Solar Cells

ATLAS
Device Simulation Framework

Simulation and Design
Solar cells are simulated within TCAD process simulation (ATHENA) and device simulation (ATLAS) frameworks. This presentation will cover:

1. The software architecture
2. Optical capabilities
3. Electronic and electro-optical capabilities
4. Solar cell technology examples
What is ATHENA?

- ATHENA process simulation framework enables process and integration engineers to develop and optimize semiconductor manufacturing processes
- ATHENA provides an easy to use, modular, and extensible platform for simulating ion implantation, diffusion, etch, deposition, lithography, oxidation, and silicidation of semiconductor materials
- ATHENA replaces costly wafer experiments with simulations to deliver shorter development cycles and higher yields
ATHENA Framework Architecture

- SSuprem4
  2D CORE PROCESS SIMULATOR

- Optolith
  2D OPTICAL LITHOGRAPHY SIMULATOR

- MC Implant
  ADVANCED MONTE-CARLO IMPLANTATION SIMULATOR

- Elite
  ADVANCED PHYSICAL ETCHING AND DEPOSITION SIMULATOR

- MC Deposit/Etch
  2D MONTE-CARLO DEPOSITION AND ETCH MODULE
SSuprem4 is the state-of-the-art 2D process simulator widely used in semiconductor industry for design, analysis and optimization of Si, SiGe and compound semiconductor technologies.

SSuprem4 accurately simulates all major process steps using a wide range of advanced physical models for diffusion, implantation, oxidation, silicidation and epitaxy.
MC Implant is a physically based 3D ion implantation simulator to model stopping and ranges in crystalline and amorphous materials.

It accurately predicts implant profiles and damage for all major ion/target combinations.
- Elite is an advanced 2D moving boundary topography simulator for modeling physical etch, deposition, reflow and CMP planarization processes.

- MC Etch/Depo is an advanced topology simulator. It includes several Monte Carlo based models for simulation of various etch and deposit processes which use a flux of atomic particles.
Optolith is a non-planar 2D lithography simulator that models all aspects of submicron lithography:
- Imaging
- Exposure
- Photoresist bake
- Development

Optolith is fully interfaced to all commercial IC layout tools conforming to GDSII and CIF formats.
Key Features

- Fast and accurate simulation of all critical fabrication steps used in CMOS, bipolar, SiGe/SiGeC, SiC, SOI, III-V, optoelectronic, and power device technologies
- Accurately predicts geometry, dopant distributions, and stresses in the device structure
- Easy to use software integrates plotting capabilities, automatic mesh generation, graphical input of process steps, and easy import of legacy TMA process decks
- Focused TCAD support team of Ph.D. physicists continuously developing models for new semiconductor technology advances
- Enables IDMs, foundries, and fabless companies to optimize semiconductor processes for the right combination of speed, yield, breakdown, leakage current, and reliability
- Accelerates time to production for new process development as well as equipment upgrades
What is ATLAS?

- ATLAS device simulation framework enables device technology engineers to simulate the electrical, optical, and thermal behavior of semiconductor devices.
- ATLAS provides a physics-based, easy to use, modular, and extensible platform to analyze DC, AC, and time domain responses for all semiconductor based technologies in 2 and 3 dimensions.
- Device designs for simulation may be created directly within ATLAS, drawn in DevEdit, or imported from the ATHENA framework.
ATLAS Framework Architecture

- **SILICON-BASED**
  - TFT2D/3D
  - Ferro

- **ADVANCED MATERIALS**
  - VCSEL
  - LASER
  - LED

- **S-Pisces/Device3D**

- **Blaze2D/3D**

Device Simulator Required Frameworks:
- Quantum2D/3D: Quantum Confinement Effects
- Noise: Semiconductor Noise
- Luminous2D/3D: Optoelectronic Device
- Giga2D/3D: Non-Isothermal Device
- MixedMode2D/3D: Combined Device and Circuit

Analysis Modules:
- C-Interpreter: User-defined models
S-Pisces/Device3D - 2D & 3D Device Simulator for Silicon Materials

- S-Pisces/Device3D is a 2D/3D device simulator for silicon based technologies that incorporates both drift-diffusion and energy balance transport equations.
- A large selection of physical models are available for DC, AC and time domain simulation.
- Typical applications include MOS, bipolar and BiCMOS technologies.
Blaze/Device3D simulates devices fabricated using advanced materials.

It includes a library of compound semiconductors which includes ternary and quaternary materials.

Blaze/Device3D has built-in models for graded and abrupt heterojunctions, and simulates structures such as MESFETS, HEMT’s and HBT’s.
Luminous 2D/3D – Optoelectronic Device Module

- Luminous 2D/3D is an advanced device module specially designed to model light absorption and photogeneration in planar and non-planar semiconductor devices.
- These features enable Luminous to account for arbitrary topologies, internal and external reflections, refractions and diffraction, polarization dependencies, and dispersion.

A lenslet above the photodetector have been defined to focus the light into the device.
- TFT2D/3D is an advanced device technology simulator equipped with the physical models and specialized numerical techniques required to simulate amorphous or polysilicon devices including thin film transistors.

- Specialized applications include large area display electronics and solar cells.
Organic Solar Module

- Organic Solar is a module which runs with Blaze in the ATLAS framework and enables the simulation of electrical and optical properties of organic solar cells, photodetectors and image sensors.
- Organic Solar incorporates features from the Luminous module, which allows the steady-state dc, ac, and transient simulation of electrical and optical behavior.
- Organic Solar borrows defect distributions from the TFT module which allows simulation of amorphous materials.
- Organic Solar incorporates properties unique to organic semiconductors: exciton behavior, Langevin recombination, Frenkel-Poole and hopping conduction mobility models.
Giga2D/3D combined with S-Pisces or Blaze device simulators allows simulation of local thermal effects.

Models in Giga2D/3D include heat generation, heat flow, lattice heating, heat sinks, and effects of local temperature on physical constants.

Thermal and electrical physical effects are coupled through self-consistent calculations.
MixedMode2D/3D works with S-Pisces or Blaze to simulate circuits that include physically-based devices in addition to compact analytical models.

Physically-based devices are used when accurate compact models do not exist, when devices that play a critical role must be simulated with very high accuracy, or when devices have non-electrical properties – such as optical devices.

MixedMode can have up to 100 nodes, 300 elements, and 10 ATLAS devices.

The circuit is defined using a SPICE netlist.
Quantum provides a set of powerful models for simulation of various effects of quantum confinement of carriers in semiconductor devices.

- A Schrodinger - Poisson solver allows calculation of bound state energies and wave functions self consistently with electrostatic potential.
- A Quantum moment models allow simulation of confinement effects on carrier transport effects on transport.
Key Features

- Accurately characterize physics-based devices for electrical, optical, and thermal performance without costly split-lot experiments
- Solve yield and process variation problems for optimal combination of speed, power, density, breakdown, leakage, luminosity, or reliability
- Fully integrated with ATHENA process simulation software, comprehensive visualization package, extensive database of examples, and simple device entry
- Choose from the largest selection of silicon, III-V, II-VI, IV-IV, or polymer/organic technologies including CMOS, bipolar, high voltage power device, VCSEL, TFT, optoelectronic, LASER, LED, CCD, sensor, fuse, NVM, ferro-electric, SOI, Fin-FET, HEMT, and HBT
- Worldwide offices support TCAD with process and device physicists
- Partner with a focused, committed, stable industry leader with active development roadmap for new technology enhancements
What is Virtual Wafer FAB?

VWF is designed for engineers who need to automate process to Spice simulation in one single simulation environment and to distribute predictive technological information across a corporation.

- Automated simulation split-lot experiments
- Process and device calibration
- Device and circuit performance optimization
- Process aware compact model
- Direct prediction of process variation on circuit performance
CMOS layout driven ring oscillator simulation was done in VWF. Key circuit figures of merit (i.e., frequency of the ring oscillator) can be plotted versus process splits.
Impact of Process Variation on Circuit Performance

Response Surface Model of ring oscillator frequency as a function of gate oxidation time and Vt implant dose.
Impact of Process Variation on Circuit Performance

Ring oscillator frequency yield analysis, based on user defined input distribution of each process parameter.
Optical Capabilities for Solar Cell Simulation

ATLAS
Device Simulation Framework
Light Simulation Physics Options

- Ray Tracing Method (RTM)
- Transfer Matrix Method (TMM)
- Beam Propagation Method (BPM)
- Finite Difference Time Domain (FDTD)

Ray traces from RTM simulation

Optical Intensity resulting from FDTD simulation
Defining Light Source Shapes

- Uniform and gaussian illumination
- Circular and elliptical optical source
- User defined optical source

Definition of the beam is free and unlimited using an ascii file

Gaussian source intensity with non-normal incidence and periodic boundaries
Defining Light Source Shapes

Diffusive Reflection (Gaussian, Lorenzian and Lambertian).
Defining 3D and 2D virtual or real lenses

2D lens created either by ATHENA or DevEdit

3D lenses created with VICTORY Cell

A lenslet above the photodetector have been defined to focus the light into the device.
Defining Multi-Spectral Optical Sources

- User-defined spectrum in ascii text file
- AM0 and Am1.5 solar spectra are built in
Miscellaneous Optical Capabilities

- Anti-Reflective coating
- C-Interpreter generated photogeneration rates
- Import photogeneration file in ATLAS
- Built-in and user defined optical index of refraction
- Diffusive Interface
- Arbitrary angle of incidence

Note that the anti-reflective coating does not need to be physically present in the simulated device as it can be simulated mathematically.
Direct import of photogeneration rate in ATLAS, calculated by an external optical simulator and resulting IV curve.
Electro-Optical Capabilities for Solar Cell Simulation

ATLAS
Device Simulation Framework

SILVACO
4/13/09
Electrical Capabilities

- DC, AC, transient, and spectral responses of general device structures can be simulated in the presence of arbitrary optical sources.
- Incorporates ANSI-C C-interpreter module for user-defined physical models definition.
- User defined material and parameters
- Non-local band-to-band tunnelling as well as trap assisted tunnelling model

Heterojunction GaAs/AlGaAs tunnel diode simulation using a nonLOCAL Band to band tunneling model. The composition fraction was varied (xcomp=0 correspond to a GaAs/GaAs tunnel junction)
Defect states in the band gap of non-crystalline materials
Users can specify activation energy, and capture cross-sections or lifetimes for electrons and holes
MixedMode simulation
Exciton dissociation model for Organic Solar cell

Density of states can be used using build-in or C-interpreter function
MixedMode Simulation of a Solar Cell

IV curves with series and shunt resistors
Solar Cell Technology Examples

ATLAS
Device Simulation Framework
Applications

1. III-V solar cell simulation
   GaInP/GaAs
   GaInP/GaAs/Ge

2. Cu(In,Ga)Se2 solar cell simulation
   CIGS/CdS/ZnO

3. Silicon based solar cell simulation
   Crystalline Silicon
   Amorphous Silicon
   Hydrogenated Silicon

4. Organic solar cell simulation
   OC1C10-PPV/PCBM (20:80 wt %) BHJ solar cell

5. Dye-sensitized solar cell simulation
GaInP/GaAs dual junction Solar cells are composed of two Solar Cells (GaInP and GaAs) and a tunnel junction. The tunnel Junction acts as a resistor. The Voc of a Dual junction Solar Cell is expected to be the sum of each Voc of individual Solar Cell with Jsc being the lowest from the two.

GaAs Solar Cell  
Jsc=36mA/cm²  Voc=1.03V

GaInP Solar Cell  
Jsc=13mA/cm²  Voc=1.29V
GaAs/GaAs tunnel diode simulation. Two enclosing barrier layers were added to minimize dopant diffusion. A non-local band-to-band tunneling model is used.

J_{peak} values of the tunnel diode vary from 3.5 mA/cm$^2$ to 220 mA/cm$^2$ when the p-n junction doping varies from 1.4e19/cm$^3$ to 1.8e19/cm$^3$. 

GaAs tunnel junction

J_{peak} values of the tunnel diode vary from 3.5 mA/cm$^2$ to 220 mA/cm$^2$ when the p-n junction doping varies from 1.4e19/cm$^3$ to 1.8e19/cm$^3$. 
Simulated IV characteristics of the dual solar cell versus doping concentration of the tunnel p-n junction. When the tunnel diode doping is high enough, the GaInP/GaAs Solar Cell exhibits $J_{sc}=12.55\,\text{mA/cm}^2$ and $V_{oc}=2.32\,\text{V}$, as expected, validating the band-to-band model used.
For Jsc < Jpeak (p-n doping > 1.7e19/cm³), the tunnel diode acts almost like a resistor and no loss in efficiency of the solar cell can be observed.

For Jsc > Jpeak (p-n doping < 1.7e19/cm³), the tunnel diode works in a region where thermal current dominates and a high current drop occurs over the tunnel diode. The produced dip in the current can severely lower the maximum power output of the solar cell.
Instead of using a non-local band-to-band tunneling model, a special treatment of the GaAs/GaAs tunnel diode in ATLAS allows very similar results with a significant reduction of the simulation time. Below is a simulation comparison of a single GaInP solar cell and GaAs tunnel diode with and without using a non-local tunneling model.
1- GaInP/GaAs/Ge Triple Solar Cell Simulation

External Quantum Efficiency EQE

IV characteristics of single and triple cell
Simulation of EQE of Ge solar were done in VWF as a function of optical models as well as solar cell design parameters.
Oscillation in EQE is observed when the Transfer Matrix Method (TMM) is used, since interferences are taken into account. Substrate reflection plays a significant role and is very well captured by the simulation.
1- Ge Solar Cell

EQE depends also on surface velocity recombination as well as GaInP thickness.
2- Cu(In,Ga)Se2 Solar Cell

Accurate electrical and optical material parameters as well as the capability of taking into account defects and grain boundaries are the key to get accurate simulation results of Cu(In,Ga)Se2 solar cell.
2- Cu(In,Ga)Se2 Solar Cell

Structure, IV characteristics, EQE and band diagram of the simulated Cu(In,Ga)Se2 solar cell.

FF=79.37  Eff=16.75%
Voc variation as a function of semiconductor Interface recombination velocity and conduction band offset

Source: Device Physics Of Cu(In,Ga)Se2 Thin-Film Solar Cells, dissertation from Markus Gloeckler, Colorado State University
IV crossover (between IV dark and IV under illumination) depends on CdS defect states characteristics decay energy.
2- Cu(In,Ga)Se₂ Solar Cell

Optimization and calibration can be done in VWF.(Virtual Wafer Fab). Below is the Response Surface model of the Efficiency as well as The Field Factor as a function of two variables: Thickness of CdS and ΔEg of CIGS
Real lenses can be defined either by using a process simulator like ATHENA or VICTORY as well as a device editor like DevEdit. Virtual lenses can also be defined directly within ATLAS.
3- Silicon Based Solar Cell

Real lenses can be defined either by using a process simulator like ATHENA or VICTORY as well as a device editor like DevEdit. Virtual lenses can also be defined directly within ATLAS.

Virtual lens defined in ATLAS.
Examination of the lenslet can be done by contouring the index of refraction

Optical intensity using FDTD method as a function of the lenslet radius
Comparison of amorphous and crystalline solar cells. The same structure was used for both simulations, but defects were introduced in the amorphous silicon material.
Textured solar cell was created using ATHENA and DevEdit and simulated with Finite Difference Time Domain (FDTD) and Ray Tracing Method (RTM).
The most common defect in a-Si:H is dangling bond. These dangling bond states are amphoteric and located around the middle of the band gap.
3- a-Si:H/uc-Si:H Solar Cell

Ray traces as a function of the wavelength.

- 0.3um
- 0.4um
- 0.5um
- 0.6um
- 0.7um
- 0.8um
3- a-Si:H/uc-Si:H Solar Cell

Photogeneration rate as a function of the wavelength.

- 0.3um
- 0.4um
- 0.5um
- 0.6um
- 0.7um
- 0.8um
Tandem a-Si:H/uc-Si:H simulation showing the influence of diffusive interface as well as semiconductor/semiconductor interface recombination velocity (only applied on the top cell) on IV key figure of merits.

Tandem a-Si:H/uc-Si:H simulation showing the influence of diffusive interface as well as semiconductor/semiconductor interface recombination velocity (only applied on the top cell) on EQE.

Absorbed light generates excess excitons which diffuse and dissociate to form electron holes pairs. Simulation parameters were taken from Koster et al., Physical Review B, Vol 72, 2005 pp085205-1 085205-9.

![Graph showing Organic Solar Cell Characteristics](image)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band Gap</td>
<td>$E_g$</td>
<td>1.34</td>
<td>eV</td>
</tr>
<tr>
<td>Electron mobility</td>
<td>$\mu_n$</td>
<td>$2.5 \times 10^{-3}$</td>
<td>cm$^3$/Vs</td>
</tr>
<tr>
<td>Hole mobility</td>
<td>$\mu_p$</td>
<td>$3.0 \times 10^{-4}$</td>
<td>cm$^3$/Vs</td>
</tr>
<tr>
<td>Eff. density of states</td>
<td>Nc/Nv</td>
<td>$2.5 \times 10^{19}$</td>
<td>cm$^{-3}$</td>
</tr>
<tr>
<td>Relative permittivity</td>
<td>$\varepsilon_r$</td>
<td>3.4</td>
<td></td>
</tr>
<tr>
<td>Pair distance</td>
<td>A.SINGLET</td>
<td>1.3</td>
<td>nm</td>
</tr>
<tr>
<td>Decay Rate</td>
<td>KNRS.EXCITON</td>
<td>$1.5 \times 10^6$</td>
<td>s$^{-1}$</td>
</tr>
</tbody>
</table>

Table 1: Suggested Parameter Values
Optimization was done using the optimizer feature of DeckBuild.
4- Peak Power and Fill Factor in an Organic Solar Cell

- $I_{\text{max}} = 20.2 \text{ A/m}^2$
- $V_{\text{max}} = 0.66 \text{ V}$
- Fill Factor $= 0.57$

Function 1 = Power
4- Langevin Recombination at Short Circuit

Langevin recombination rate and singlet exciton density at short circuit under illumination
5- Dye-sensitized Solar Cell Simulation

Schematic representation of the principle of the dye-sensitized photovoltaic cell to indicate the electron energy level in the different phases. Ref (1).


Optical refractive index of TiO2 and Dye/TiO2 material

Absorption spectrum of the N3 dye in ethanol solution (--) and of a N3 dye-sensitized nanocrystalline TiO2 electrode (-*-). Ref. (2).

Simulation and measurements of IV characteristics of dye-sensitized solar cell

5- Dye-sensitized Solar Cell Simulation

Ray traces and optical intensity of dye-sensitized solar cell

Light injection into 1 nanocrystalline TiO2 particle and optical intensity distribution

Light injection into 2 nanocrystalline TiO2 particles and optical intensity distribution
Summary

- In conclusion, Silvaco TCAD tools provide a complete solution for researchers interested in solar cell technology. It enables researchers to study the electrical properties of solar cells under illumination in both two and three dimensional domains. The simulated properties include IV characteristics, spectral response, quantum efficiency, photogeneration rates, potential distribution, etc. The software is capable of simulating any type of solar cell as well as solar cells with textured surfaces. The calibration task is now very convenient and easy thanks to VWF.

- Silvaco is the one-stop vendor for all companies interested in advance solar cell technology simulation solutions.