Project and Thesis Folder 2023

- Pillars of the Institute for Microelectronics
 - Teaching: Programming in Python and C/C++
 - Simulation: Numerical simulation of semiconductor devices and processes
 - Experiments: Development of characterization equipment and techniques
- Unique chance to improve teaching quality and scientific research
- Potential to earn some extra money
- Optional seminars and practical courses:
 - 360.245 Computational Electronics
 - 360.238 Experimental Device Characterization in Microelectronics
 - 360.230 Emerging Devices
 - 360.206 Programming
- Bachelor Thesis
- Master Thesis



Atomated Data Extraction From Graphs



Supervisor:

Balázs Bámer

Contact:

bamer@iue.tuwien.ac.at 01-58801-36077

Project BB1

- Data extraction from scientific papers is currently done manually or semi-automatically with uncertain accuracy
- An automated tool using image processing and possibly AI methods could dramatically improve this process

Possible Tasks:

- Investigate different methods for various plot styles
- Implement image processing and/or AI algorithms for data extraction
- Extend an existing UI or create a new one

- Programming in C++
- Image processing, for example OpenCV
- Optionally deep learning
- Desktop user interfaces



Extraction of Topography Information from SEM Images



Supervisor:

Balázs Bámer

Contact: <u>bamer@iue.tuwien.ac.at</u> 01-58801-36077

Project BB2

- Use many of SEM images and scan them to identify the topography after a certain process, which is defined by equipment settings
- This will allow us to use machine learning to map the equipment settings to the final topography from these samples

Possible Tasks:

- Design image pre-processing suitable for a wide range of SEM images
- Design and teach a deep learning network for predicting topography based on equipment settings

- Programming in C++
- Image processing, for example OpenCV
- Deep learning



Simulate Sensors Based on 2D Materials



Supervisor:

Lado Filipovic

Contact: <u>filipovic@iue.tuwien.ac.at</u> 01-58801-36036

Project LF1

- 2D materials are heavily investigated for their application in disease detection, both as biosensors and gas sensors
- Simulation of such devices helps to understand the novel materials and to design novel sensor applications

Tasks:

- Perform simulations on bio-sensors or gas sensors which are based on 2D materials
- Compare and improve models by calibrating to measurements

Electrolyte

receptor

gate

dielectric

molecules

Reference Electrode

target

biomolecules

Required knowledge:

- Programming (Python, C, C++)
- (Rudimentary) understanding and profound interest in semiconductor physics

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Measuring Gas Sensors based on 2D Materials



Supervisor:

Lado Filipovic

Contact: <u>filipovic@iue.tuwien.ac.at</u> 01-58801-36036

Project LF2

- 2D materials such as the graphene family of materials (graphene, graphene oxide, etc.) and MoS₂ have shown potential for use as a gas sensor
- Combined characterizations and modeling are essential in order to better understand the capabilities of these films for sensing

Tasks:

- Perform characterizations of the electrical behavior of several devices under varying ambient conditions
- Write scripts to control the measurement setup

- Basic knowledge of Python
- Interest in sensor physics



Physical Modeling of Novel Semiconductor Devices



Supervisor:

Lado Filipovic

Contact: <u>filipovic@iue.tuwien.ac.at</u> 01-58801-36036

Project LF3

To investigate new devices, based on novel materials such as 2D materials and Perovskites, physical modeling tools are essential

• We are developing a framework in C++ to model electron transport in semiconductors under various scattering phenomena

Tasks:

 Implement models for different types of electron scattering mechanisms in C++

- Programming in C++
- (Rudimentary) understanding and profound interest in semiconductor physics





- -Secondary Electron Path
- Characteristic X-Ray

Modeling Atomic Layer Deposition (ALD)



Supervisor:

Lado Filipovic

Contact:

filipovic@iue.tuwien.ac.at 01-58801-36036

Project LF4

- ALD is a crucial step in modern semiconductor fabrication
- The fundamental aspect of ALD is that the films grown by it show self-limiting behavior
- This type of growth is not directly available from Level-set based simulators

Tasks:

- Develop a mathematical model for self-limiting growth within the Level-set method
- Implement this model in an existing simulator

- Programming in C++
- Knowledge of Finite Differences is a plus
- Familiarity with semiconductor processing is NOT necessary





Machine Learning for Process TCAD



Supervisor:

Lado Filipovic

Contact:

filipovic@iue.tuwien.ac.at 01-58801-36036

Project LF5

- Physical process simulations are memory- and time-intensive, giving rise to the need for emulation
- Emulation, or process compact modeling, allows to accelerate simulations for many processes
- Machine learning can be applied to train a compact model which is based on physical or experimental results

Tasks:

- Use machine learning to generate a compact model based on physical data
- Implementation of the model in an in-house process TCAD framework ViennaPS
- Test the model under various conditions

Required knowledge:

- Programming in C/C++, Python
- Interest in solid state physics and/or semiconductor process engineering

Reinforcement Learning in ML





Physical Modeling of MOSFETs based on 2D Materials



Supervisor:

Theresia Knobloch

Contact:

knobloch@iue.tuwien.ac.at 01-58801-36059

Project TK1

- 2D material-based FETs offer performance improvements for next-generation integrated circuits.
- We have adapted industrial device simulators to describe the device behavior of 2D FETs.

Possible Tasks:

- Compare simulated transfer characteristics based on different simulation methods
- Include the anisotropic permittivity of 2D materials in our model
- Study the impact of the contact geometry of prototype FETs on the device performance
- Study the impact of charge trapping on the FET reliability.
- Compare the simulation results to measurement data

Required knowledge:

- Programming with Python
- Interest in semiconductor physics

Institute for Microelectronics – TU Wien Gußhausstraße 27-29/E360, 1040 Vienna, Austria





Calculating Tunnel Currents through Novel Gate Insulators



Supervisor:

Theresia Knobloch

Contact:

knobloch@iue.tuwien.ac.at 01-58801-36059

Project TK2

- As the thickness of the gate insulator is scaled down gate leakage currents become a major problem.
- We have implemented a semi-classical model in a compact Python simulator (<u>Comphy</u>) to describe the leakage currents through novel gate stacks.

Possible Tasks:

- Adapt the model to describe complex gate stacks consisting of combinations of insulators
- Adapt the model to include the van der Waals gap
- Benchmark gate leakage currents for different combinations of metal-insulator-semiconductors

- Programming with Python
- Interest in semiconductor physics





Visualizing Research Results for the General Public



Supervisor:

Theresia Knobloch

Contact:

knobloch@iue.tuwien.ac.at 01-58801-36059

Project TK3

- Science communication is highly important to make new research insights visible and understandable for a broad public audience.
- Using the open-source, professional rendering and animation software <u>Blender</u> we are working to create videos to describe our findings in a scientifically accurate yet easily accessible way.

Possible Tasks:

- Create an animation for the fabrication of 2D material-based FETs
- Create an animation about charge transport through a FET and the impact of charge trapping

- Programming with Python
- Creativity
- Interest in semiconductor physics and processes
- Some first steps with Blender are an asset







Algorithm for Electron-Electron Scattering in Monte Carlo Device Simulation



Supervisor:

Hans Kosina

Contact: kosina@iue.tuwien.ac.at 01-58801-36013

Project HK1

- Hot carriers occuring in integrated transistors cause a degradation of the electrical characteristics
- Understanding on this degradation effect requires knowledge of the energy distribution of the carriers
 - This distribution is strongly affected by electron scattering (EES)
- The aim of this work is to implement a novel algorithm for EES in the Vienna Monte Carlo (VMC) simulator

Possible Tasks:

- Implement a recently developed algorithm for EES in the VMC simulator
- Test the implementation against other models and implementations

Required knowledge:

- Programming in C
- Interest in semiconductor physics

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Simulate Large Structures using ViennaLS



Supervisor:

Paul Manstetten Xaver Klemenschits

Contact:

manstetten@iue.tuwien.ac.at 01-58801-36016

Project PM1

- ViennaLS is a high-performance level set engine tailored towards micro-electronic fabrication simulations
- Its full capabilities have not yet been explored on a modern high performance computer
- Simulations of even large ICs should be possible

Tasks:

 Benchmark large scale simulations using ViennaLS on our new high performance cluster (2x 20 Cores, 768GB RAM)

Required knowledge:

• Advanced Knowledge of C++



Simulation of Spintronic Memory Device



Supervisor:

Roberto L. de Orio

Contact: orio@iue.tuwien.ac.at 01-58801-36068

Project RO1

- Magnetoresistive random access memory (MRAM) is a new memory technology under development
- In MRAM, a bit is stored as a magnetization direction in a magnetic layer
- Simulation of MRAM devices is an interesting and challenging task

Tasks:

- Simulation of MRAM cells for different conditions and parameters
- Extend an in-house simulation tool to incorporate new features

- Programming in C/C++
- Interest in modeling and simulation
- Familiarity with MRAM is NOT necessary



Compact Modeling for Spintronic Memory Device



Supervisor:

Roberto L. de Orio

Contact: orio@iue.tuwien.ac.at 01-58801-36068

Project RO2

- Magnetoresistive random access memory (MRAM) is a new memory technology under development
- In MRAM, a bit is stored as a magnetization direction in a magnetic layer
- Compact models are important for simulation of MRAM-based circuits

Tasks:

- Development of models suitable for simulation of MRAM circuits
- Extend available tools to incorporate new features

- Programming in Python
- Knowledge of circuit simulation and HDL languages is a plus
- Familiarity with MRAM is NOT necessary





MRAM Circuit Simulation



Supervisor:

Roberto L. de Orio

Contact:

orio@iue.tuwien.ac.at 01-58801-36068

Project RO3

- Magnetoresistive random access memory (MRAM) is a new memory technology under development
- In MRAM, a bit is stored as a magnetization direction in a magnetic layer
- Circuit simulation (spice-like) is a fundamental step during design of new technologies

Tasks:

- Simulation of basic circuits for MRAM
- Investigation of possible simulation tools and framework

- Basic circuit simulation
- Knowledge of HDL languages is a plus
- Familiarity with MRAM is NOT necessary





Simulation Framework Development



Supervisor:

Roberto L. de Orio Theresia Knobloch

Contact: orio@iue.tuwien.ac.at

01-58801-36068

Project RO4

- Analysis of differential equation systems using numerical methods (e.g. spatial and time discretization schemes)
- Simulation of semiconductor devices
 - Drift-diffusion model
 - Modeling of physical parameters

Task:

 Development of an academic simulation framework using Python

Required knowledge:

- Basic knowledge of semiconductor devices
- Programming in Python
- Interest in semiconductor devices and numerical simulations

 $\nabla^{2}\psi = q(n - p - C)/\varepsilon$ $\nabla \cdot (\mu_{n}n\nabla\psi - \mu_{n}V_{T}\nabla n) + \frac{\partial n}{\partial t} = -R ,$ $\nabla \cdot (\mu_{p}p\nabla\psi + \mu_{p}V_{T}\nabla p) - \frac{\partial p}{\partial t} = R .$







Atomistic Modeling: Interaction of Oxide Defects with Electric Fields



Supervisor:

Dominic Waldhoer

Contact:

waldhoer@iue.tuwien.ac.at 01-58801-36055

Project DW1

- Oxide defects in MOSFETs can act as charge trapping sites, causing various reliability issues like the Bias Temperature Instability (BTI)
- In our current BTI models the electric field across the gate oxide only affects the charge trapping levels of the defect
- However, the electric field can also interact with the charge distribution of the defect and potentially alter transition barriers between different defect states
- Density Functional Theory (DFT) allows us to simulate individual defects at an atomistic level and quantify these effects theoretically

Tasks:

- Use DFT to investigate the impact of electric fields on defect transition barriers due to dipole interaction
- Deduce a simplified model from your results which can be used in device simulators

Required knowledge:

- Solid understanding of electrodynamics and quantum mechanics
- Linux, Programming in Python



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Atomistic Modeling: Extending the 4-State Defect Model



Supervisor:

Dominic Waldhoer

Contact: waldhoer@iue.tuwien.ac.at 01-58801-36055

Project DW2

- Bias Temperature Instability (BTI) and Random Telegraph Noise (RTN) are caused by oxide defects which can trap/emit electric charges from/to the device substrate
- These defects are usually described by a 4-state Markov chain
- Although this 4-state model accounts for many experimental findings, it cannot explain certain observed defect behaviors like volatility or double capture/emission events
- *Density Functional Theory (DFT)* is an invaluable tool for the atomistic modeling of defects. DFT can be used to search for additional defect states and predict how these new states change the observable defect behavior

Tasks:

- Use DFT to identify possible defect states which can account for defect volatility and/or double capture/emission events
- Include these states in a Markov chain model and simulate the resulting RTN signals

- Solid understanding of physics
- Linux, Programming in Python





Web Interface to Control Defect Probing Instruments for Transistor Single-Defect Spectroscopy



Supervisor:

Michael Waltl

Contact: waltl@iue.tuwien.ac.at 01-58801-36050

Project MW1

- Electrical characterization of single defects in MOSFETs
- Use Defect Probing Instrument (right) developed at IuE
- Measurement sequences controlled by jobserver
- Jobserver communicates with SQL database

Tasks:

- Develop a web interface in Python (Django)
- Control of measurement flow
- Configuration of measurement tool
- Live tracking of measurement data

Requirements:

- Basic knowledge of Python
- Handling of UNIX operating system







Hardware- and Software Development for Defect Probing Instrument



Supervisor:

Michael Waltl

Contact: waltl@iue.tuwien.ac.at 01-58801-36050

Project MW2

- Electrical characterization of single defects in MOSFETs
- Defect Probing Instrument (right) developed at IuE
- Communicates with measurement host via USB interface

Tasks:

- Development of a calibration tool for DPI
- Development of a switching matrix
- Femto-ampere measurements
- Stepping motor controller and autofocus
- Enhancement of current control modul
- Application of zoom-and-scan method for single defect spectroscopy
- Driver development for general purpose measurement instruments (wafer prober, Keithleys, etc.)

Requirements:

- Knowledge of programming languages C/C++ and Python
- Profound knowledge of hardware development and PCB design







CSE & HPC: Quantum Monte Carlo Simulator on Supercomputers



Supervisor:

Josef Weinbub

Contact:

weinbub@iue.tuwien.ac.at 01-58801-36053

Project JW2

- Development of new highly parallel C++ Monte Carlo Simulator
- Several parallelization layers: MPI/OpenMP/CUDA
- Tailored to Supercomputers

Tasks: (several options based on one of the following)

- Switchable OpenMP/CUDA kernels
- MPI domain decomposition
- Structure generator
- Performance studies: Algorithms, data structures ..
- Automated testing pipelines

and many more ..

Required knowledge: (at least one of the following)

- C++
- MPI
- OpenMP
- CUDA



Atomistic Simulations



Supervisor:

Christoph Wilhelmer

Contact: wilhelmer@iue.tuwien.ac.at 01-58801-36002

Project CW2

- Ab-initio simulations on an atomistic level are needed to identify the properties of defects
- In this context, Density Functional Theory (DFT) is used to calculate e.g. the energetic position of defects, activation energies, ...

Possible Tasks:

- Analyze defect creation and H migration in SiO₂
- Characterize new and emerging technologies and materials
- Explore new simulation approaches

- Solid knowledge/interest in physics
- Postprocessing data (bash/python/...)



