightarrow d \) orbital interactions.

<table>
<thead>
<tr>
<th>Param</th>
<th>GaAs all.mat</th>
<th>InAs all.mat</th>
<th>InGaAs all.mat</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma )</td>
<td>( V_{p_p \sigma \Sigma Ga} )</td>
<td>( V_{p_p \sigma \Sigma In} )</td>
<td>( V_{p_p \sigma \Sigma Galn} )</td>
</tr>
<tr>
<td></td>
<td>4.1508</td>
<td>4.3106</td>
<td>4.2018</td>
</tr>
<tr>
<td></td>
<td>( V_{p_p \sigma \Sigma As} )</td>
<td>( V_{p_p \sigma \Sigma Ga} )</td>
<td>( V_{p_p \sigma \Sigma In} )</td>
</tr>
<tr>
<td>( \pi )</td>
<td>( V_{p_p \pi \Pi Ga} )</td>
<td>( V_{p_p \pi \Pi In} )</td>
<td>( V_{p_p \pi \Pi Galn} )</td>
</tr>
<tr>
<td></td>
<td>-1.14274</td>
<td>-1.2890</td>
<td>-1.3245</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( V_{p_p \delta \Delta Ga} )</td>
<td>( V_{p_p \delta \Delta In} )</td>
<td>( V_{p_p \delta \Delta Galn} )</td>
</tr>
<tr>
<td></td>
<td>-1.8743</td>
<td>-1.7314</td>
<td>-1.7684</td>
</tr>
</tbody>
</table>

The final bowing interactions in Table 4.9 shows parameters applied to the \( d \rightarrow t \rightarrow d \) orbital interactions. The \( s \rightarrow t \rightarrow d \) and \( p \rightarrow t \rightarrow d \) orbital interactions were shown in the previous tables. The \( d \)-orbital forms sigma, pi, and delta bonds so all of these are listed.

Table 4.9: Bowing effects for the \( d \rightarrow t \rightarrow d \) orbital interactions.

<table>
<thead>
<tr>
<th>Param</th>
<th>GaAs all.mat</th>
<th>InAs all.mat</th>
<th>InGaAs all.mat</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma )</td>
<td>( V_{d_d \sigma \Sigma Ga} )</td>
<td>( V_{d_d \sigma \Sigma In} )</td>
<td>( V_{d_d \sigma \Sigma Galn} )</td>
</tr>
<tr>
<td></td>
<td>1.2700</td>
<td>1.5846</td>
<td>1.4286</td>
</tr>
<tr>
<td></td>
<td>( V_{d_d \sigma \Sigma As} )</td>
<td>( V_{d_d \sigma \Sigma Ga} )</td>
<td>( V_{d_d \sigma \Sigma In} )</td>
</tr>
<tr>
<td>( \pi )</td>
<td>( V_{d_d \pi \Pi Ga} )</td>
<td>( V_{d_d \pi \Pi In} )</td>
<td>( V_{d_d \pi \Pi Galn} )</td>
</tr>
<tr>
<td></td>
<td>2.5054</td>
<td>2.71799</td>
<td>2.6708</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( V_{d_d \delta \Delta Ga} )</td>
<td>( V_{d_d \delta \Delta In} )</td>
<td>( V_{d_d \delta \Delta Galn} )</td>
</tr>
<tr>
<td></td>
<td>0.8517</td>
<td>0.5051</td>
<td>0.5817</td>
</tr>
</tbody>
</table>

4.6 Bowing results

New all.mat files were generated for varying compositions of In and GaAs, from 5% to 95% in steps of 5% of each and these were used to simulate new \( E - k \) plots. A few of these are included in Figs. 4.12 - 4.15. Note from Fig. 4.12 that the band-diagram generated from the all.mat file with the added bowing parameter effects
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

shows a notably smaller band gap. Recall that this was the goal, as the InGaAs band gap from the first simulations was too large to be real.

(a) Simulation using only the VCA model. \( E_g = 1.3764 \text{ eV} \).

(b) Simulation with bowing effects included. \( E_g = 1.3491 \text{ eV} \).

Figure 4.12: NEMO5 bandstructure results for In=0.05 GaAs=0.95 composition with and without bowing effects included.

Fig. 4.13 has compositions similar to the standard indium 53% concentration and shows a band gap a lot closer to the 0.74 eV expected when the bowing effects are included in the simulation.
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

(a) Simulation using only the VCA model. $E_g = 0.9260$ eV.

(b) Simulation with bowing effects included. $E_g = 0.7816$ eV.

Figure 4.13: NEMO5 bandstructure results for In=0.50 GaAs=0.50 composition with and without bowing effects included.

Fig. 4.14 corresponds to the indium 53%, gallium 47% concentration and shows a band gap even closer to the 0.74 eV expected with the bowing effects included in the simulation as the band gap is measured to be $E_g = 0.7662$ eV in this case.
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

Figure 4.14: NEMO5 bandstructure results for In=0.53 GaAs=0.47 composition with bowing effects included. $E_g = 0.7662$ eV.

Fig. 4.15 shows the same trends as the previous two figures.

(a) Simulation using only the VCA model. $E_g = 0.4290$ eV.

(b) Simulation with bowing effects included. $E_g = 0.4002$ eV.

Figure 4.15: NEMO5 bandstructure results for In=0.95 GaAs=0.05 composition with and without bowing effects included.
Next, the composition was plotted against the band gap for a plot similar to the one made by Luisier et al. (Fig. 4.11). Note that Luisier et al. actually plotted the $x$-axis incorrectly.

As seen from Fig. 4.16, band gap increases with decreased indium concentration. There is a slight bow to this data as a result of the bowing parameter application, and it matches up almost perfectly with data from both Luisier et al. and Ioffe. [15, 16]

![Graph showing electron band gap of $In_x Ga_{1-x}As$ at room temperature as a function of the In concentration $x$ as plotted after applying the bowing effects and comparing to the Ioffe and Luisier data.][15, 16]

**Figure 4.16:** Electron band gap of $In_x Ga_{1-x}As$ at room temperature as a function of the In concentration $x$ as plotted after applying the bowing effects and comparing to the Ioffe and Luisier data. [15, 16]
4.7 Second NEMO5 Attempts at Benchmarking Homojunctions

The next step after creating this new *all.mat* file with the edited tight-binding parameters was to run the simulations again. The InGaAs results are included in Fig. 4.18. The new simulated data is seen to be an extremely close fit to the experimental data which makes this exercise a success. Note that the device labeled "low-doped, too thin" had contact regions of 16 unit cells which was determined to be not wide enough for the simulation to produce NDR. The contact regions were extended to 20 unit cells; subsequently NDR with a peak current density comparable with the experiment was observed.

![Figure 4.17: InGaAs device structure with doping. [14]](image)
CHAPTER 4. NEMO5 SIMULATION RESULTS: AN INGAAS BOWING PARAMETER STUDY

Figure 4.18: InGaAs devices simulated with the new all.mat file and plotted against real data from Pawlik et al. [14]

Table 4.10 shows the new simulated data for the InGaAs structures. As stated above and now seen in this table, an extremely tight fit to the tunneling current is seen for the simulations, especially for the highly-doped devices. This validates the revised NEMO models wholly.

**Table 4.10:** Device doping and output current density peak summary for InGaAs structure as simulated with the new all.mat file. [14]

<table>
<thead>
<tr>
<th>Device</th>
<th>$N_D \times 10^{19} \text{ cm}^{-3}$</th>
<th>$N_A \times 10^{19} \text{ cm}^{-3}$</th>
<th>Exp. $J_P /\text{cm}^2$</th>
<th>NEMO $J_P /\text{cm}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>InGaAs – 1</td>
<td>1.6</td>
<td>0.57</td>
<td>14 A</td>
<td>20.4 kA</td>
</tr>
<tr>
<td>InGaAs – 2</td>
<td>3</td>
<td>1</td>
<td>360 A</td>
<td>483</td>
</tr>
<tr>
<td>InGaAs – 3</td>
<td>1.6</td>
<td>4.5</td>
<td>7 kA</td>
<td>8.8 kA</td>
</tr>
<tr>
<td>InGaAs – 4</td>
<td>3</td>
<td>5</td>
<td>56 kA</td>
<td>61.3 kA</td>
</tr>
<tr>
<td>InGaAs – 5</td>
<td>4.3</td>
<td>8</td>
<td>210 kA</td>
<td>207 kA</td>
</tr>
<tr>
<td>InGaAs – 6</td>
<td>7</td>
<td>9.6</td>
<td>975 kA</td>
<td>686 kA</td>
</tr>
</tbody>
</table>

Following this data match, a second experiment was run to simulate an exper-
imental device that had initially been meant to be an InGaAs TFET \((N_D \times 1E19 \text{ cm}^{-3}, N_A \times 1E19 \text{ cm}^{-3})\) with a 100 nm intrinsic region. Due to miscommunication with the grower, the intrinsic region was instead grown to 10 nm, so when the device was tested it showed NDR. A NEMO5 simulation was performed varying the intrinsic region thicknesses. The simulated results are plotted along with the experimental results in Fig.4.20. Not surprisingly the 10 nm intrinsic region is the tightest match.

![InGaAs device structure with doping.](image)

**Figure 4.19:** InGaAs device structure with doping. [14]
Figure 4.20: InGaAs devices with varying intrinsic (referred to as "i") region thicknesses plotted against experimental data from Pawlik et al. [14]
Chapter 5

VASP Benchmarking Results

A number of VASP tests were run with the primary goal of determining the software's limitations. Note that Appendix B shows the methodology for performing a simple VASP run using MedeA.

5.1 Lattice Constant Variations

One of the first experiments run in VASP 5.4 was to vary the lattice constant input for GaAs and InAs and observe the results in terms of the band diagrams. Note that all VASP simulations were performed in the Materials Design MedeA environment.

A screening DFT simulation was performed. The k-point spacing was 0.5/Å in a Γ-centered Monkhorst-Pack mesh. This resulted in a 4x4x4 grid. The planewave cutoff was 280 eV and a GGA-PBE exchange correlation was used. Fig. 5.1 shows the results for the GaAs simulations. The primary take-away is that the band gap grows larger as the lattice constant is increased. Fig. 5.1(a) is no longer a semiconductor and Fig. 5.1(c) shows an indirect band gap not consonant with GaAs as it is generally known.
This same experiment was conducted using InAs as the material and parallel observations can be made about the effects of increasing the lattice constant on the band gap from Fig. 5.2.

5.2 The Effects of Varying the Functional: Part 1

The simulation functionals refers to the simulation calculation methods used. Simulations were performed for GaAs and InAs using different functionals to determine
which corresponded the closest to reality. The functionals of interest were: DFT with GGA-PBE, HSE06 with GGA-PBE, and Hartree-Fock.

Recall that Luisier et al. mentioned that in their NEMO simulations the band gap and effective masses of InAs and GaAs could not be reproduced without spin-orbit coupling being included in the calculations. If this effect was not included the band gap and effective mass were both predicted larger than reality. For this reason, spin-orbit was turned on for the following simulations to increase accuracy, though the trade-off is an increase in computation time. The settings described in Section 5.1 for k-point spacing and planewave cutoff were used again. The change was the functional, which is accordingly noted.

5.2.1 GaAs VASP Simulation Results

Note that the expected band gap, $E_g$, for GaAs is approximately 1.424 eV at 300 K. Fig. 5.3 - 5.5 are all DFT simulations. Fig. 5.3 is the simple DFT with GGA-PBE and added spin orbit and predicts a band gap of 0.3804 eV. Fig. 5.4 is the DFT calculated during the HSE06 simulation and predicts a band gap of 0.5467 eV. Fig. 5.5 is the DFT calculated during the Hartree-Fock simulation and predicts a band gap of 0.1531 eV. They all significantly underestimate the band gap. These simulations were extremely quick to compute, taking approximately one minute each, but are not accurate enough to be useful.
CHAPTER 5. VASP BENCHMARKING RESULTS

(a) Energy band diagram.  
(b) Density of States.

Figure 5.3: VASP simulation of GaAs using DFT with GGA-PBE with spin-orbit.

(a) Energy band diagram.  
(b) Density of States.

Figure 5.4: VASP simulation of GaAs DFT as an artifact of the HSE06 simulation. Again with spin-orbit included.
CHAPTER 5. VASP BENCHMARKING RESULTS

(a) Energy band diagram.
(b) Density of States.

Figure 5.5: VASP simulation of GaAs DFT as an artifact of the Hartree-Fock simulation. Again with spin-orbit included.

Next, Fig. 5.6 represents the GaAs $E - k$ as simulated using the HSE06 meta-GGA method with spin orbit coupling turned on. The band gap predicted with this method is 1.5029 eV which is very close to the 1.424 eV expected. This simulation took approximately two days to complete on a two-core four-thread machine, so it is significantly more cumbersome computationally.

(a) Energy band diagram.
(b) Density of States.

Figure 5.6: VASP simulation of GaAs using HSE06 with spin-orbit.
Finally, Fig. 5.7 contains the GaAs band diagram as simulated using the Hartree-Fock method. This also took approximately two days to complete, but with a predicted band gap of 4.582 eV that is substantially larger than the 1.44 eV predicted theoretically. The fact that the peak is extremely sharp is a simulation artifact.

![Energy band diagram and Density of States](image)

(a) Energy band diagram. (b) Density of States.

**Figure 5.7**: VASP simulation of GaAs using Hartree-Fock with spin-orbit.

### 5.2.2 InAs VASP Simulation Results

The same simulations as done for GaAs in section 5.1.1 were repeated for an InAs unit cell. Note that the expected band gap in this case is approximately 0.354 eV.

[16]

Fig. 5.8 shows a band diagram generated using DFT with GGA-PBE and spin orbit. There is no discernible band gap in this $E - k$ plot. Clearly this is not real as InAs is a known semiconductor.
CHAPTER 5. VASP BENCHMARKING RESULTS

Figure 5.8: VASP simulation of InAs using DFT with spin-orbit coupling included.

Fig. 5.9 includes the band diagram from the HSE06 with spin orbit simulation. The band gap extracted from the $E - k$ plot is 0.4816 eV which is not far off from the expected band gap 0.354 eV.

Figure 5.9: VASP simulation of InAs using HSE06 with spin-orbit.

Fig. 5.10 shows a band diagram generated using the Hartree-Fock method with spin orbit. Not only is this band gap extremely large (>5 eV), but it also simulated

76
InAs as an indirect band gap material, which is not true.

![Energy band diagram](image1)

![Density of States](image2)

**Figure 5.10:** VASP simulation of InAs using Hartree-Fock with spin-orbit.

### 5.2.3 Reflections on Varying the Functional

From the data seen in Sections 5.2.1 and 5.2.2 it is clear that the HSE06 with GGA simulation method (a type of meta-GGA) was the most promising, while the Hartree-Fock the least useful (as well as time-consuming). In conclusion, the Hartree-Fock method is not a viable method of predicting material characteristics such as energy band gap, possibly because it requires more computational power or the simulation was not set up correctly.

### 5.3 The Effects of Varying the Functional: Part 2

More materials were simulated using both HSE06 with GGA and DFT with GGA with spin orbit turned on for all simulations. These results are included in Table 5.1.
CHAPTER 5. VASP BENCHMARKING RESULTS

Table 5.1: Materials simulated in VASP using HSE06 with GGA and DFT with GGA with spin orbit turned on. Note that the PWC is the plane-wave cutoff which refers to the distance the energy is simulated away from atom. The farther or larger this is, the more likely the simulation will converge to reality due to an increase in resolution, but also the longer the computation time. Note that the k-point spacing was 0.5/Å in a Γ-centered Monkhorst-Pack mesh, resulting in a 4x4x4 grid.

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice (Å)</th>
<th>Calc $E_g$ (ev)</th>
<th>Real $E_g$ (ev)</th>
<th>Gap Type</th>
<th>PWC (eV)</th>
<th>Functional</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>5.6339</td>
<td>0.4104</td>
<td>1.424</td>
<td>direct</td>
<td>0.0327</td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.3601</td>
<td></td>
<td>direct</td>
<td></td>
<td>DFT GGA_BEB</td>
</tr>
<tr>
<td>InAs</td>
<td>6.048</td>
<td>0</td>
<td>0.354</td>
<td>direct</td>
<td>239.21</td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.3523</td>
<td></td>
<td>direct</td>
<td></td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td>GaSb</td>
<td>6.118</td>
<td>0</td>
<td>0.726</td>
<td>direct</td>
<td>282.69</td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.6077</td>
<td></td>
<td>direct</td>
<td></td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td>InP</td>
<td>5.8687</td>
<td>0.5411</td>
<td>1.344</td>
<td>direct</td>
<td>255.04</td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.3723</td>
<td></td>
<td>direct</td>
<td></td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td>AlAs</td>
<td>5.62</td>
<td>1.147</td>
<td>2.153</td>
<td>indirect</td>
<td>240.3</td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.8871</td>
<td></td>
<td>indirect</td>
<td></td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td>Ge</td>
<td>5.65</td>
<td>0.0001</td>
<td>0.661</td>
<td>direct</td>
<td>310.29</td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.7291</td>
<td></td>
<td>indirect</td>
<td></td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td>AlSb</td>
<td>6.1347</td>
<td>0.8767</td>
<td>1.615</td>
<td>indirect</td>
<td>240.3</td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.5577</td>
<td></td>
<td>indirect</td>
<td></td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td>GaP</td>
<td>5.4505</td>
<td>1.4581</td>
<td>2.26</td>
<td>indirect</td>
<td>286.69</td>
<td>DDFT GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.1886</td>
<td></td>
<td>indirect</td>
<td></td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td>AlP</td>
<td>5.451</td>
<td>1.3775</td>
<td>2.45</td>
<td>indirect</td>
<td>255.04</td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.1624</td>
<td></td>
<td>indirect</td>
<td></td>
<td>HSE06 GGA_PBE</td>
</tr>
<tr>
<td>Si</td>
<td>5.431</td>
<td>0.41418</td>
<td>1.12</td>
<td>indirect</td>
<td>255.04</td>
<td>DFT GGA_PBE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.0845</td>
<td></td>
<td>indirect</td>
<td></td>
<td>HSE06 GGA_PBE</td>
</tr>
</tbody>
</table>

From Table 5.1, as well as the results of the previous section, HSE06 is decidedly worth the extra simulation time as its results are significantly more likely to simulate reality. The **boldface** entries in Table 5.1 highlight the best fits, which in the case of these simulations were always found using the HSE06 GGA_PBE method.

5.4 Some Effects of Changing the Lattice Constant

The ultimate goal of this research is to lay the foundations for simulating TMD material interfaces. A few designed experiments using these materials were run to begin setting up VASP functionality in this regard. DFT with GGA with spin-orbit
CHAPTER 5. VASP BENCHMARKING RESULTS

turned on was the primary simulation method, chosen for its computation speed.

Fig. 5.11 shows 16 $E - k$ curves for MoS$_2$ where the lattice constant was varied in steps of 1% up to 15%. This type of variation would happen in reality through the addition of strain to the material system. The top (solid black) line in this plot corresponds to the generic lattice constant of MoS$_2$, 3.16 Å. The shift in minimum energy to different Brillouin zones is noteworthy for further analysis beyond the scope of this report.

![Figure 5.11](image)

**Figure 5.11:** VASP DFT with GGA simulation of MoS$_2$ band diagrams varying with lattice constant. The top (solid black) line corresponds to the original lattice constant.

Fig. 5.12 plots the data from Fig. 5.11, as well as from the same designed experiment run for WTe$_2$. 
Figure 5.12: VASP DFT GGA simulation data of the MoS$_2$ and WTe$_2$ lattice constant variation designed experiment explained above. vdW corresponds to a setting in the simulation where van der Waals forces are applied.

The final plot, seen in Fig. 5.13 shows the MoS$_2$ bandstructures as simulated in NEMO5 and VASP 5.4 plotted together. The reason for the discrepancies in the data lines is that the tight-binding parameters used for generating the data set in NEMO5 do not correspond exactly to the VASP 5.4 simulation results. The relevance of these results is that the difference between the two data sets can be calculated to generate a new set of bowing parameters.
Figure 5.13: VASP 5.4 van der Waals DFT GGA simulation data of MoS$_2$ plotted against NEMO5 MoS$_2$ simulations. Spin-orbit is applied during both simulations.
Chapter 6

Conclusions

6.1 Summary of Work

This thesis has set the groundwork necessary for successful fabrication of TFETs with TMD channels at RIT. For such work to become a reality, simulations have to first be performed so as to reduce fabrication cost and increase the likeliness of generating functioning devices. Quantum simulations were identified as a necessity over TCAD simulations through a thorough study of simulation results performed by other groups. The study discussed in this paper is by Jiang et al. [10].

The goal of quantum simulations are $E - k$ plots and $I - V$ characteristics that correspond to "real" or experimental data. This means that the simulated data must converge onto reality; the Jacobian iterative method was considered as an example algorithm used by the NEMO5 simulation package to achieve convergence. NEMO5 and VASP 5.4 were both considered and used for the first time at RIT in device design capacity in this thesis. The understanding developed of both is crucial for further work in designing TFET devices.

Previous Esaki diode data was simulated in NEMO5 and the match to reality was poor. To determine why this was so, the band gaps for the material systems were simulated: for GaAs and InAs as simulated by NEMO5, reasonable results were seen, but the band gap for InGaAs was significantly higher than the reality. This
was fixed by developing an understanding of the virtual crystal approximation model used as the tight-binding parameters in NEMO5, and then editing these parameters to contain the effects of bowing parameters as described in Luisier et al. [15]. The Esaki diode data was simulated using the newly generated model containing the bowing effects and the results were seen to match reality closely. Thus, the understanding of the bowing effects and how they can be applied to create a calibrated simulation model in NEMO5 is considered a huge find in this study.

Preliminary VASP 5.4 band gap calculations were performed for various III-Vs and other common semiconductors. An experiment was run to determine the most accurate simulation method and the HSE06 with GGA simulation method (a type of meta-GGA) was determined to be the most promising, while the Hartree-Fock the least useful (as well as time-consuming). The Hartree-Fock method is not a viable method of predicting material characteristics such as energy band gap, possibly because it requires more computational power.

Lattice constant variation effects in VASP 5.4 were considered for both standard III-V and MoS$_2$ and WTe$_2$ systems. More work should be done in this regard if there is any interest in the effects of strain on 2D materials. Finally, VASP 5.4 and NEMO5 results for MoS$_2$ bandstructure simulations were plotted together, which is the first step to calculating a set of bowing parameters for this material system.

### 6.2 Future Work

As this thesis has been merely a first look at using NEMO5 and VASP 5.4 for quantum simulations at the Rochester Institute of Technology, there is substantially more work to do in terms of benchmarking both software packages before actual TMD TFETs can be simulated meaningfully. The ultimate goal is, of course, fabrication of such devices.

Some suggestions for more immediate work include a study of bowing parameters
for other material systems, specifically TMDs. Sharma et al., Mourada and Czycholl, Zhao et al., and Kang et al. are all suggested as good starting materials in this regard [40, 41, 42, 43]. Another item is to edit the newly created all.mat InGaAs file to remove the $d$-orbital effects and analyze the results to determine the necessity of the $d$-orbital for a true simulation. This is especially useful as the matrix corresponding to the new file would be smaller and thus take less time to simulate, but the accuracy difference between the two simulations must be considered.

Further necessary VASP benchmarking includes developing an understanding of the basic TMD Brillouin zones and the way VASP goes about traversing these, as well as running more standard simulations for TMD energy band diagrams. Also necessary is the further development of a super-cell structure in VASP as this is necessary to simulate compounds such as InGaAs.
References


REFERENCES


REFERENCES


Appendix A: Hohenburg-Kohn Theorem Proof

[1]

Proof: if $\Psi \neq \Psi'$ then $\rho \neq \rho'$.

Assume $\Psi \neq \Psi'$ and $\rho = \rho'$, and prove that this is untrue.

$\Psi$ is the ground state of $\hat{H}$ with ground energy $E_{gs}$,
and $\Psi'$ is the ground state of $\hat{H}'$ with ground energy $E'_{gs}$.

Assuming the same number of electrons:

$$\hat{H} = T + W + V$$  \hspace{1cm} (A.1)

and

$$\hat{H}' = T + W + V'$$  \hspace{1cm} (A.2)

so

$$\hat{H} = \hat{H}' - V' + V.$$  \hspace{1cm} (A.3)

Applying the variational principle:

$$E_{gs} = |\Psi\rangle\langle\hat{H}|\Psi\rangle < |\Psi'\rangle\langle\hat{H}'|\Psi'\rangle = \langle\Psi'|\hat{H}' - V' + V|\Psi'\rangle = E'_{gs} + \int \rho'(\bar{r})[v'(\bar{r}) - v(\bar{r})]d\bar{r}.$$  \hspace{1cm} (A.4)

Now repeat the argument, starting with $\Psi'$:

$$E'_{gs} < E_{gs} + \int \rho(\bar{r})[v'(\bar{r}) - v(\bar{r})]d\bar{r}.$$  \hspace{1cm} (A.5)

Assuming $\rho = \rho'$, add the previous statements:

$$E'_{gs} + E_{gs} < E'_{gs} + E_{gs}$$  \hspace{1cm} (A.6)

This is clearly a contradiction. Therefore, $\rho \neq \rho'$ has been proven.
Appendix B: Brief Guide to Using MedeA 2.22.2 for VASP 5.4 Simulations

B.1 Part 1: MedeA Set-Up

Begin by opening runJobServer and runTaskServer from the Materials Design folder. Once these are loaded, open MedeA 2.22.2. These options can be seen in Fig. B.1.

![Materials Design folder](image)

**Figure B.1:** Materials Design folder as seen running Windows 10 Pro.

Next, click on Tools and load InfoMaticA and VASP 5.4 from the drop-down menu. These two tools will appear up top as extra drop-down menus.

Now click Job Control and Select Server to select the relevant server. The default in this example scenario is the local server which refers to the laptop MedeA is installed on, but other servers can be called as well, and these will appear here. Note that it is also possible to point to a remote machine for execution, but this is beyond the scope of this example.
B.2 Part 2: Cell Set-Up

Select *InfoMaticA* and load the *Search* function. The *InfoMaticA* Search menu will appear. Click *Add New Criterion* from the bottom half of this menu and select *Formula* from the drop-down menu. Type the molecule of interest into the box which appears. In this example case this is indium arsenide (InAs). The relevant existing structures in the library will appear in the top half of the search menu, as seen in Fig. B.2. If there are multiple results, as is the case in this example, click *Edit* and *Find Median Structures* to narrow it down to one selection.

![Figure B.2: InfoMaticA Search menu as seen after selecting InAs for this example.](image)

Next, right click on the molecule that is left and select *View*. A figure will appear
APPENDIX B. BRIEF GUIDE TO USING MEDEA 2.22.2 FOR VASP 5.4 SIMULATIONS

in MedeA which can be rotated by clicking the molecule and dragging the cursor; this is the molecule in question. The molecule in its initial state, as seen in Fig. B.3(a), is bond-less; to add bonds right-click on it and select Edit bonds. Click OK if the bond parameters correspond to what is known about the molecule; this will result in Fig. B.3(b).

Figure B.3: (a) The InAs molecule chosen as seen without bonds applied. (b) The InAs molecule chosen as seen with bonds applied.

To edit things such as the lattice constant (\(A=6.048\) Å for InAs remains unchanged in this example case) or to add, move, or remove atoms, right click the cell in question again and click Edit Cell. After this, the cell has been set up and VASP is ready to be run.

B.3 Part 3: Structural Optimization using VASP 5.4

The cell must now be minimized, and this is done with VASP 5.4. Click VASP 5.4 from the menu bar and select Run. The menu which will appear is seen in Fig. B.4. All the settings in Fig. B.4 correspond to the standard for Standard Optimization. Specifically, these include turning on Relax atom positions, Allow cell
volumes to change, and Allow cell shape to change; the functional can be changed to any functional of interest, though the Density functional with the GGA – PBEsol exchange correlation selected is one of the fastest to run; Spin – orbit magnetic can be turned on or off from the Magnetism option (note that turning it on will increase simulation time substantially); Standard 500 is the simplest Precision to run. The Spacing of k − points can be edited under the SCF menu (0.5 1/Å is standard for InAs). Do not forget to edit the Title to something meaningful before running the simulation by clicking Run.

Figure B.4: General setup for Structural Optimization of the chosen InAs molecule.

A Submit VASP Job menu will appear where the server Queue may be chosen, as well as the Number of processors and Priority of the job at hand. This can be seen in Fig. B.5. The Number of processors is dependent on the machine the chosen server is running on (in the case of this example “minint-3famcr” has an Intel Core i5-5200U Processor, which corresponds to two cores and four threads, so two is the maximum number of Processors available). The greatest Priority is 1 and the lowest is 10. Do not forget to add a relevant comment describing the job about to be run.
B.4 Part 4: Viewing and Controlling the Job requested

To view the job, open an Internet browser and type 127.0.0.1:32000/index.html into the search bar. The resulting page is seen in Fig. B.6.

Figure B.5: The pre-run menu.

Figure B.6: The Materials Design JobServer menu.
To see the status of the current job, click Jobs. After the job in question is shown as Finished, load it into MedeA by clicking File and selecting Open structure from job.

B.5 Part 5: Band Structure and Density of States using VASP 5.4

To acquire meaningful data such as Band structure or Density of states information using VASP, start by clicking on VASP 5.4 from the menu again. Next, select Single − point, followed by whichever Properties are of interest. In this case, Band structure and Density of states are both selected. As before, select the Functional of interest as well as the Precision. Fig. B.7 shows a sample set-up.

![MedeA: Run VASP 5.4](image)

**Figure B.7:** Sample set-up of band structure and density of states run for the InAs model chosen.

Proceed to Run, view and control the job as before.
B.6 Part 6: Analysis

Click *Analysis* from the top menu, followed by the property of interest (in this case *Band structure* or *Density of States*), and choose the relevant job. These files can be exported for further analysis by clicking *Analysis*, *Export*, and finally *File Select* and selecting the relevant file.
Appendix C: NEMO5 Sample Device Simulation Files

The following files correspond to InGaAs-6 which was simulated in this study.

C.1 Typical Material and Structure definition

Material { crystal_structure = zincblende
doping_density = 7E19
doping_type = N
name = GaInAs
x=0.47
regions = (3)
tag = InGaAs_highDoping }
Material { crystal_structure = zincblende
doping_density = 7E19
doping_type = N
name = GaInAs
x=0.47
regions = (2)
tag = InGaAs_lowDoping }
Material { crystal_structure = zincblende
doping_density = 9.6E19
doping_type = P
name = GaInAs
x=0.47
regions = (1)
tag = GaSb_high_doping }
C.2 Domain definition

Domain { base_material = InGaAs_lowDoping
crystal_direction1 = (1,0,0)
crystal_direction2 = (0,1,0)
crystal_direction3 = (0,0,1)
dimension = (48,1,1)
leads = (source_contact, drain_contact)
name = device
output = (xyz, coupling)
periodic = (false, true, true)
regions = (1, 2, 3)
space_orientation_dir1 = (1,0,0)
space_orientation_dir2 = (0,1,0)
starting_cell_coordinate = (0,0,0)
type = pseudomorphic }

C.3 Contact definitions

source contact, source source contact, source source source contact
source mode contact, source source mode contact
drain contact, drain drain contact, drain drain drain contact
drain mode contact

C.4 Mesh Domain definition

Domain{
mesh_from_domain = device
name = fem_device
number_of_refinement_steps = 1
refinement_regions = (1,2,3)
type = finite_elements
periodic = (false,true,true)}
Domain{
mesh_from_domain = drain_contact
name = fem_drain_contact
number_of_refinement_steps = 1
periodic = (false,false,false)
refinement_regions = (2,3)
type = finite_elements}
Domain{
mesh_from_domain = drain_drain_contact
name = fem_drain_drain_contact
number_of_refinement_steps = 1
periodic = (false,false,false)
refinement_regions = (2,3)
type = finite_elements}

C.5 Region definition

Geometry{Region{
max = (9.38992,2,2)//represents 16 UC of InGaAs per div, a=0.58687 nm
min = (-20,0,0) //Hopefully I don’t need to change this #.
priority = 1
region_number = 1
shape = cuboid}
Region{
  max = (18.77984,2,2) //represents 16 UC of InGaAs per div, a=0.58687 nm
  min = (9.38992,0,0)
  priority = 1
  region_number = 2
  shape = cuboid}
Region{
  max = (40,2,2)
  min = (18.77984,0,0)//represents 16 UC of InGaAs per div, a=0.58687 nm
  priority = 2
  region_number = 3
  shape = cuboid}}

C.6 QTBM Solver definition

  solver{
    type = MetaPoissonQTBM5
    name = QTBM
    active_regions = (1,2,3)
    clean_all_in_reinit = true
    contact_domains = (source_contact,drain_contact)
    contact_aux = (source_source_mode_contact)
    output = (JE,NE,current,ldosn1d,ldosp1d)
    tb_basis = sp3d5sstar
    energy_grid_constructor = QTBM:adaptive_grid_generator
    number_of_MPI_ranks_in_real_space = 1
    density_solver = QTBM:Transformation1
    derivative_of_density_solver = QTBM:Transformation1

solve_on_single_replica = true
solver_type = compression
with_poisson = true
no_file_output = true
dbg_output_job_list = false
regions_adjacent_to_source_electrode = 1
regions_adjacent_to_drain_electrode = 3
source_voltage = 0.0
drain_voltage = 0.0
ramper_voltage (-0.65,-0.6,-0.55,-0.5,-0.45,-0.4,-0.35,-0.3,-0.25,-0.2,-0.15,-0.1,-0.05,0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.5,0.55,0.6,0.65,0.7,0.75,0.8,0.85)
ramper_contact = source
no_integration_for_transmission = true
system_type = quasi_1D
kxmax = 0.5
kxmin = 0
kymax = 0.5
kymin = 0
number_of_k_points = 14
degeneracy_factor = 4
non_rectangular_energy = true
laplacian = (x)
bands_number_of_nodes = (100)
number_of_eigenvalues = 80
number_of_eigenvalues_to_use = 16
output_line_corners = [(0, 0.2, 0.2), (40, 0.2, 0.2)]
number_1D_output_points = 100
homogeneous_initial_potential = 0.3
selfconsistent_algorithm = fast
electron_hole_model = true
electron_hole_heuristics = omen_smooth
particle_source = hole
particle_drain = electron
iteration_output = false
poisson_max_iterations = 24
bandstructure_smart_parallelization = true
parallelize_adaptive_grid_construction = true
residual_criterion = 1.e-5}